Supplementary Material (ESI) for Chemical Communications

Cyclopentathiadiazines, new heterocyclic materials from cyclic enaminonitriles.

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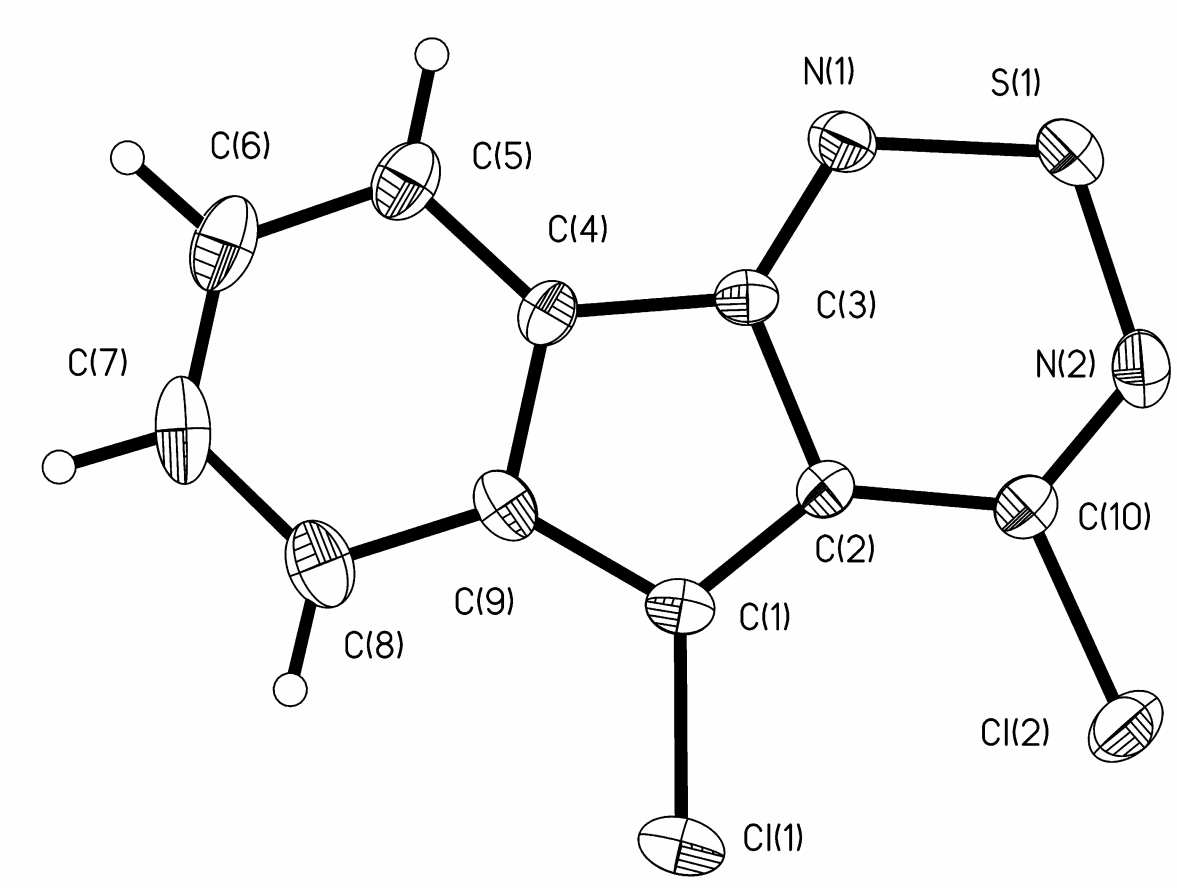
Crystal data and structure refinement for **4**.



4

Supplementary Material (ESI) for Chemical Communications

Table 1. Crystal data and structure refinement for **4**.

