Supplementary Information

The synthesis of thia-6-oxa-6aλ^4-seleno-3-azapentalene and a 3*H*-1,2,4-dithiazole

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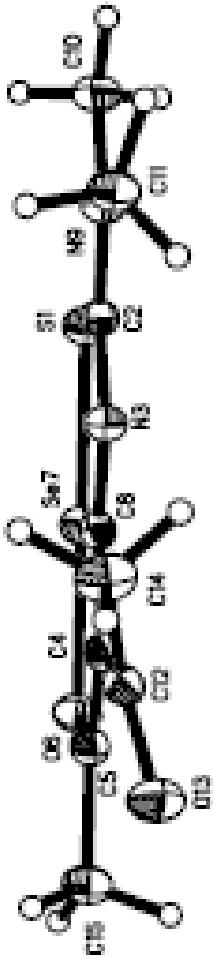

Figure S1 X-ray crystal structure of **3a** (thermal ellipsoid drawing).

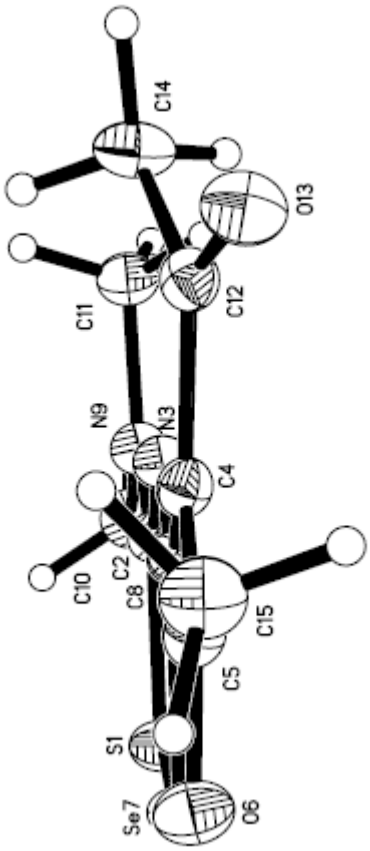

Figure S2 X-ray crystal structure of **3a** (thermal ellipsoid drawing).

Table S1 Crystal data and structure refinement for **3a**

Empirical formula	$C_{12}H_{12}N_2O_2S\,Se$
Formula weight	327.26
Temperature	190(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P\,2_1/c$
Unit cell dimensions	a = 7.6506(8) Å
	b = 18.5206(18) Å β = 110.451(5) º
	c = 8.4687(8) Å
Volume	1124.33(19) Å^3
Z, Calculated density	4, 1.933 Mg/m^3
Absorption coefficient	3.519 mm^{-1}
F(000)	656
Crystal size	0.21 x 0.19 x 0.16 mm
θ range for data collection	3.0 to 27.5 º
Limiting indices	$-6 \le h \le 9$, $-23 \le k \le 23$, $-10 \le l \le 10$
Reflections collected / unique	13403 / 2517 [R_{int} = 0.0198]
Completeness to θ =	27.48 98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6029 and 0.5253
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2517 / 0 / 140
Goodness-of-fit on F^2	1.078
Final R indices [I>2σ(I)]	$R1$ = 0.0224, $wR2$ = 0.0560
R indices (all data)	$R1$ = 0.0267, $wR2$ = 0.0582
Largest diff. peak and hole	0.319 and -0.471 e. Å^{-3}

Table S2. Selected bond lengths [Å] and angles [°] for **3a**.

