Supporting Materials

Tables of atom coordinates, thermal parameters and bonding geometry for the X-ray crystal structure of **5e**. This material is available free of charge via the Internet at http://pubs.acs.org.

Table Supp1. Crystal data and structure refinement for **5e**.

Identification code	3hla	
Empirical formula	C16 H16 N2 O S	
Formula weight	284.37	
Temperature	168(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.660(3) Å	α= 90°.
	b = 13.574(4) Å	β= 94.587(4)°.
	c = 9.227(3) Å	γ = 90°.
Volume	1331.0(7) Å^3	
Z	4	
Density (calculated)	1.419 Mg/m^3	
Absorption coefficient	0.240 mm^{-1}	
F(000)	600	
Crystal size	0.51 x 0.46 x 0.44 mm^3	
Theta range for data collection	2.43 to 26.43°.	
Index ranges	-13<=h<=13, -16<=k<=14, -11<=l<=11	
Reflections collected	16733	
Independent reflections	2724 [R(int) = 0.0229]	
Completeness to theta = 26.43°	99.6 %	
Max. and min. transmission	0.9019 and 0.8875	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2724 / 0 / 182	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0955	
R indices (all data)	R1 = 0.0457, wR2 = 0.1016	
Largest diff. peak and hole	0.279 and -0.268 e.Å^{-3}	

Table Supp2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5e**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	150(1)	7987(1)	1680(1)	34(1)
C(2)	-761(2)	7081(1)	600(2)	35(1)
N(3)	-860(1)	6184(1)	1366(1)	32(1)
C(4)	356(2)	5744(1)	1602(2)	34(1)
N(5)	1284(1)	6269(1)	2523(1)	30(1)
C(6)	1247(1)	7196(1)	2601(2)	29(1)
C(31)	-1618(1)	6184(1)	2544(2)	29(1)
C(32)	-2760(2)	6670(1)	2445(2)	36(1)
C(33)	-3539(2)	6619(1)	3530(2)	40(1)
C(34)	-3222(2)	6072(1)	4757(2)	37(1)
C(35)	-2101(2)	5591(1)	4879(2)	33(1)
C(36)	-1303(2)	5665(1)	3792(2)	30(1)
O(30)	-4059(1)	6072(1)	5775(2)	54(1)
C(37)	-3744(3)	5540(2)	7050(3)	78(1)
C(61)	2194(1)	7717(1)	3560(2)	29(1)
C(62)	2415(2)	8700(1)	3403(2)	39(1)
C(63)	3305(2)	9169(1)	4300(2)	44(1)
C(64)	3995(2)	8662(1)	5352(2)	39(1)
C(65)	3784(2)	7681(1)	5517(2)	39(1)
C(66)	2890(2)	7210(1)	4635(2)	34(1)

Table Supp3. Bond lengths [Å] and angles [°] for **5e**.

S(1)-C(6)	1.7568(16)
S(1)-C(2)	1.8149(17)
C(2)-N(3)	1.417(2)
N(3)-C(31)	1.405(2)
N(3)-C(4)	1.428(2)
C(4)-N(5)	1.441(2)
N(5)-C(6)	1.261(2)
C(6)-C(61)	1.470(2)
C(31)-C(36)	1.369(2)
C(31)-C(32)	1.380(2)
C(32)-C(33)	1.352(2)
C(33)-C(34)	1.373(2)
C(34)-O(30)	1.347(2)
C(34)-C(35)	1.359(2)
C(35)-C(36)	1.370(2)
O(30)-C(37)	1.398(2)
C(61)-C(62)	1.365(2)
C(61)-C(66)	1.375(2)
C(62)-C(63)	1.366(3)
C(63)-C(64)	1.357(3)
C(64)-C(65)	1.362(3)
C(65)-C(66)	1.362(2)
C(6)-S(1)-C(2)	99.09(8)
N(3)-C(2)-S(1)	111.47(11)
C(31)-N(3)-C(2)	117.11(13)
C(31)-N(3)-C(4)	116.97(13)
C(2)-N(3)-C(4)	109.47(13)
N(3)-C(4)-N(5)	117.07(13)
C(6)-N(5)-C(4)	120.30(14)
N(5)-C(6)-C(61)	119.49(14)
N(5)-C(6)-S(1)	127.23(12)
C(61)-C(6)-S(1)	113.28(12)
C(36)-C(31)-C(32)	117.16(15)