Identification code	sm106am	
Empirical formula	C10 H4 Cl2 N2 S	
Formula weight	255.11	
Temperature	299(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.888(4) Å	α= 68.241(9)°.
	b = 8.696(5) Å	β= 83.001(10)°.
	c = 9.612(5) Å	γ = 70.332(10)°.
Volume	503.5(5) $Å^3$	
Z	2	
Density (calculated)	1.683 Mg/m^3	
Absorption coefficient	0.812 mm^{-1}	
F(000)	256	
Crystal size	0.03 x 0.08 x 0.45 mm^3	
Theta range for data collection	2.28 to 23.31°.	
Index ranges	-7<=h<=7, -9<=k<=9, -10<=l<=9	
Reflections collected	2285	
Independent reflections	1452 [R(int) = 0.0217]	
Completeness to theta = 23.31°	99.3 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000000 and 0.620117	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1452 / 0 / 136	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1289	
R indices (all data)	R1 = 0.0670, wR2 = 0.1375	
Largest diff. peak and hole	0.529 and -0.286 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cl(1)	3856(2)	2925(2)	7886(2)	66(1)
Cl(2)	2843(2)	6860(2)	5261(1)	59(1)
S(1)	851(2)	9908(1)	7937(1)	54(1)
N(1)	1169(5)	8322(4)	9572(4)	42(1)
N(2)	1551(6)	9122(5)	6579(4)	48(1)
C(1)	3032(6)	4351(5)	8850(4)	37(1)
C(2)	2409(6)	6111(5)	8303(4)	32(1)
C(3)	1863(6)	6688(5)	9621(4)	32(1)
C(4)	2209(6)	5152(5)	10949(4)	34(1)
C(5)	1932(7)	4918(6)	12470(5)	50(1)
C(6)	2409(8)	3224(7)	13488(5)	62(1)
C(7)	3099(7)	1809(7)	13029(5)	62(1)
C(8)	3387(7)	1997(6)	11538(5)	54(1)
C(9)	2923(6)	3694(5)	10476(5)	38(1)
C(10)	2191(6)	7457(5)	6833(4)	37(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

Cl(1)-C(1)	1.723(4)
Cl(2)-C(10)	1.736(4)
S(1)-N(2)	1.640(4)
S(1)-N(1)	1.641(4)
N(1)-C(3)	1.322(5)
N(2)-C(10)	1.298(5)
C(1)-C(2)	1.349(5)
C(1)-C(9)	1.454(6)
C(2)-C(10)	1.448(5)
C(2)-C(3)	1.492(5)
C(3)-C(4)	1.437(5)
C(4)-C(5)	1.398(5)
C(4)-C(9)	1.418(5)
C(5)-C(6)	1.385(7)
C(6)-C(7)	1.376(7)
C(7)-C(8)	1.378(7)
C(8)-C(9)	1.402(6)
N(2)-S(1)-N(1)	110.67(17)
C(3)-N(1)-S(1)	119.1(3)
C(10)-N(2)-S(1)	122.1(3)
C(2)-C(1)-C(9)	110.9(3)
C(2)-C(1)-Cl(1)	128.8(3)
C(9)-C(1)-Cl(1)	120.3(3)
C(1)-C(2)-C(10)	136.1(3)
C(1)-C(2)-C(3)	106.6(3)
C(10)-C(2)-C(3)	117.3(3)
N(1)-C(3)-C(4)	126.3(3)
N(1)-C(3)-C(2)	126.0(3)
C(4)-C(3)-C(2)	107.8(3)
C(5)-C(4)-C(9)	120.5(4)
C(5)-C(4)-C(3)	132.4(4)
C(9)-C(4)-C(3)	107.0(3)
C(6)-C(5)-C(4)	117.8(4)