Se(1)-C(3)	1.9182(17)
Se(1)-O(5)	2.1647(13)
Se(1)-S(1)	2.3097(6)
S(1)-C(1)	1.7348(18)
C(1)-N(6)	1.329(2)
C(1)-N(2)	1.339(2)
N(2)-C(3)	1.318(2)
C(3)-C(4)	1.412(2)
C(4)-C(5)	1.425(2)
C(4)-C(9)	1.479(2)
O(5)-C(5)	1.274(2)
C(5)-C(11)	1.501(3)
N(6)-C(8)	1.457(2)
N(6)-C(7)	1.461(2)
O(9)-C(9)	1.222(2)
C(9)-C(10)	1.498(3)
C(3)-Se(1)-O(5)	80.28(6)
C(3)-Se(1)-S(1)	86.46(5)
O(5)-Se(1)-S(1)	166.70(4)
C(1)-S(1)-Se(1)	93.25(6)
N(6)-C(1)-N(2)	118.83(16)
N(6)-C(1)-S(1)	119.98(13)
N(2)-C(1)-S(1)	121.19(13)
C(3)-N(2)-C(1)	119.67(16)
N(2)-C(3)-C(4)	125.22(16)
N(2)-C(3)-Se(1)	119.41(13)
C(4)-C(3)-Se(1)	115.37(12)
C(3)-C(4)-C(5)	115.06(15)
C(3)-C(4)-C(9)	123.79(15)
C(5)-C(4)-C(9)	121.15(16)
C(5)-O(5)-Se(1)	110.58(11)
O(5)-C(5)-C(4)	118.66(16)
O(5)-C(5)-C(11)	116.00(16)
C(4)-C(5)-C(11)	125.32(17)
C(1)-N(6)-C(8)	120.35(15)
C(1)-N(6)-C(7)	121.00(16)
C(8)-N(6)-C(7)	118.62(15)
O(9)-C(9)-C(4)	120.70(17)
O(9)-C(9)-C(10)	118.41(17)
C(4)-C(9)-C(10)	120.89(16)

Symmetry transformations used to generate equivalent atoms:

Table S3. Bond lengths [Å] and angles [º] for **3a**.

Se(1)-C(3)	1.9182(17)
Se(1)-O(5)	2.1647(13)
Se(1)-S(1)	2.3097(6)
S(1)-C(1)	1.7348(18)
C(1)-N(6)	1.329(2)
C(1)-N(2)	1.339(2)
N(2)-C(3)	1.318(2)
C(3)-C(4)	1.412(2)
C(4)-C(5)	1.425(2)
C(4)-C(9)	1.479(2)
O(5)-C(5)	1.274(2)
C(5)-C(11)	1.501(3)
N(6)-C(8)	1.457(2)
N(6)-C(7)	1.461(2)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
O(9)-C(9)	1.222(2)
C(9)-C(10)	1.498(3)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(3)-Se(1)-O(5)	80.28(6)
C(3)-Se(1)-S(1)	86.46(5)
O(5)-Se(1)-S(1)	166.70(4)
C(1)-S(1)-Se(1)	93.25(6)
N(6)-C(1)-N(2)	118.83(16)
N(6)-C(1)-S(1)	119.98(13)
N(2)-C(1)-S(1)	121.19(13)
C(3)-N(2)-C(1)	119.67(16)
N(2)-C(3)-C(4)	125.22(16)
N(2)-C(3)-Se(1)	119.41(13)
C(4)-C(3)-Se(1)	115.37(12)
C(3)-C(4)-C(5)	115.06(15)
C(3)-C(4)-C(9)	123.79(15)
C(5)-C(4)-C(9)	121.15(16)
C(5)-O(5)-Se(1)	110.58(11)
O(5)-C(5)-C(4)	118.66(16)
O(5)-C(5)-C(11)	116.00(16)
C(4)-C(5)-C(11)	125.32(17)
C(1)-N(6)-C(8)	120.35(15)
C(1)-N(6)-C(7)	121.00(16)

C(8)-N(6)-C(7)	118.62(15)
N(6)-C(7)-H(7A)	109.5
N(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
N(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(6)-C(8)-H(8A)	109.5
N(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
N(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(9)-C(9)-C(4)	120.70(17)
O(9)-C(9)-C(10)	118.41(17)
C(4)-C(9)-C(10)	120.89(16)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(5)-C(11)-H(11A)	109.5
C(5)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(5)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Torsion angles [°] for **3a**.