C(36)-C(31)-N(3)	122.20(15)
C(32)-C(31)-N(3)	120.53(14)
C(33)-C(32)-C(31)	121.15(16)
C(32)-C(33)-C(34)	120.84(16)
O(30)-C(34)-C(35)	124.73(16)
O(30)-C(34)-C(33)	116.26(16)
C(35)-C(34)-C(33)	119.00(16)
C(34)-C(35)-C(36)	119.81(15)
C(31)-C(36)-C(35)	121.98(15)
C(34)-O(30)-C(37)	117.30(15)
C(62)-C(61)-C(66)	118.56(15)
C(62)-C(61)-C(6)	121.58(15)
C(66)-C(61)-C(6)	119.86(15)
C(61)-C(62)-C(63)	120.60(16)
C(64)-C(63)-C(62)	120.48(17)
C(63)-C(64)-C(65)	119.45(16)
C(64)-C(65)-C(66)	120.37(16)
C(65)-C(66)-C(61)	120.53(16)

Table Supp4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5e**. 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)	35(1)	29(1)	38(1)	5(1)	-2(1)	1(1)
C(2)	39(1)	38(1)	28(1)	3(1)	0(1)	-4(1)
N(3)	35(1)	30(1)	30(1)	0(1)	2(1)	-3(1)
C(4)	39(1)	29(1)	35(1)	-4(1)	8(1)	0(1)
N(5)	30(1)	28(1)	32(1)	1(1)	6(1)	1(1)
C(6)	28(1)	31(1)	28(1)	4(1)	6(1)	2(1)
C(31)	30(1)	25(1)	30(1)	-3(1)	-1(1)	-5(1)
C(32)	36(1)	35(1)	37(1)	5(1)	-3(1)	0(1)
C(33)	31(1)	39(1)	51(1)	6(1)	2(1)	6(1)
C(34)	36(1)	32(1)	44(1)	2(1)	10(1)	0(1)
C(35)	38(1)	25(1)	35(1)	3(1)	3(1)	1(1)
C(36)	30(1)	25(1)	35(1)	-1(1)	0(1)	1(1)
O(30)	49(1)	54(1)	62(1)	18(1)	26(1)	15(1)
C(37)	96(2)	72(2)	75(2)	36(1)	56(2)	38(2)
C(61)	26(1)	30(1)	33(1)	1(1)	6(1)	1(1)
C(62)	35(1)	33(1)	48(1)	7(1)	-1(1)	-2(1)
C(63)	38(1)	32(1)	60(1)	1(1)	1(1)	-5(1)
C(64)	28(1)	43(1)	47(1)	-8(1)	1(1)	-1(1)
C(65)	33(1)	43(1)	41(1)	-1(1)	-1(1)	7(1)
C(66)	34(1)	31(1)	38(1)	2(1)	5(1)	3(1)

Table Supp5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5e**.

	x	y	z	U(eq)
H(2A)	-1615	7345	335	42
H(2B)	-355	6956	-310	42
H(4A)	694	5648	644	41
H(4B)	250	5082	2027	41
H(32A)	-3003	7046	1601	44
H(33A)	-4314	6967	3443	48
H(35A)	-1870	5205	5717	39
H(36A)	-508	5347	3907	36
H(37A)	-4416	5609	7708	117
H(37B)	-2955	5795	7525	117
H(37C)	-3639	4843	6811	117
H(62A)	1945	9062	2664	47
H(63A)	3442	9856	4188	52
H(64A)	4619	8989	5968	47
H(65A)	4264	7322	6251	47
H(66A)	2745	6527	4764	40