C(7)-C(6)-C(5)	121.6(4)
C(6)-C(7)-C(8)	121.9(4)
C(7)-C(8)-C(9)	118.0(4)
C(8)-C(9)-C(4)	120.1(4)
C(8)-C(9)-C(1)	132.3(4)
C(4)-C(9)-C(1)	107.7(3)
N(2)-C(10)-C(2)	124.9(4)
N(2)-C(10)-Cl(2)	115.8(3)
C(2)-C(10)-Cl(2)	119.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. 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}
Cl(1)	85(1)	46(1)	72(1)	-36(1)	7(1)	-11(1)
Cl(2)	70(1)	68(1)	36(1)	-23(1)	5(1)	-15(1)
S(1)	73(1)	31(1)	52(1)	-13(1)	-5(1)	-12(1)
N(1)	45(2)	36(2)	46(2)	-17(2)	-4(2)	-8(2)
N(2)	52(2)	40(2)	40(2)	-3(2)	-2(2)	-13(2)
C(1)	34(2)	37(2)	44(2)	-21(2)	2(2)	-9(2)
C(2)	32(2)	35(2)	30(2)	-12(2)	2(2)	-11(2)
C(3)	28(2)	36(2)	36(2)	-17(2)	0(2)	-11(2)
C(4)	29(2)	42(2)	30(2)	-10(2)	-3(2)	-12(2)
C(5)	50(3)	63(3)	37(3)	-14(2)	-7(2)	-19(2)
C(6)	57(3)	81(4)	38(3)	-4(3)	-10(2)	-25(3)
C(7)	52(3)	59(3)	52(3)	17(3)	-13(2)	-24(3)
C(8)	41(3)	44(3)	64(3)	-5(2)	-8(2)	-12(2)
C(9)	26(2)	31(2)	50(3)	-9(2)	-6(2)	-7(2)
C(10)	34(2)	42(3)	36(2)	-15(2)	1(2)	-13(2)

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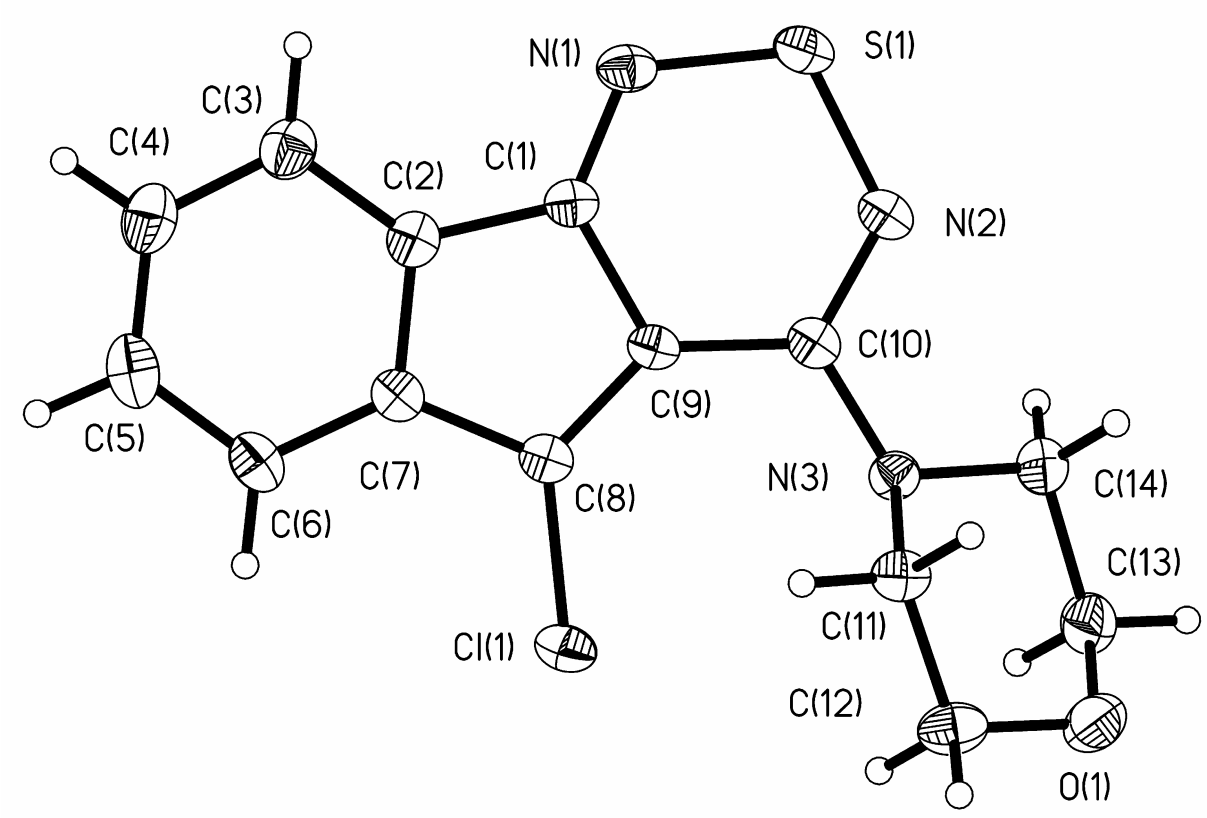
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(5)	1443	5868	12788	61
H(6)	2259	3040	14506	74
H(7)	3379	692	13746	75
H(8)	3874	1028	11245	64