C(3)-Se(1)-S(1)-C(1)	-0.62(7)
O(5)-Se(1)-S(1)-C(1)	3.66(18)
Se(1)-S(1)-C(1)-N(6)	-178.60(13)
Se(1)-S(1)-C(1)-N(2)	1.52(14)
N(6)-C(1)-N(2)-C(3)	178.11(15)
S(1)-C(1)-N(2)-C(3)	-2.0(2)
C(1)-N(2)-C(3)-C(4)	-179.90(15)
C(1)-N(2)-C(3)-Se(1)	1.2(2)
O(5)-Se(1)-C(3)-N(2)	-179.16(14)
S(1)-Se(1)-C(3)-N(2)	-0.16(13)
O(5)-Se(1)-C(3)-C(4)	1.88(12)
S(1)-Se(1)-C(3)-C(4)	-179.12(12)
N(2)-C(3)-C(4)-C(5)	178.86(15)
Se(1)-C(3)-C(4)-C(5)	-2.3(2)
N(2)-C(3)-C(4)-C(9)	-1.5(3)
Se(1)-C(3)-C(4)-C(9)	177.38(12)
C(3)-Se(1)-O(5)-C(5)	-1.30(12)
S(1)-Se(1)-O(5)-C(5)	-5.6(3)
Se(1)-O(5)-C(5)-C(4)	0.45(19)
Se(1)-O(5)-C(5)-C(11)	179.19(12)
C(3)-C(4)-C(5)-O(5)	1.1(2)
C(9)-C(4)-C(5)-O(5)	-178.55(15)
C(3)-C(4)-C(5)-C(11)	-177.53(16)
C(9)-C(4)-C(5)-C(11)	2.8(3)
N(2)-C(1)-N(6)-C(8)	-1.7(2)
S(1)-C(1)-N(6)-C(8)	178.38(13)
N(2)-C(1)-N(6)-C(7)	-179.79(16)
S(1)-C(1)-N(6)-C(7)	0.3(2)
C(3)-C(4)-C(9)-O(9)	-164.54(17)
C(5)-C(4)-C(9)-O(9)	15.1(3)
C(3)-C(4)-C(9)-C(10)	15.4(3)
C(5)-C(4)-C(9)-C(10)	-164.94(17)

Symmetry transformations used to generate equivalent atoms:

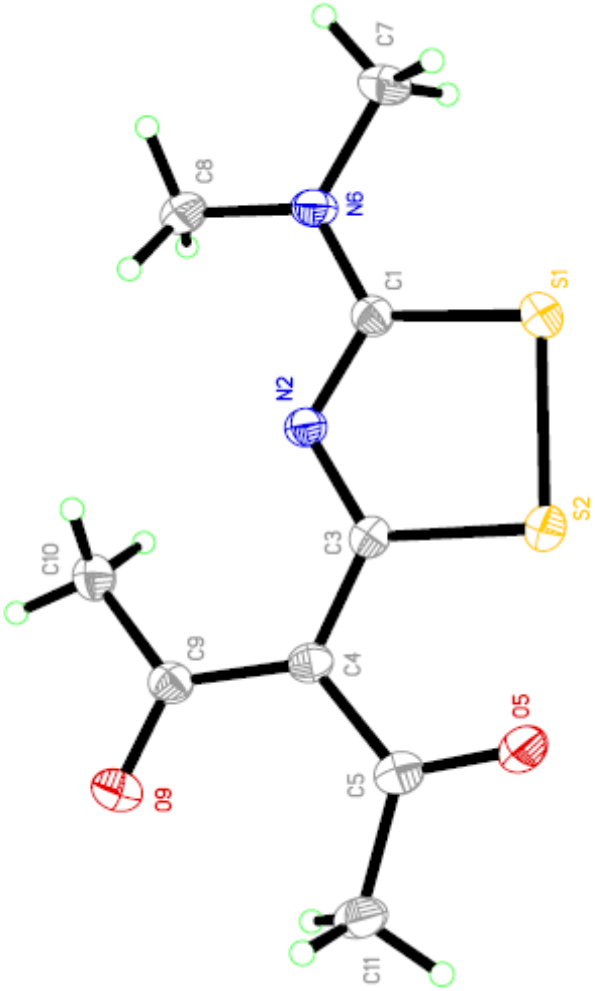

Figure S3 X-ray crystal structure of **4a** (thermal ellipsoid drawing).

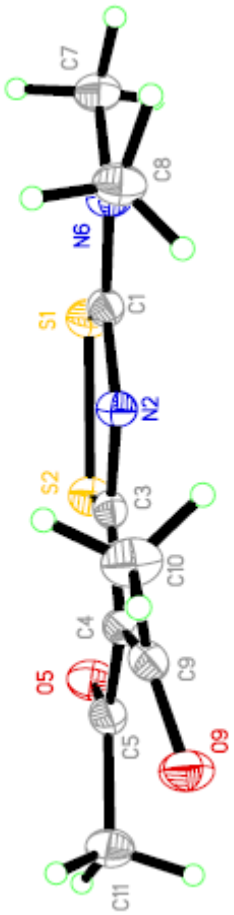

Figure S4 X-ray crystal structure of 4a (thermal ellipsoid drawing).

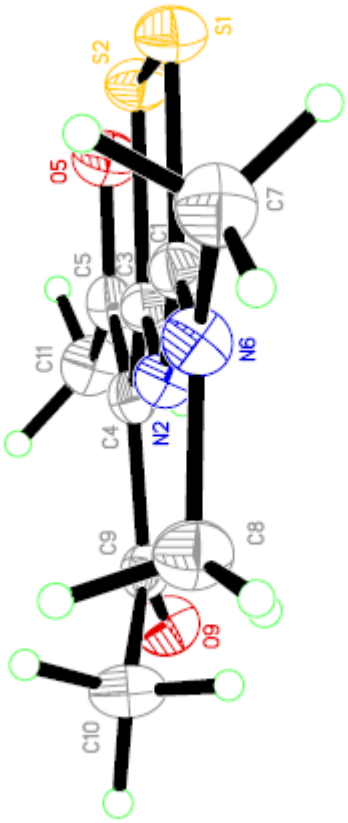

Figure S5 X-ray crystal structure of **4a** (thermal ellipsoid drawing).

Table S5. Crystal data and structure refinement for **4a**.

Empirical formula	$C_9H_{12}N_2O_2S_2$
Formula weight	244.33
Temperature	190(2) K
Wavelength	0.71069 A
Crystal system, space group	Monoclinic, $P\ 2_1/c$
Unit cell dimensions	a = 7.6627(8) Å
	b = 18.4638(18) Å β = 110.288(5) º
	c = 8.3775(8) Å
Volume	1111.74(19) Å ^{3}
Z, Calculated density	4, 1.460 Mg/m^3
Absorption coefficient	0.460 mm^{-1}
F(000)	512
Crystal size	0.40 x 0.10 x 0.06 mm
θ range for data collection	2.8 to 27.5 º
Limiting indices	$-9 \le h \le 9$, $-23 \le k \le 23$, $-10 \le l \le 10$
Reflections collected / unique	31420 / 2537 [R_{int} = 0.0249]
Completeness to θ = 27.47	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9729 and 0.8373
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2537 / 0 / 140
Goodness-of-fit on F^2	1.031
Final R indices [$I>2\sigma(I)$]	$R1$ = 0.0320, $wR2$ = 0.0802
R indices (all data)	$R1$ = 0.0412, $wR2$ = 0.0845
Largest diff. peak and hole	0.315 and -0.215 e.A^{-3}

Table S6. Selected bond lengths [Å] and angles [º] for **4a**.