Supplementary Material (ESI) for Chemical Communications

Crystal data and structure refinement for **5**.



5

Supplementary Material (ESI) for Chemical Communications

Table 1. Crystal data and structure refinement for **5**.

Identification code	sm1032am	
Empirical formula	C14 H12 Cl N3 O S	
Formula weight	305.78	
Temperature	299(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 16.356(6) Å	α= 90°.
	b = 11.871(4) Å	β= 114.333(7)°.
	c = 15.296(5) Å	γ = 90°.
Volume	2706.0(17) $Å^3$	
Z	8	
Density (calculated)	1.501 Mg/m^3	
Absorption coefficient	0.435 mm^{-1}	
F(000)	1264	
Crystal size	0.10 x 0.14 x 0.27 mm^3	
Theta range for data collection	2.19 to 23.33°.	
Index ranges	-18<=h<=16, -13<=k<=13, -16<=l<=15	
Reflections collected	5954	
Independent reflections	1957 [R(int) = 0.0582]	
Completeness to theta = 23.33°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000000 and 0.411093	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1957 / 0 / 181	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0509, wR2 = 0.1196	
R indices (all data)	R1 = 0.0834, wR2 = 0.1368	
Largest diff. peak and hole	0.331 and -0.335 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	921(1)	4277(1)	1922(1)	50(1)
S(1)	1378(1)	2686(1)	5619(1)	46(1)
N(1)	1412(2)	1739(2)	4857(2)	40(1)
N(2)	1365(2)	3959(2)	5206(2)	40(1)
N(3)	1350(2)	5275(2)	4079(2)	35(1)
O(1)	1603(2)	7586(2)	3828(2)	59(1)
C(1)	1367(2)	2076(3)	4032(3)	32(1)
C(2)	1265(3)	1352(3)	3229(3)	36(1)
C(3)	1279(3)	182(3)	3145(3)	49(1)
C(4)	1100(3)	-253(4)	2249(3)	57(1)
C(5)	904(3)	425(4)	1460(3)	55(1)
C(6)	894(3)	1585(4)	1534(3)	44(1)
C(7)	1090(2)	2047(3)	2431(3)	33(1)
C(8)	1119(2)	3211(3)	2737(3)	32(1)
C(9)	1307(2)	3261(3)	3699(2)	30(1)
C(10)	1360(2)	4163(3)	4355(3)	33(1)
C(11)	2087(3)	5656(3)	3849(3)	41(1)
C(12)	1826(3)	6746(3)	3306(3)	51(1)
C(13)	898(3)	7202(3)	4063(3)	55(1)
C(14)	1129(3)	6131(3)	4640(3)	48(1)

Table 3. Bond lengths [Å] and angles [°] for **5**.