S(1)-C(1)	1.7361(15)
S(1)-S(2)	2.1367(6)
C(1)-N(6)	1.326(2)
C(1)-N(2)	1.3279(19)
S(2)-C(3)	1.7768(15)
N(2)-C(3)	1.3288(19)
C(3)-C(4)	1.413(2)
C(4)-C(5)	1.428(2)
C(4)-C(9)	1.476(2)
O(5)-C(5)	1.265(2)
C(5)-C(11)	1.502(2)
N(6)-C(8)	1.457(2)
N(6)-C(7)	1.463(2)
C(9)-O(9)	1.2253(19)
C(9)-C(10)	1.505(2)
C(1)-S(1)-S(2)	93.14(5)
N(6)-C(1)-N(2)	120.22(14)
N(6)-C(1)-S(1)	120.74(11)
N(2)-C(1)-S(1)	119.05(12)
C(3)-S(2)-S(1)	91.37(5)
C(1)-N(2)-C(3)	117.79(13)
N(2)-C(3)-C(4)	123.70(14)
N(2)-C(3)-S(2)	118.64(11)
C(4)-C(3)-S(2)	117.66(11)
C(3)-C(4)-C(5)	114.76(13)
C(3)-C(4)-C(9)	123.67(13)
C(5)-C(4)-C(9)	121.57(13)
O(5)-C(5)-C(4)	117.98(14)
O(5)-C(5)-C(11)	117.30(14)
C(4)-C(5)-C(11)	124.70(15)
C(1)-N(6)-C(8)	120.15(13)
C(1)-N(6)-C(7)	121.05(14)
C(8)-N(6)-C(7)	118.73(13)
O(9)-C(9)-C(4)	120.38(14)
O(9)-C(9)-C(10)	118.04(14)
C(4)-C(9)-C(10)	121.58(13)

Symmetry transformations used to generate equivalent atoms:

Table S7. Bond lengths [Å] and angles [º] for **4a**.

S(1)-C(1)	1.7361(15)
S(1)-S(2)	2.1367(6)
C(1)-N(6)	1.326(2)
C(1)-N(2)	1.3279(19)
S(2)-C(3)	1.7768(15)
N(2)-C(3)	1.3288(19)
C(3)-C(4)	1.413(2)
C(4)-C(5)	1.428(2)
C(4)-C(9)	1.476(2)
O(5)-C(5)	1.265(2)
C(5)-C(11)	1.502(2)
N(6)-C(8)	1.457(2)
N(6)-C(7)	1.463(2)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-O(9)	1.2253(19)
C(9)-C(10)	1.505(2)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(1)-S(1)-S(2)	93.14(5)
N(6)-C(1)-N(2)	120.22(14)
N(6)-C(1)-S(1)	120.74(11)
N(2)-C(1)-S(1)	119.05(12)
C(3)-S(2)-S(1)	91.37(5)
C(1)-N(2)-C(3)	117.79(13)
N(2)-C(3)-C(4)	123.70(14)
N(2)-C(3)-S(2)	118.64(11)
C(4)-C(3)-S(2)	117.66(11)
C(3)-C(4)-C(5)	114.76(13)
C(3)-C(4)-C(9)	123.67(13)
C(5)-C(4)-C(9)	121.57(13)
O(5)-C(5)-C(4)	117.98(14)
O(5)-C(5)-C(11)	117.30(14)
C(4)-C(5)-C(11)	124.70(15)
C(1)-N(6)-C(8)	120.15(13)
C(1)-N(6)-C(7)	121.05(14)
C(8)-N(6)-C(7)	118.73(13)
N(6)-C(7)-H(7A)	109.5
N(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5

N(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(6)-C(8)-H(8A)	109.5
N(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
N(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(9)-C(9)-C(4)	120.38(14)
O(9)-C(9)-C(10)	118.04(14)
C(4)-C(9)-C(10)	121.58(13)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(5)-C(11)-H(11A)	109.5
C(5)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(5)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S8. Torsion angles [°] for **4a**.

S(2)-S(1)-C(1)-N(6)	-178.72(12)
S(2)-S(1)-C(1)-N(2)	1.42(12)
C(1)-S(1)-S(2)-C(3)	-0.80(7)
N(6)-C(1)-N(2)-C(3)	178.60(13)
S(1)-C(1)-N(2)-C(3)	-1.54(19)
C(1)-N(2)-C(3)-C(4)	179.50(13)
C(1)-N(2)-C(3)-S(2)	0.68(19)
S(1)-S(2)-C(3)-N(2)	0.26(12)
S(1)-S(2)-C(3)-C(4)	-178.63(11)
N(2)-C(3)-C(4)-C(5)	178.36(13)
S(2)-C(3)-C(4)-C(5)	-2.82(18)
N(2)-C(3)-C(4)-C(9)	-2.4(2)
S(2)-C(3)-C(4)-C(9)	176.41(11)
C(3)-C(4)-C(5)-O(5)	1.4(2)
C(9)-C(4)-C(5)-O(5)	-177.86(13)
C(3)-C(4)-C(5)-C(11)	-176.92(14)
C(9)-C(4)-C(5)-C(11)	3.8(2)
N(2)-C(1)-N(6)-C(8)	-3.2(2)
S(1)-C(1)-N(6)-C(8)	176.99(11)
N(2)-C(1)-N(6)-C(7)	179.92(13)
S(1)-C(1)-N(6)-C(7)	0.1(2)
C(3)-C(4)-C(9)-O(9)	-164.03(14)
C(5)-C(4)-C(9)-O(9)	15.1(2)
C(3)-C(4)-C(9)-C(10)	16.2(2)
C(5)-C(4)-C(9)-C(10)	-164.62(15)

Symmetry transformations used to generate equivalent atoms:

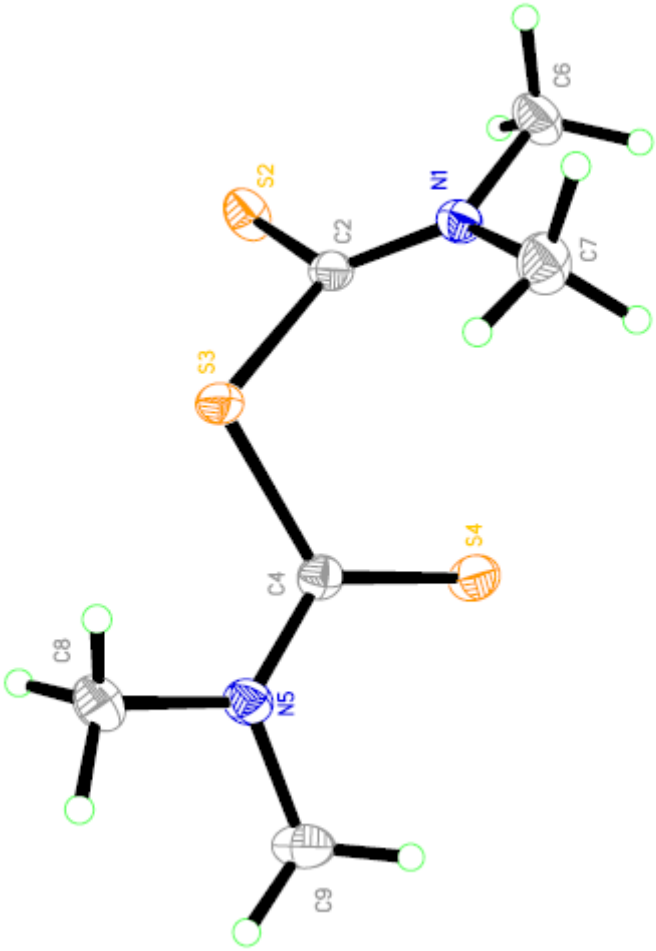

Figure S6 X-ray crystal structure of **5** (thermal ellipsoid drawing).