Cl(1)-C(8)	1.712(4)
S(1)-N(2)	1.636(3)
S(1)-N(1)	1.638(3)
N(1)-C(1)	1.296(4)
N(2)-C(10)	1.320(5)
N(3)-C(10)	1.384(4)
N(3)-C(11)	1.459(5)
N(3)-C(14)	1.468(4)
O(1)-C(12)	1.417(5)
O(1)-C(13)	1.417(5)
C(1)-C(2)	1.452(5)
C(1)-C(9)	1.486(5)
C(2)-C(3)	1.395(5)
C(2)-C(7)	1.402(5)
C(3)-C(4)	1.378(6)
C(4)-C(5)	1.375(6)
C(5)-C(6)	1.382(6)
C(6)-C(7)	1.386(5)
C(7)-C(8)	1.453(5)
C(8)-C(9)	1.375(5)
C(9)-C(10)	1.446(5)
C(11)-C(12)	1.502(5)
C(13)-C(14)	1.505(5)
N(2)-S(1)-N(1)	110.93(16)
C(1)-N(1)-S(1)	118.5(2)
C(10)-N(2)-S(1)	123.0(3)
C(10)-N(3)-C(11)	117.6(3)
C(10)-N(3)-C(14)	117.1(3)
C(11)-N(3)-C(14)	110.7(3)
C(12)-O(1)-C(13)	110.0(3)
N(1)-C(1)-C(2)	125.6(3)
N(1)-C(1)-C(9)	126.5(3)
C(2)-C(1)-C(9)	107.6(3)

C(3)-C(2)-C(7)	120.7(3)
C(3)-C(2)-C(1)	131.8(4)
C(7)-C(2)-C(1)	107.4(3)
C(4)-C(3)-C(2)	117.3(4)
C(5)-C(4)-C(3)	122.1(4)
C(4)-C(5)-C(6)	121.1(4)
C(5)-C(6)-C(7)	118.0(4)
C(6)-C(7)-C(2)	120.6(3)
C(6)-C(7)-C(8)	131.2(3)
C(2)-C(7)-C(8)	108.1(3)
C(9)-C(8)-C(7)	110.5(3)
C(9)-C(8)-Cl(1)	129.7(3)
C(7)-C(8)-Cl(1)	119.8(3)
C(8)-C(9)-C(10)	134.3(3)
C(8)-C(9)-C(1)	106.3(3)
C(10)-C(9)-C(1)	119.1(3)
N(2)-C(10)-N(3)	118.1(3)
N(2)-C(10)-C(9)	121.5(3)
N(3)-C(10)-C(9)	120.3(3)
N(3)-C(11)-C(12)	109.0(3)
O(1)-C(12)-C(11)	112.0(3)
O(1)-C(13)-C(14)	112.7(4)
N(3)-C(14)-C(13)	107.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

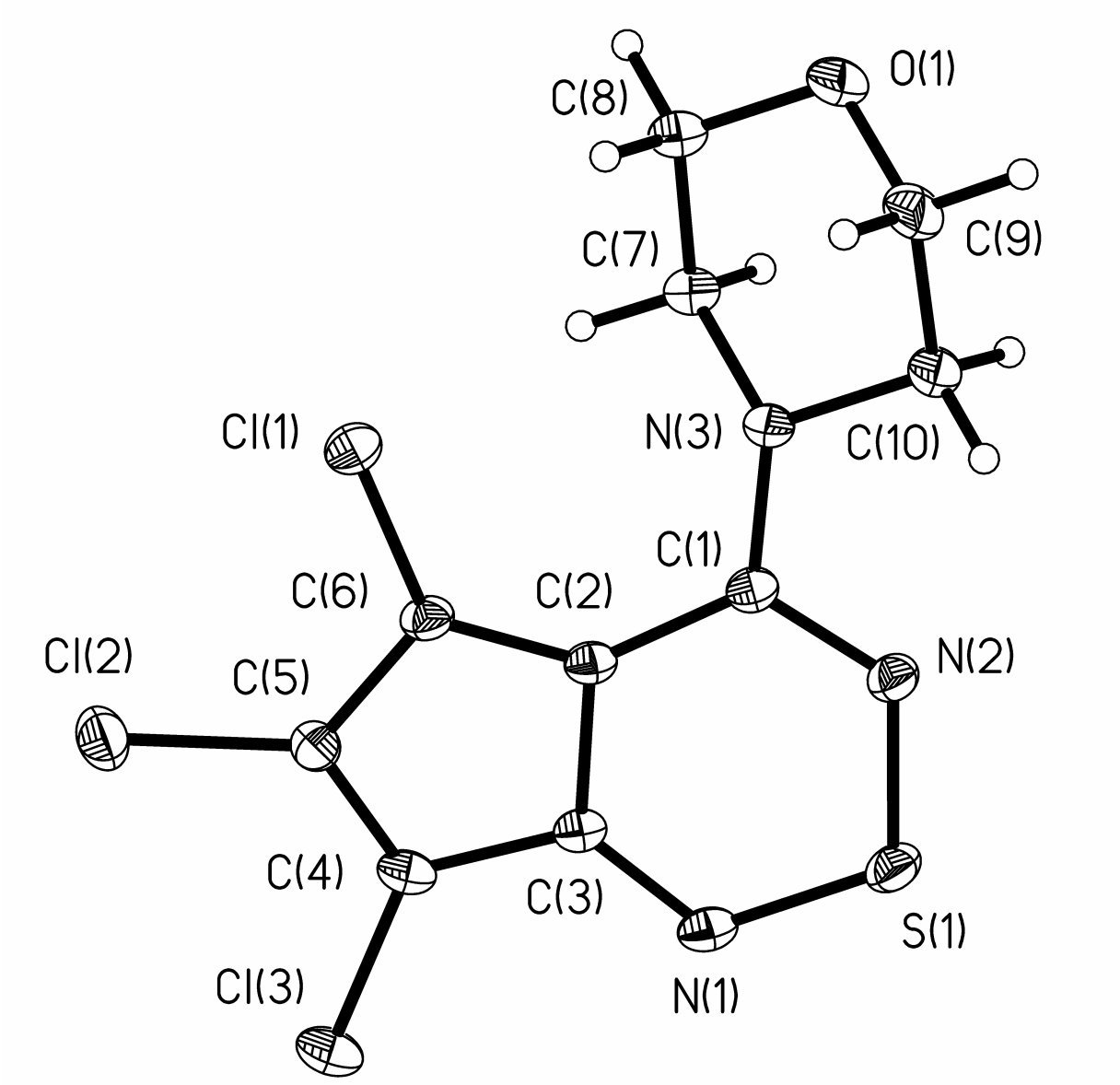
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	58(1)	53(1)	35(1)	11(1)	15(1)	3(1)
S(1)	51(1)	53(1)	35(1)	9(1)	18(1)	0(1)
N(1)	31(2)	46(2)	38(2)	10(2)	9(2)	-1(2)
N(2)	38(2)	50(2)	32(2)	3(2)	15(2)	1(2)
N(3)	34(2)	36(2)	39(2)	1(2)	19(2)	-1(2)
O(1)	66(2)	43(2)	64(2)	5(2)	23(2)	-5(2)
C(1)	18(2)	39(2)	34(2)	6(2)	6(2)	1(2)
C(2)	20(2)	41(2)	42(2)	-1(2)	8(2)	2(2)
C(3)	44(3)	44(2)	52(3)	-1(2)	13(2)	3(2)
C(4)	53(3)	47(2)	67(3)	-10(2)	22(3)	3(2)
C(5)	43(3)	66(3)	53(3)	-20(2)	17(2)	-2(2)
C(6)	33(3)	60(3)	37(2)	-5(2)	14(2)	-2(2)
C(7)	19(2)	43(2)	37(2)	1(2)	12(2)	3(2)
C(8)	20(2)	42(2)	34(2)	4(2)	11(2)	3(2)
C(9)	19(2)	40(2)	30(2)	5(2)	10(2)	-1(2)
C(10)	19(2)	44(2)	33(2)	2(2)	9(2)	1(2)
C(11)	31(3)	48(2)	43(2)	6(2)	13(2)	-1(2)
C(12)	38(3)	54(3)	58(3)	16(2)	19(2)	0(2)
C(13)	68(4)	47(2)	52(3)	-3(2)	26(3)	8(2)
C(14)	57(3)	44(2)	45(3)	-5(2)	23(2)	-4(2)

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

	x	y	z	U(eq)
H(3)	1404	-285	3673	59
H(4)	1111	-1029	2177	68
H(5)	776	98	865	66
H(6)	760	2042	999	52
H(11A)	2215	5093	3463	50
H(11B)	2623	5764	4435	50
H(12A)	2319	7010	3165	61
H(12B)	1315	6617	2701	61
H(13A)	367	7076	3475	66
H(13B)	757	7782	4425	66
H(14A)	1638	6254	5248	57
H(14B)	624	5884	4769	57

Supplementary Material (ESI) for Chemical Communications

Crystal data and structure refinement for **8**.



8

Supplementary Material (ESI) for Chemical Communications

Table 1. Crystal data and structure refinement for **8**.

Identification code	sm761am	
Empirical formula	C10 H8 Cl3 N3 O S	
Formula weight	324.60	
Temperature	299(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.2261(10) Å	α= 98.589(3)°.
	b = 8.9133(12) Å	β= 93.045(3)°.
	c = 10.0492(13) Å	γ = 99.426(2)°.
Volume	629.35(15) $Å^3$	
Z	2	
Density (calculated)	1.713 Mg/m^3	
Absorption coefficient	0.883 mm^{-1}	
F(000)	328	
Crystal size	0.09 x 0.20 x 0.29 mm^3	
Theta range for data collection	2.06 to 23.26°.	
Index ranges	-8<=h<=8, -9<=k<=8, -9<=l<=11	
Reflections collected	2820	
Independent reflections	1768 [R(int) = 0.0145]	
Completeness to theta = 23.26°	98.2 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000000 and 0.386569	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1768 / 0 / 164	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0965	
R indices (all data)	R1 = 0.0364, wR2 = 0.0988	
Extinction coefficient	0.011(3)	
Largest diff. peak and hole	0.248 and -0.321 $e.Å^{-3}$	

Supplementary Material (ESI) for Chemical Communications

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4934(1)	5497(1)	6561(1)	55(1)
Cl(2)	8265(1)	5154(1)	8772(1)	59(1)
Cl(3)	7838(1)	7275(1)	11807(1)	56(1)
S(1)	2157(1)	9203(1)	10849(1)	47(1)
O(1)	733(3)	8198(3)	4328(2)	63(1)
N(1)	4105(3)	8649(3)	11194(2)	43(1)
N(2)	1548(3)	8861(3)	9249(2)	42(1)
N(3)	1919(3)	7973(2)	7012(2)	40(1)
C(1)	2534(3)	8138(3)	8361(2)	36(1)
C(2)	4113(3)	7497(3)	8778(2)	36(1)
C(3)	4867(3)	7882(3)	10209(2)	36(1)
C(4)	6462(4)	7155(3)	10351(3)	41(1)
C(5)	6638(4)	6306(3)	9130(3)	40(1)
C(6)	5198(4)	6504(3)	8165(2)	39(1)
C(7)	3257(4)	8551(3)	6077(3)	46(1)
C(8)	2521(5)	7837(4)	4648(3)	57(1)
C(9)	-565(5)	7654(4)	5236(3)	60(1)
C(10)	62(4)	8349(3)	6684(3)	47(1)

Table 3. Bond lengths [Å] and angles [°] for **8**.

Cl(1)-C(6)	1.709(2)
Cl(2)-C(5)	1.702(3)
Cl(3)-C(4)	1.704(3)
S(1)-N(1)	1.604(3)
S(1)-N(2)	1.614(2)
O(1)-C(8)	1.414(4)
O(1)-C(9)	1.422(4)
N(1)-C(3)	1.314(3)
N(2)-C(1)	1.329(3)
N(3)-C(1)	1.383(3)
N(3)-C(10)	1.467(3)
N(3)-C(7)	1.471(3)
C(1)-C(2)	1.427(4)
C(2)-C(6)	1.376(4)
C(2)-C(3)	1.480(3)
C(3)-C(4)	1.423(4)
C(4)-C(5)	1.366(4)
C(5)-C(6)	1.435(4)
C(7)-C(8)	1.512(4)
C(9)-C(10)	1.509(4)
N(1)-S(1)-N(2)	111.88(11)
C(8)-O(1)-C(9)	110.0(2)
C(3)-N(1)-S(1)	118.25(19)
C(1)-N(2)-S(1)	122.47(19)
C(1)-N(3)-C(10)	117.7(2)
C(1)-N(3)-C(7)	118.2(2)
C(10)-N(3)-C(7)	109.9(2)
N(2)-C(1)-N(3)	117.1(2)
N(2)-C(1)-C(2)	121.7(2)
N(3)-C(1)-C(2)	121.1(2)
C(6)-C(2)-C(1)	135.6(2)
C(6)-C(2)-C(3)	105.6(2)
C(1)-C(2)-C(3)	118.8(2)

N(1)-C(3)-C(4)	126.0(2)
N(1)-C(3)-C(2)	126.0(2)
C(4)-C(3)-C(2)	107.8(2)
C(5)-C(4)-C(3)	107.7(2)
C(5)-C(4)-Cl(3)	126.6(2)
C(3)-C(4)-Cl(3)	125.6(2)
C(4)-C(5)-C(6)	109.4(2)
C(4)-C(5)-Cl(2)	126.6(2)
C(6)-C(5)-Cl(2)	124.0(2)
C(2)-C(6)-C(5)	109.4(2)
C(2)-C(6)-Cl(1)	129.3(2)
C(5)-C(6)-Cl(1)	121.2(2)
N(3)-C(7)-C(8)	108.9(2)
O(1)-C(8)-C(7)	111.1(2)
O(1)-C(9)-C(10)	112.1(3)
N(3)-C(10)-C(9)	108.4(2)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. 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}
Cl(1)	70(1)	62(1)	32(1)	-8(1)	-1(1)	25(1)
Cl(2)	59(1)	57(1)	65(1)	10(1)	-1(1)	25(1)
Cl(3)	59(1)	68(1)	39(1)	12(1)	-15(1)	8(1)
S(1)	50(1)	59(1)	31(1)	-2(1)	7(1)	11(1)
O(1)	76(2)	84(2)	36(1)	11(1)	-6(1)	33(1)
N(1)	49(1)	49(1)	27(1)	2(1)	2(1)	2(1)
N(2)	42(1)	50(1)	33(1)	1(1)	3(1)	10(1)
N(3)	42(1)	49(1)	29(1)	6(1)	-1(1)	12(1)
C(1)	39(1)	36(1)	31(1)	3(1)	2(1)	2(1)
C(2)	39(1)	40(1)	27(1)	3(1)	0(1)	3(1)
C(3)	39(1)	38(1)	28(1)	5(1)	3(1)	2(1)
C(4)	45(2)	45(1)	32(1)	9(1)	-6(1)	2(1)
C(5)	40(1)	42(1)	40(2)	9(1)	2(1)	9(1)
C(6)	48(2)	41(1)	28(1)	0(1)	1(1)	7(1)
C(7)	52(2)	54(2)	35(2)	10(1)	4(1)	12(1)
C(8)	70(2)	73(2)	32(2)	8(1)	5(1)	25(2)
C(9)	58(2)	75(2)	46(2)	4(2)	-15(1)	21(2)
C(10)	48(2)	56(2)	37(2)	5(1)	-3(1)	15(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(7A)	4478	8283	6280	55
H(7B)	3403	9664	6175	55
H(8A)	3396	8213	4024	68
H(8B)	2428	6727	4547	68
H(9A)	-702	6541	5140	72
H(9B)	-1786	7905	5003	72
H(10A)	134	9458	6805	56
H(10B)	-835	7935	7279	56

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