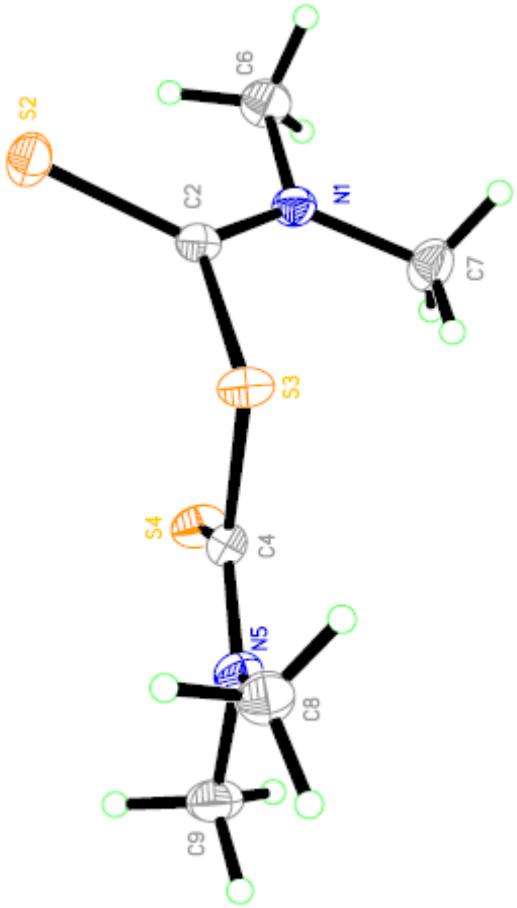

Figure S7 X-ray crystal structure of **5** (thermal ellipsoid drawing).

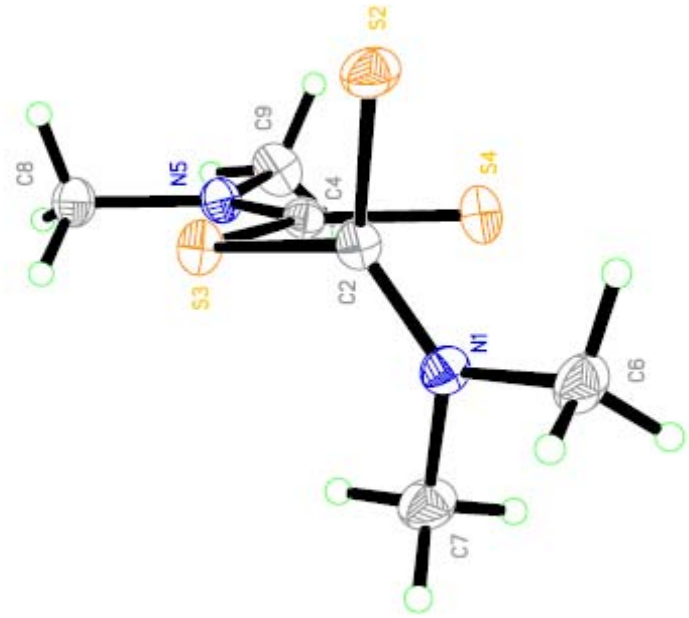

Figure S8 X-ray crystal structure of **5** (thermal ellipsoid drawing).

Table S9. Crystal data and structure refinement for **5**.

Empirical formula	$C_6H_{12}N_2S_{1.96}Se_{1.04}$
Formula weight	257.01
Temperature	190(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P* 2(1)/c
Unit cell dimensions	*a* = 10.1624(10) Å
	b = 7.4766(7) Å β = 111.027(5) º
	c = 14.1240(14) Å
Volume	1001.68(17) $Å^3$
Z, Calculated density	4, 1.704 Mg/m^3
Absorption coefficient	4.237 mm^{-1}
F(000)	515
Crystal size	0.41 x 0.24 x 0.14 mm
θ range for data collection	3.1 to 27.5 º
Limiting indices	$-13 \le h \le 13$, $-9 \le k \le 9$, $-18 \le l \le 18$
Reflections collected / unique	29933 / 2293 [R_{int} = 0.0180]
Completeness to θ=	27.48 99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5884 and 0.2755
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2293 / 0 / 108
Goodness-of-fit on F^2	1.143
Final *R* indices [$I>2\sigma(I)$]	*R*1 = 0.0236, *wR*2 = 0.0475
R indices (all data)	*R*1 = 0.0277, *wR*2 = 0.0486
Extinction coefficient	0.0043(5)
Largest diff. peak and hole	0.266 and -0.300 e. $Å^{-3}$

Table S10. Selected bond lengths [Å] and angles [º] for **5**.

N(1)-C(2)	1.321(2)
N(1)-C(7)	1.466(2)
N(1)-C(6)	1.466(2)
S(2)-C(2)	1.7593(18)
C(2)-S(3)	1.8818(17)
S(3)-C(4)	1.8559(18)
S(4)-C(4)	1.7236(18)
C(4)-N(5)	1.339(2)
N(5)-C(9)	1.466(2)
N(5)-C(8)	1.467(2)
C(2)-N(1)-C(7)	126.07(16)
C(2)-N(1)-C(6)	120.78(16)
C(7)-N(1)-C(6)	113.15(15)
N(1)-C(2)-S(2)	125.35(13)
N(1)-C(2)-S(3)	118.69(13)
S(2)-C(2)-S(3)	115.51(10)
C(4)-S(3)-C(2)	100.50(8)
N(5)-C(4)-S(4)	124.43(14)
N(5)-C(4)-S(3)	111.49(13)
S(4)-C(4)-S(3)	124.07(10)
C(4)-N(5)-C(9)	119.67(16)
C(4)-N(5)-C(8)	123.51(16)
C(9)-N(5)-C(8)	116.64(15)

Symmetry transformations used to generate equivalent atoms:

Table S11. Bond lengths [Å] and angles [°] for **5**.

N(1)-C(2)	1.321(2)
N(1)-C(7)	1.466(2)
N(1)-C(6)	1.466(2)
S(2)-C(2)	1.7593(18)
C(2)-S(3)	1.8818(17)
S(3)-C(4)	1.8559(18)
S(4)-C(4)	1.7236(18)
C(4)-N(5)	1.339(2)
N(5)-C(9)	1.466(2)
N(5)-C(8)	1.467(2)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(2)-N(1)-C(7)	126.07(16)
C(2)-N(1)-C(6)	120.78(16)
C(7)-N(1)-C(6)	113.15(15)
N(1)-C(2)-S(2)	125.35(13)
N(1)-C(2)-S(3)	118.69(13)
S(2)-C(2)-S(3)	115.51(10)
C(4)-S(3)-C(2)	100.50(8)
N(5)-C(4)-S(4)	124.43(14)
N(5)-C(4)-S(3)	111.49(13)
S(4)-C(4)-S(3)	124.07(10)
C(4)-N(5)-C(9)	119.67(16)
C(4)-N(5)-C(8)	123.51(16)
C(9)-N(5)-C(8)	116.64(15)
N(1)-C(6)-H(6A)	109.5
N(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
N(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
N(1)-C(7)-H(7A)	109.5
N(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
N(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(5)-C(8)-H(8A)	109.5

N(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
N(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(5)-C(9)-H(9A)	109.5
N(5)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
N(5)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S12. Torsion angles [º] for **5**.

C(7)-N(1)-C(2)-S(2)	175.58(15)
C(6)-N(1)-C(2)-S(2)	-4.5(3)
C(7)-N(1)-C(2)-S(3)	3.6(3)
C(6)-N(1)-C(2)-S(3)	-176.51(14)
N(1)-C(2)-S(3)-C(4)	-79.45(15)
S(2)-C(2)-S(3)-C(4)	107.77(10)
C(2)-S(3)-C(4)-N(5)	-172.31(13)
C(2)-S(3)-C(4)-S(4)	6.85(13)
S(4)-C(4)-N(5)-C(9)	-4.3(3)
S(3)-C(4)-N(5)-C(9)	174.89(14)
S(4)-C(4)-N(5)-C(8)	-179.22(14)
S(3)-C(4)-N(5)-C(8)	-0.1(2)

Symmetry transformations used to generate equivalent atoms: