

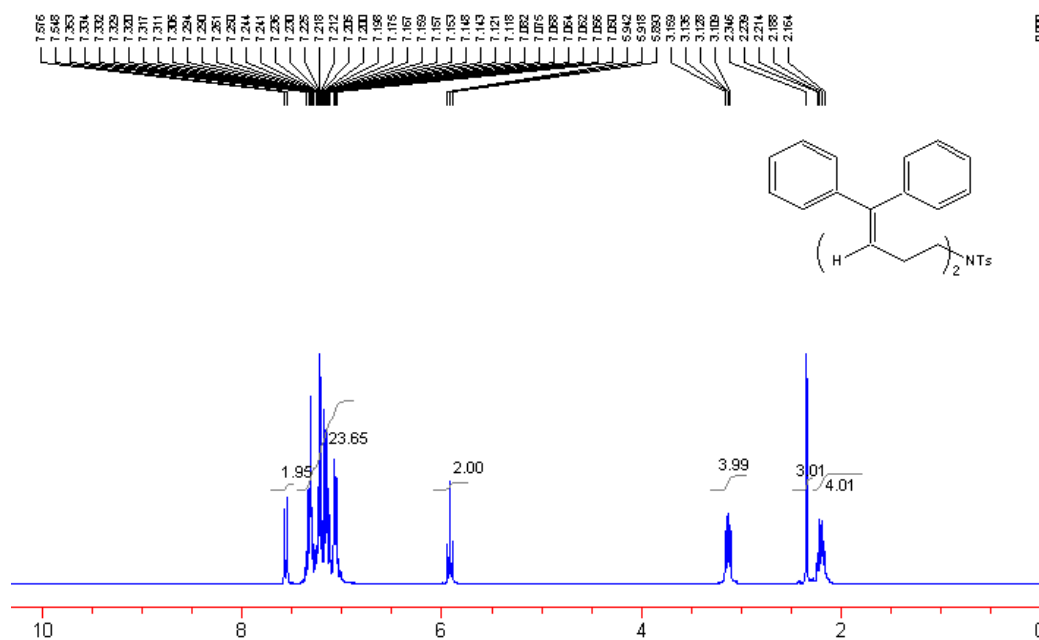
Supporting Information

Ring-opening Reactions of MCPs with Sulfonamides Promoted by Metal Triflate Lewis Acids

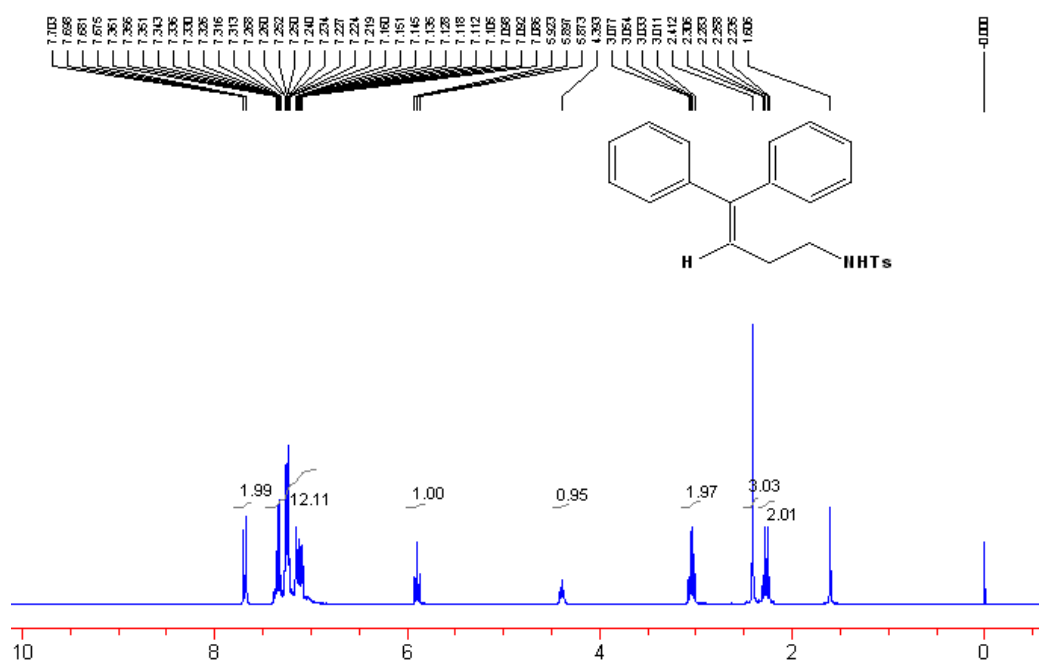
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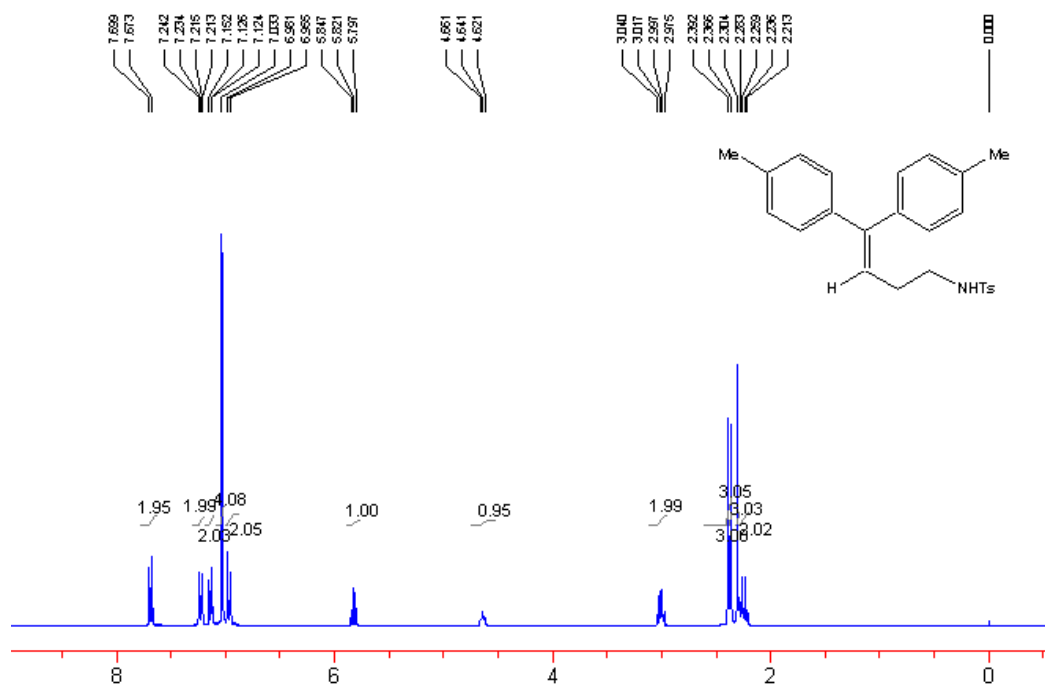
¹ H NMR charts of compounds	S2-S11
X-ray data of 5f .	S12-S21



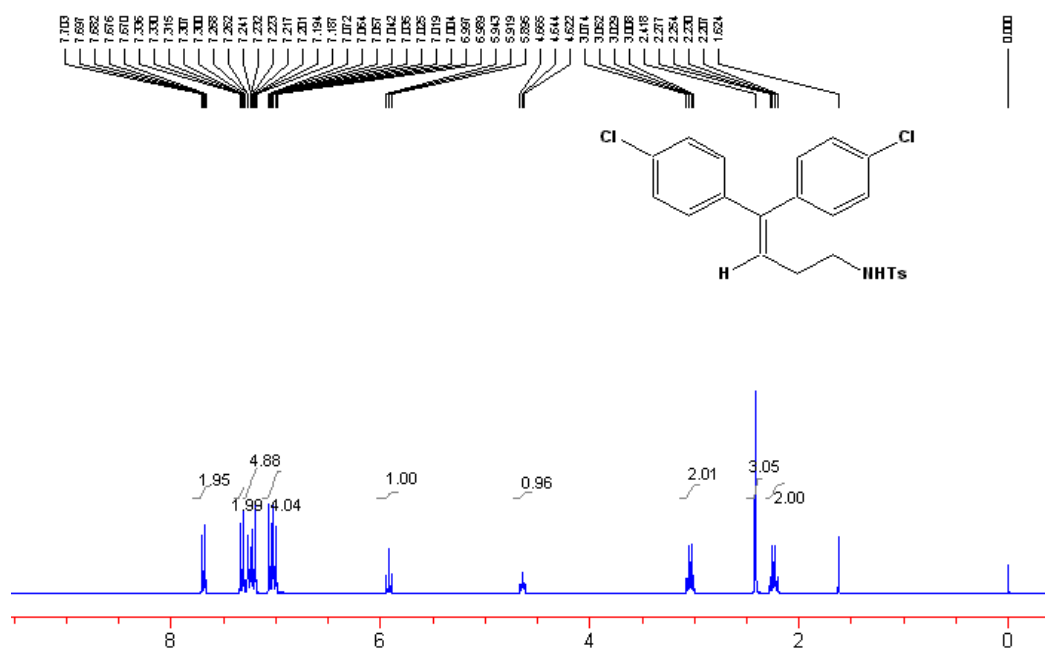
The ¹H NMR spectrum of **4a**.



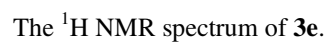
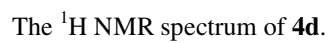
The ¹H NMR spectrum of **3a**.

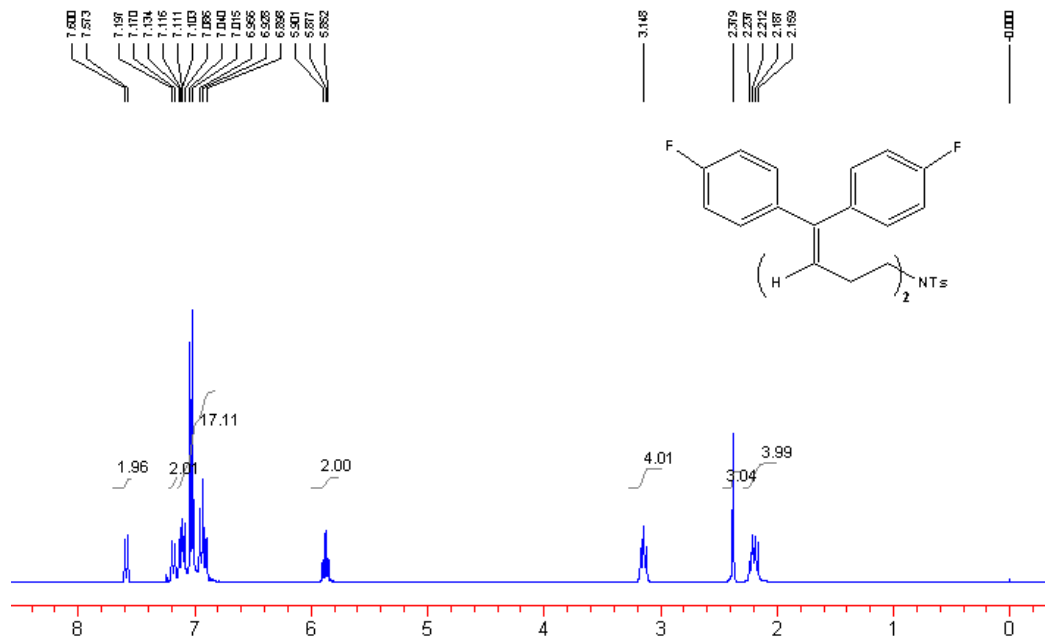


The ¹H NMR spectrum of **3b**.

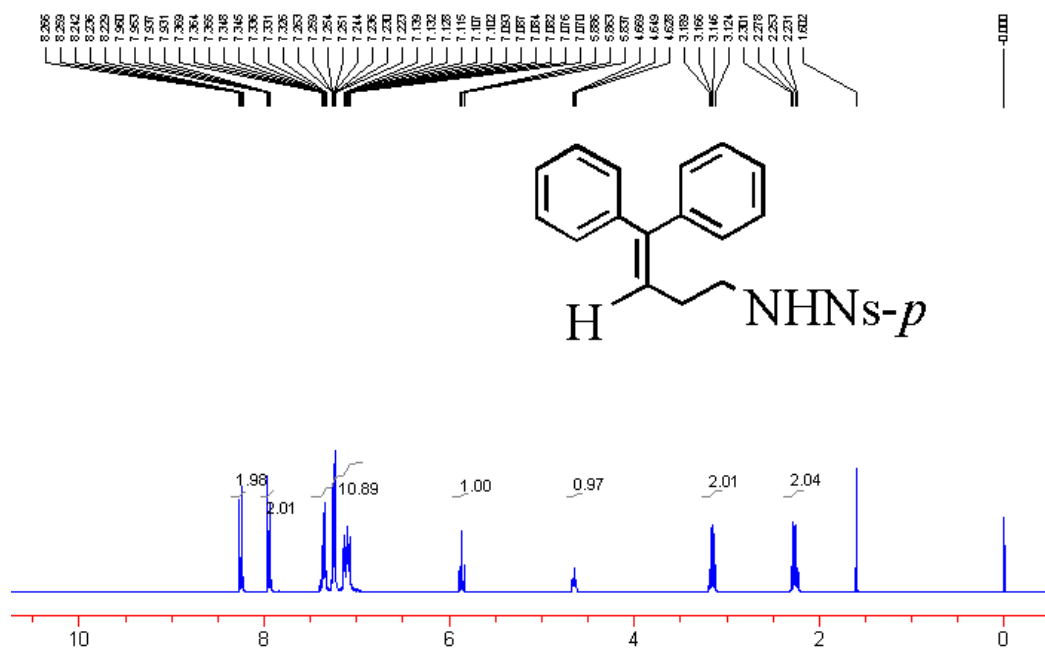


The ¹H NMR spectrum of **3d**.

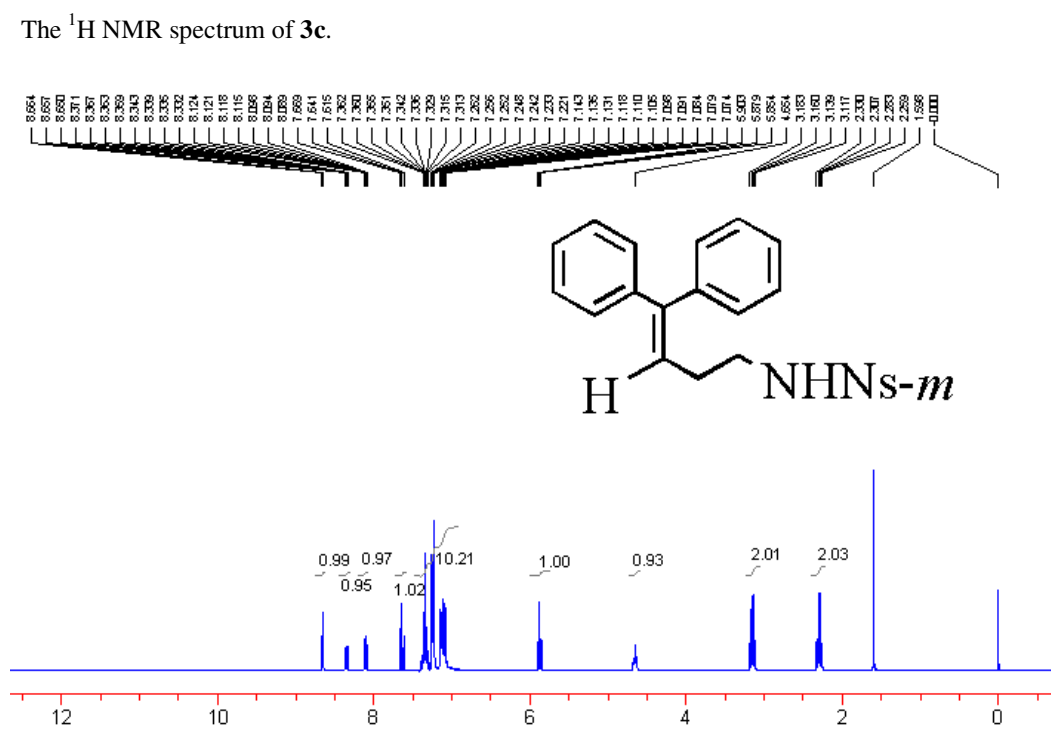
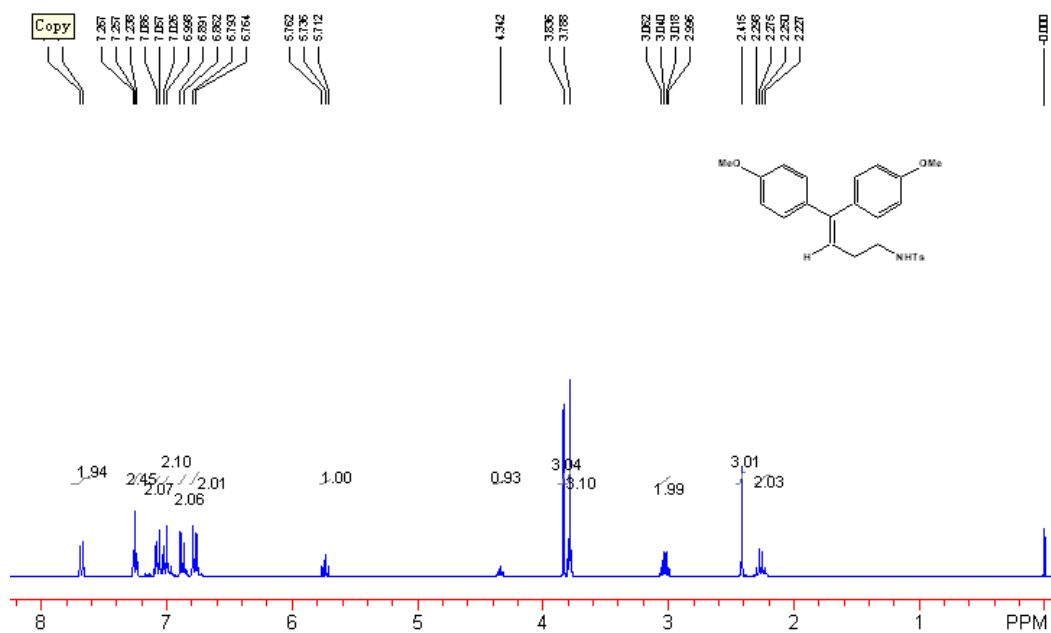


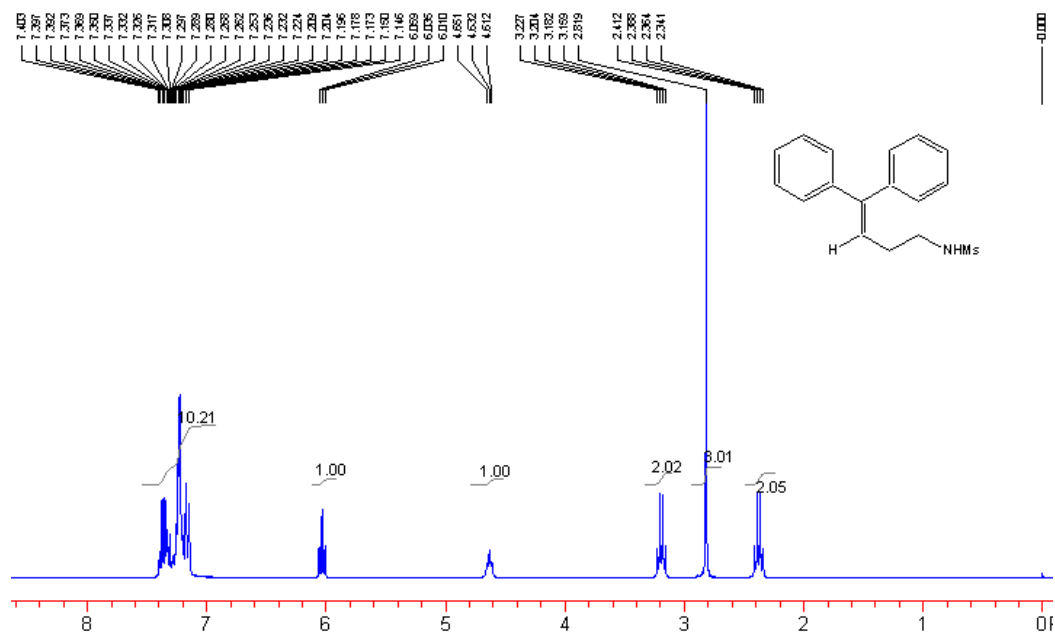


The ¹H NMR spectrum of **4e**.

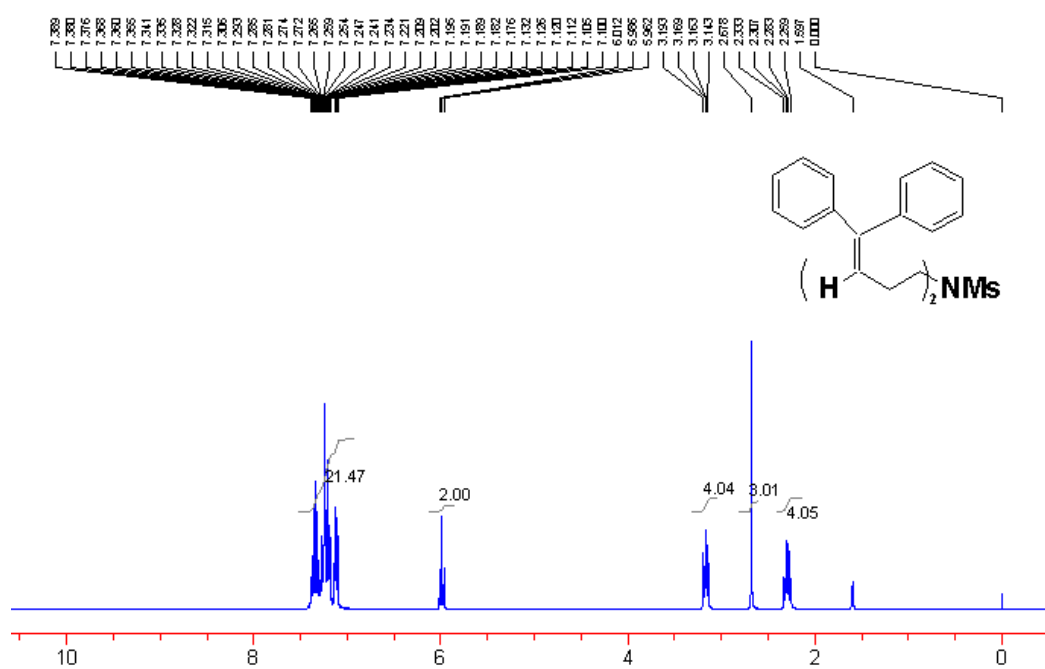


The ¹H NMR spectrum of **3j**.

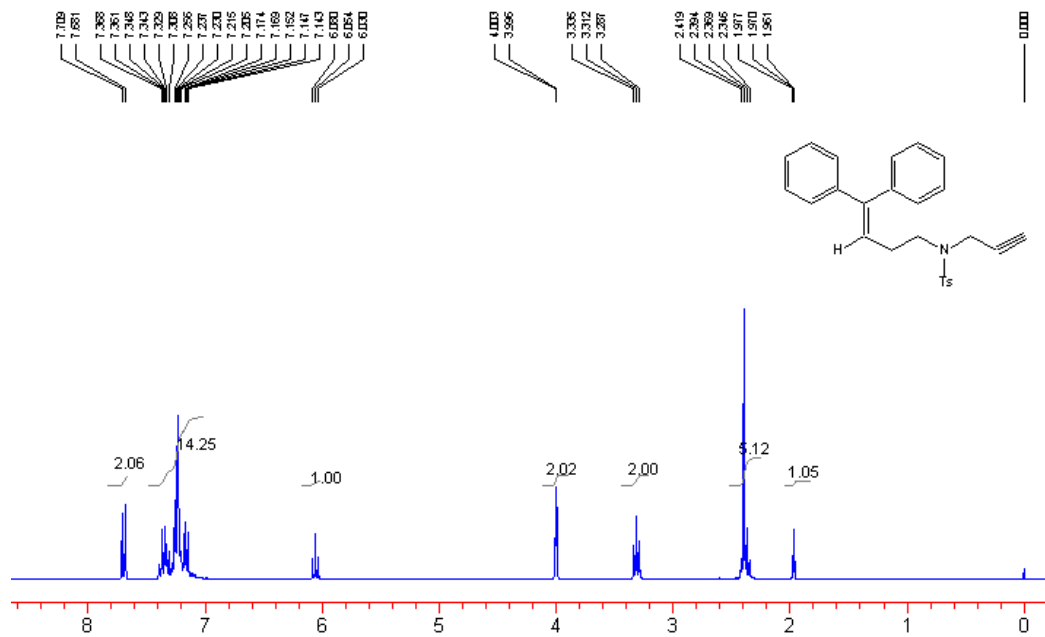




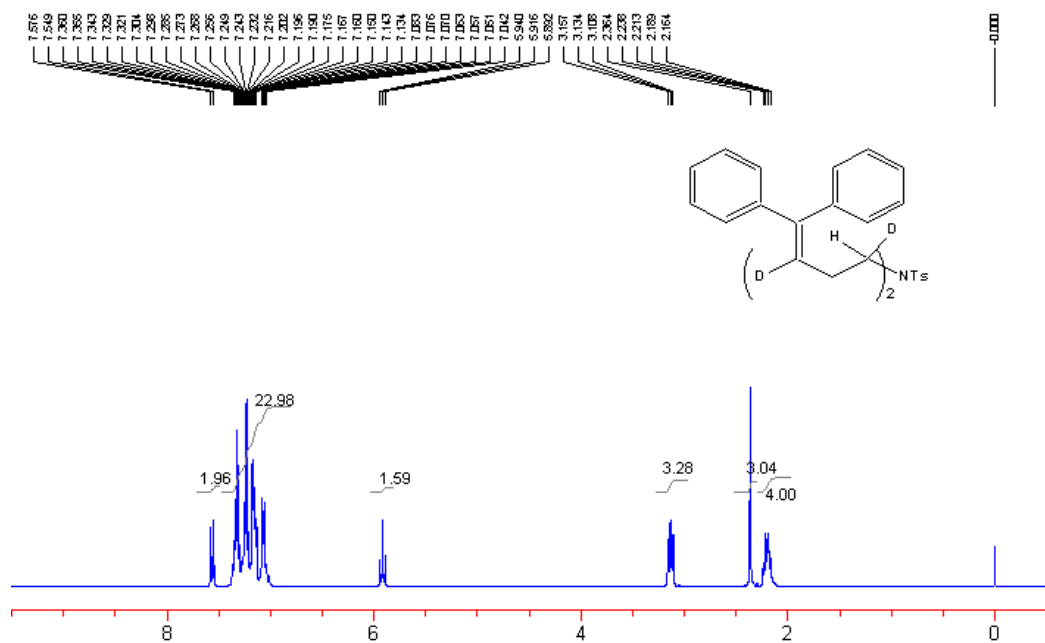
The ¹H NMR spectrum of **3I**.



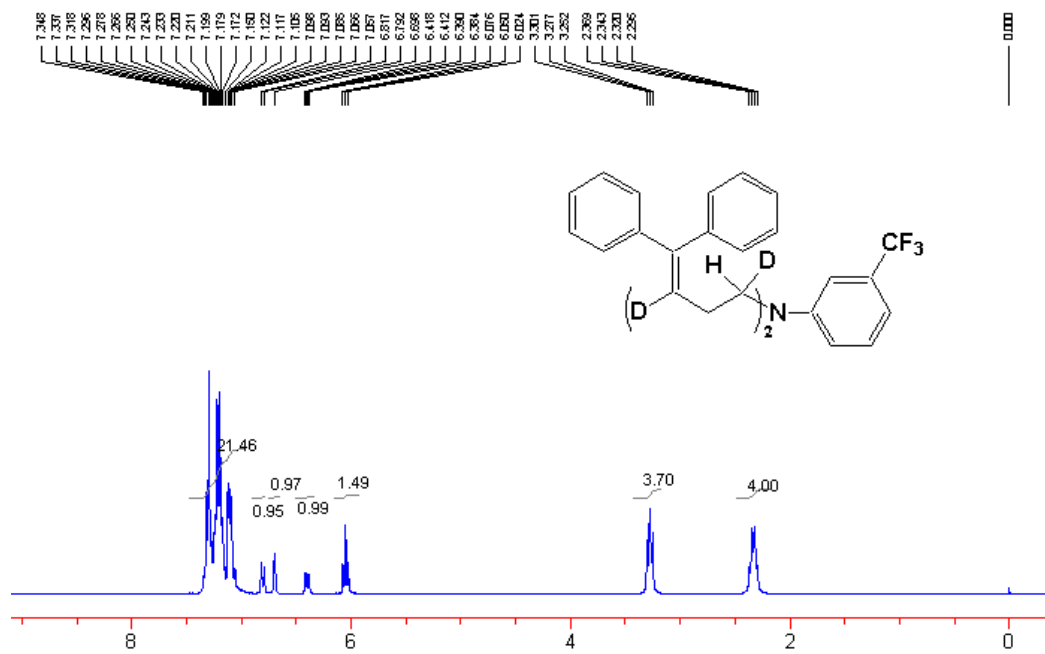
The ¹H NMR spectrum of **4I**.



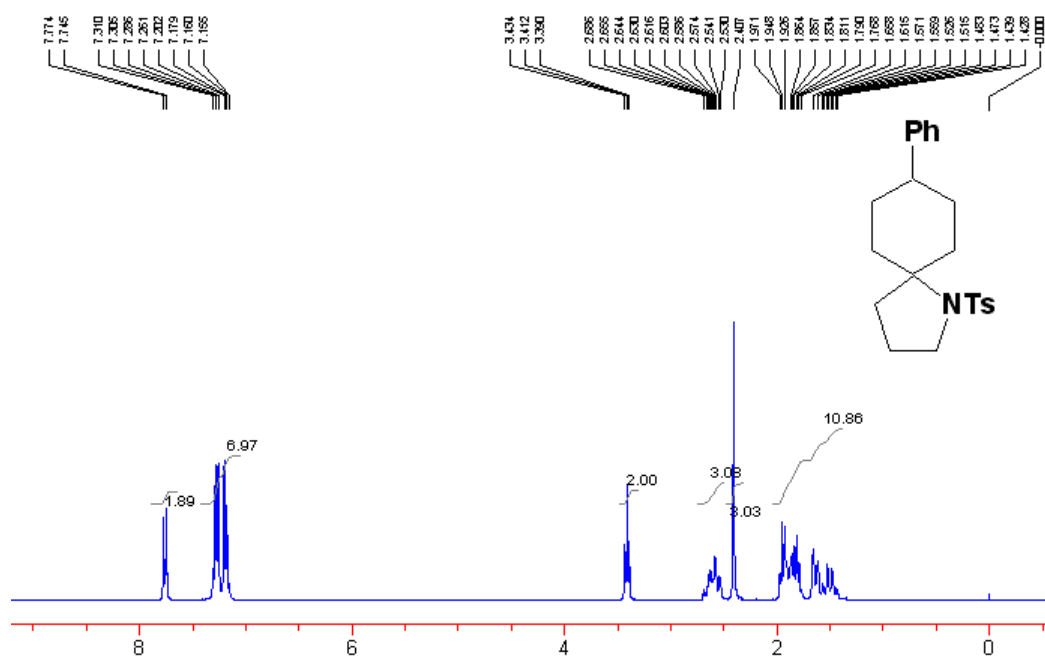
The ¹H NMR spectrum of **3m**.



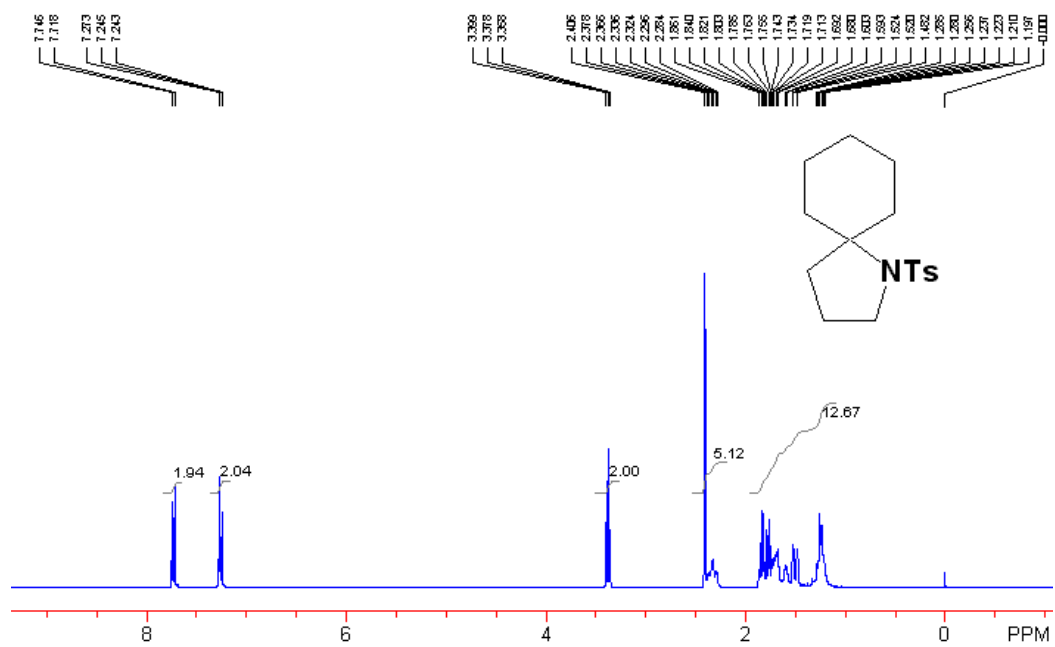
The ¹H NMR spectrum of **4a-d**.



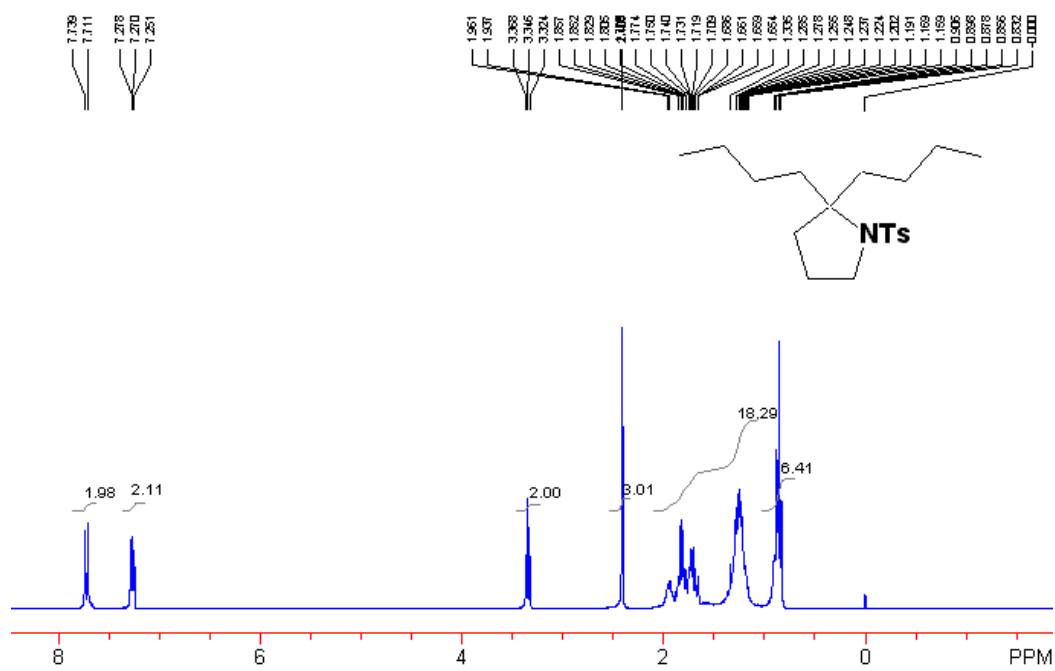
The ^1H NMR spectrum of **4i-d**.



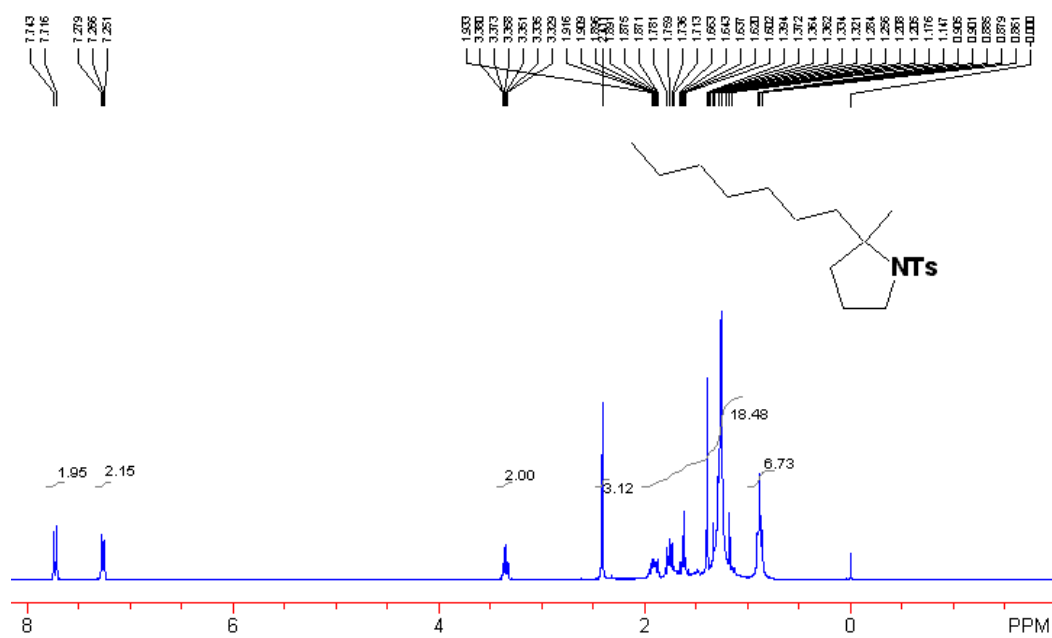
The ^1H NMR spectrum of **5f**.



The ^1H NMR spectrum of **5g**.



The ^1H NMR spectrum of **5h**.



The ^1H NMR spectrum of **5i**.

Table 1. Crystal data and structure refinement for cd23267.

Identification code	cd23267
Empirical formula	C22 H27 N O2 S
Formula weight	369.51
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 5.9875(5) Å alpha = 90 deg. b = 19.9377(18) Å beta = 94.585(2) deg. c = 15.8348(14) Å gamma = 90 deg.
Volume	1884.3(3) Å ³
Z, Calculated density	4, 1.303 Mg/m ³
Absorption coefficient	0.188 mm ⁻¹
F(000)	792
Crystal size	0.510 x 0.248 x 0.217 mm
Theta range for data collection	1.65 to 28.30 deg.
Limiting indices	-7<=h<=7, -26<=k<=17, -20<=l<=21
Reflections collected / unique	11377 / 4350 [R(int) = 0.0572]
Completeness to theta = 28.30	93.2 %
Absorption correction	Sadabs
Max. and min. transmission	1.00000 and 0.25534
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4350 / 4 / 343
Goodness-of-fit on F ²	0.914
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1150
R indices (all data)	R1 = 0.0788, wR2 = 0.1235
Largest diff. peak and hole	0.434 and -0.310 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd23267. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
S	6796 (1)	8146 (1)	8288 (1)	40 (1)
O(1)	5542 (2)	8684 (1)	7878 (1)	53 (1)
O(2)	5610 (3)	7650 (1)	8719 (1)	63 (1)
N(1)	8248 (3)	7793 (1)	7610 (1)	37 (1)
C(1)	9541 (5)	7191 (1)	7867 (2)	55 (1)
C(2)	11160 (6)	7127 (2)	7201 (2)	79 (1)
C(3)	10005 (5)	7415 (1)	6429 (2)	55 (1)
C(4)	8493 (3)	7989 (1)	6700 (1)	34 (1)
C(5)	9623 (4)	8670 (1)	6639 (1)	42 (1)
C(6)	9774 (4)	8894 (1)	5724 (1)	49 (1)
C(7)	7498 (4)	8888 (1)	5226 (1)	40 (1)
C(8)	6481 (4)	8192 (1)	5258 (1)	40 (1)
C(9)	6250 (4)	7978 (1)	6173 (1)	40 (1)
C(10)	7568 (4)	9162 (1)	4335 (1)	40 (1)
C(11)	5808 (5)	9541 (1)	3977 (2)	50 (1)
C(12)	5864 (5)	9828 (1)	3187 (2)	60 (1)
C(13)	7685 (5)	9737 (1)	2736 (2)	59 (1)
C(14)	9403 (6)	9346 (2)	3063 (2)	65 (1)
C(15)	9357 (4)	9061 (1)	3857 (1)	55 (1)
C(16)	8710 (3)	8508 (1)	9069 (1)	34 (1)
C(17)	8051 (4)	8577 (1)	9879 (1)	45 (1)
C(18)	9410 (4)	8914 (1)	10483 (1)	51 (1)
C(19)	11425 (4)	9182 (1)	10301 (1)	42 (1)
C(20)	12077 (4)	9098 (1)	9494 (1)	48 (1)
C(21)	10732 (4)	8760 (1)	8881 (1)	46 (1)
C(22)	12878 (6)	9562 (2)	10954 (2)	64 (1)

Table 3. Bond lengths [Å] and angles [deg] for cd23267.

S-O(2)	1.4226(15)
S-O(1)	1.4343(15)
S-N(1)	1.5990(17)
S-C(16)	1.771(2)
N(1)-C(1)	1.468(3)
N(1)-C(4)	1.510(2)
C(1)-C(2)	1.494(4)
C(1)-H(1)	0.93(3)
C(1)-H(2)	0.94(3)
C(2)-C(3)	1.471(4)
C(2)-H(3)	0.980(19)
C(2)-H(4)	0.99(3)
C(3)-C(4)	1.540(3)
C(3)-H(5)	0.993(18)
C(3)-H(6)	1.01(2)
C(4)-C(5)	1.524(3)
C(4)-C(9)	1.524(3)
C(5)-C(6)	1.527(3)
C(5)-H(7)	0.98(2)
C(5)-H(8)	1.026(19)
C(6)-C(7)	1.519(3)
C(6)-H(9)	1.00(2)
C(6)-H(10)	0.97(2)
C(7)-C(10)	1.516(3)
C(7)-C(8)	1.519(3)
C(7)-H(11)	0.89(2)
C(8)-C(9)	1.527(3)
C(8)-H(12)	0.95(2)
C(8)-H(13)	0.99(2)
C(9)-H(14)	0.96(2)
C(9)-H(15)	0.96(2)
C(10)-C(15)	1.375(3)
C(10)-C(11)	1.381(3)
C(11)-C(12)	1.379(3)
C(11)-H(16)	0.89(3)
C(12)-C(13)	1.362(4)
C(12)-H(17)	0.92(2)
C(13)-C(14)	1.360(4)
C(13)-H(18)	0.88(2)
C(14)-C(15)	1.382(3)
C(14)-H(19)	0.87(3)
C(15)-H(20)	0.93(2)
C(16)-C(21)	1.366(3)
C(16)-C(17)	1.378(3)
C(17)-C(18)	1.379(3)
C(17)-H(21)	0.93(2)
C(18)-C(19)	1.372(3)
C(18)-H(22)	0.96(2)
C(19)-C(20)	1.376(3)
C(19)-C(22)	1.502(3)
C(20)-C(21)	1.385(3)
C(20)-H(23)	0.99(2)
C(21)-H(24)	0.88(2)
C(22)-H(25)	0.923(18)
C(22)-H(26)	0.917(18)
C(22)-H(27)	0.90(3)
O(2)-S-O(1)	118.25(10)
O(2)-S-N(1)	109.58(10)
O(1)-S-N(1)	108.53(8)
O(2)-S-C(16)	105.58(9)
O(1)-S-C(16)	107.34(9)
N(1)-S-C(16)	107.00(9)
C(1)-N(1)-C(4)	112.74(17)

C(1)-N(1)-S	118.44(14)
C(4)-N(1)-S	128.82(13)
N(1)-C(1)-C(2)	103.4(2)
N(1)-C(1)-H(1)	110.2(15)
C(2)-C(1)-H(1)	114.5(16)
N(1)-C(1)-H(2)	111.0(19)
C(2)-C(1)-H(2)	112.1(19)
H(1)-C(1)-H(2)	106(2)
C(3)-C(2)-C(1)	105.3(2)
C(3)-C(2)-H(3)	98(3)
C(1)-C(2)-H(3)	111(3)
C(3)-C(2)-H(4)	114.2(15)
C(1)-C(2)-H(4)	111.7(15)
H(3)-C(2)-H(4)	116(3)
C(2)-C(3)-C(4)	107.8(2)
C(2)-C(3)-H(5)	108.8(18)
C(4)-C(3)-H(5)	110.2(18)
C(2)-C(3)-H(6)	115.8(13)
C(4)-C(3)-H(6)	112.4(13)
H(5)-C(3)-H(6)	102(2)
N(1)-C(4)-C(5)	111.57(15)
N(1)-C(4)-C(9)	111.72(16)
C(5)-C(4)-C(9)	110.77(17)
N(1)-C(4)-C(3)	100.26(16)
C(5)-C(4)-C(3)	111.71(19)
C(9)-C(4)-C(3)	110.43(18)
C(4)-C(5)-C(6)	112.39(18)
C(4)-C(5)-H(7)	107.5(12)
C(6)-C(5)-H(7)	110.5(12)
C(4)-C(5)-H(8)	106.6(11)
C(6)-C(5)-H(8)	109.4(11)
H(7)-C(5)-H(8)	110.3(16)
C(7)-C(6)-C(5)	111.9(2)
C(7)-C(6)-H(9)	112.1(13)
C(5)-C(6)-H(9)	108.0(13)
C(7)-C(6)-H(10)	110.8(13)
C(5)-C(6)-H(10)	107.3(13)
H(9)-C(6)-H(10)	106.6(18)
C(10)-C(7)-C(8)	113.68(17)
C(10)-C(7)-C(6)	112.96(19)
C(8)-C(7)-C(6)	109.54(19)
C(10)-C(7)-H(11)	104.9(13)
C(8)-C(7)-H(11)	108.4(13)
C(6)-C(7)-H(11)	107.0(13)
C(7)-C(8)-C(9)	110.79(18)
C(7)-C(8)-H(12)	108.6(12)
C(9)-C(8)-H(12)	111.7(13)
C(7)-C(8)-H(13)	107.9(12)
C(9)-C(8)-H(13)	111.3(12)
H(12)-C(8)-H(13)	106.3(17)
C(4)-C(9)-C(8)	111.89(17)
C(4)-C(9)-H(14)	109.5(12)
C(8)-C(9)-H(14)	107.7(12)
C(4)-C(9)-H(15)	111.5(12)
C(8)-C(9)-H(15)	102.9(12)
H(14)-C(9)-H(15)	113.2(18)
C(15)-C(10)-C(11)	117.2(2)
C(15)-C(10)-C(7)	122.7(2)
C(11)-C(10)-C(7)	120.1(2)
C(12)-C(11)-C(10)	121.7(3)
C(12)-C(11)-H(16)	119.4(16)
C(10)-C(11)-H(16)	118.8(16)
C(13)-C(12)-C(11)	120.0(3)
C(13)-C(12)-H(17)	125.2(16)
C(11)-C(12)-H(17)	114.8(16)
C(14)-C(13)-C(12)	119.3(3)
C(14)-C(13)-H(18)	123.7(17)
C(12)-C(13)-H(18)	116.9(17)

C(13)-C(14)-C(15)	120.8(3)
C(13)-C(14)-H(19)	121(2)
C(15)-C(14)-H(19)	118(2)
C(10)-C(15)-C(14)	120.9(3)
C(10)-C(15)-H(20)	118.6(13)
C(14)-C(15)-H(20)	120.4(14)
C(21)-C(16)-C(17)	119.4(2)
C(21)-C(16)-S	122.21(15)
C(17)-C(16)-S	118.24(16)
C(16)-C(17)-C(18)	119.8(2)
C(16)-C(17)-H(21)	117.4(14)
C(18)-C(17)-H(21)	122.7(13)
C(19)-C(18)-C(17)	121.6(2)
C(19)-C(18)-H(22)	120.0(13)
C(17)-C(18)-H(22)	118.4(14)
C(18)-C(19)-C(20)	117.8(2)
C(18)-C(19)-C(22)	121.5(2)
C(20)-C(19)-C(22)	120.7(2)
C(19)-C(20)-C(21)	121.2(2)
C(19)-C(20)-H(23)	119.2(12)
C(21)-C(20)-H(23)	119.6(12)
C(16)-C(21)-C(20)	120.1(2)
C(16)-C(21)-H(24)	120.6(14)
C(20)-C(21)-H(24)	119.2(14)
C(19)-C(22)-H(25)	108(2)
C(19)-C(22)-H(26)	111(2)
H(25)-C(22)-H(26)	86(3)
C(19)-C(22)-H(27)	114.3(19)
H(25)-C(22)-H(27)	105(3)
H(26)-C(22)-H(27)	127(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd23267.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
S	36(1)	52(1)	31(1)	-1(1)	7(1)	-6(1)
O(1)	44(1)	75(1)	41(1)	-5(1)	0(1)	20(1)
O(2)	65(1)	77(1)	51(1)	-4(1)	19(1)	-35(1)
N(1)	44(1)	38(1)	29(1)	3(1)	4(1)	5(1)
C(1)	74(2)	44(2)	47(2)	7(1)	3(1)	11(1)
C(2)	105(3)	72(2)	60(2)	9(2)	16(2)	48(2)
C(3)	62(2)	57(2)	47(1)	-1(1)	13(1)	17(1)
C(4)	37(1)	37(1)	26(1)	1(1)	5(1)	-1(1)
C(5)	46(1)	49(1)	32(1)	3(1)	-2(1)	-12(1)
C(6)	60(2)	50(2)	34(1)	5(1)	-3(1)	-19(1)
C(7)	51(1)	40(1)	30(1)	-1(1)	6(1)	8(1)
C(8)	37(1)	52(1)	31(1)	-2(1)	-2(1)	-6(1)
C(9)	40(1)	46(1)	35(1)	-1(1)	3(1)	-11(1)
C(10)	53(1)	35(1)	30(1)	-2(1)	1(1)	1(1)
C(11)	59(2)	52(2)	39(1)	-3(1)	-2(1)	9(1)
C(12)	81(2)	52(2)	44(1)	4(1)	-16(1)	11(2)
C(13)	94(2)	48(2)	33(1)	6(1)	-6(1)	-17(2)
C(14)	72(2)	84(2)	39(1)	4(1)	11(1)	-5(2)
C(15)	60(2)	66(2)	38(1)	6(1)	5(1)	13(1)
C(16)	38(1)	35(1)	28(1)	2(1)	5(1)	0(1)
C(17)	46(1)	54(2)	35(1)	5(1)	11(1)	-7(1)
C(18)	64(2)	62(2)	27(1)	-3(1)	10(1)	-4(1)
C(19)	50(1)	42(1)	33(1)	1(1)	1(1)	2(1)
C(20)	42(1)	61(2)	42(1)	-4(1)	7(1)	-11(1)
C(21)	43(1)	67(2)	30(1)	-5(1)	9(1)	-6(1)
C(22)	70(2)	75(2)	47(2)	-17(2)	-2(2)	-10(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd23267.

	x	y	z	U(eq)
H(1)	10200(40)	7242(12)	8412(17)	69(8)
H(2)	8600(50)	6812(16)	7885(19)	101(11)
H(3)	12360(60)	7462(19)	7290(30)	190(20)
H(4)	11660(40)	6658(14)	7137(16)	74(8)
H(5)	9080(40)	7060(12)	6131(18)	107(11)
H(6)	11000(40)	7559(11)	5977(15)	64(7)
H(7)	11120(30)	8635(10)	6933(13)	43(6)
H(8)	8670(30)	9006(10)	6944(12)	36(5)
H(9)	10480(40)	9348(12)	5733(14)	59(7)
H(10)	10810(40)	8592(11)	5472(14)	55(7)
H(11)	6630(30)	9171(10)	5482(12)	42(6)
H(12)	5080(40)	8193(10)	4934(13)	44(6)
H(13)	7450(30)	7879(10)	4969(12)	41(6)
H(14)	5650(30)	7529(11)	6162(12)	45(6)
H(15)	5240(30)	8306(10)	6369(13)	42(6)
H(16)	4590(40)	9592(13)	4262(16)	72(9)
H(17)	4590(40)	10058(13)	3000(15)	70(8)
H(18)	7640(40)	9923(12)	2235(16)	68(8)
H(19)	10630(50)	9308(15)	2809(18)	99(11)
H(20)	10560(40)	8812(10)	4087(13)	47(6)
H(21)	6650(40)	8409(11)	9985(13)	51(6)
H(22)	8950(40)	8939(11)	11048(14)	58(7)
H(23)	13560(40)	9269(10)	9356(13)	53(6)
H(24)	11230(30)	8693(10)	8378(14)	51(6)
H(25)	12960(60)	9317(16)	11450(16)	131(14)
H(26)	12040(50)	9865(14)	11231(19)	120(13)
H(27)	14310(50)	9613(14)	10827(19)	95(11)

Table 6. Torsion angles [deg] for cd23267.

O(2)-S-N(1)-C(1)	-44.8(2)
O(1)-S-N(1)-C(1)	-175.22(19)
C(16)-S-N(1)-C(1)	69.2(2)
O(2)-S-N(1)-C(4)	134.70(17)
O(1)-S-N(1)-C(4)	4.24(19)
C(16)-S-N(1)-C(4)	-111.30(17)
C(4)-N(1)-C(1)-C(2)	16.9(3)
S-N(1)-C(1)-C(2)	-163.6(2)
N(1)-C(1)-C(2)-C(3)	-29.9(3)
C(1)-C(2)-C(3)-C(4)	33.0(4)
C(1)-N(1)-C(4)-C(5)	-116.1(2)
S-N(1)-C(4)-C(5)	64.5(2)
C(1)-N(1)-C(4)-C(9)	119.3(2)
S-N(1)-C(4)-C(9)	-60.1(2)
C(1)-N(1)-C(4)-C(3)	2.3(2)
S-N(1)-C(4)-C(3)	-177.14(17)
C(2)-C(3)-C(4)-N(1)	-21.5(3)
C(2)-C(3)-C(4)-C(5)	96.8(3)
C(2)-C(3)-C(4)-C(9)	-139.4(3)
N(1)-C(4)-C(5)-C(6)	-176.93(19)
C(9)-C(4)-C(5)-C(6)	-51.8(3)
C(3)-C(4)-C(5)-C(6)	71.8(2)
C(4)-C(5)-C(6)-C(7)	54.4(3)
C(5)-C(6)-C(7)-C(10)	175.36(19)
C(5)-C(6)-C(7)-C(8)	-56.8(3)
C(10)-C(7)-C(8)-C(9)	-174.35(19)
C(6)-C(7)-C(8)-C(9)	58.2(3)
N(1)-C(4)-C(9)-C(8)	178.58(18)
C(5)-C(4)-C(9)-C(8)	53.5(3)
C(3)-C(4)-C(9)-C(8)	-70.8(2)
C(7)-C(8)-C(9)-C(4)	-57.6(3)
C(8)-C(7)-C(10)-C(15)	-90.0(3)
C(6)-C(7)-C(10)-C(15)	35.6(3)
C(8)-C(7)-C(10)-C(11)	91.3(2)
C(6)-C(7)-C(10)-C(11)	-143.1(2)
C(15)-C(10)-C(11)-C(12)	-2.2(3)
C(7)-C(10)-C(11)-C(12)	176.5(2)
C(10)-C(11)-C(12)-C(13)	0.3(4)
C(11)-C(12)-C(13)-C(14)	2.1(4)
C(12)-C(13)-C(14)-C(15)	-2.5(4)
C(11)-C(10)-C(15)-C(14)	1.8(4)
C(7)-C(10)-C(15)-C(14)	-176.9(2)
C(13)-C(14)-C(15)-C(10)	0.5(4)
O(2)-S-C(16)-C(21)	149.57(19)
O(1)-S-C(16)-C(21)	-83.4(2)
N(1)-S-C(16)-C(21)	32.9(2)
O(2)-S-C(16)-C(17)	-35.18(19)
O(1)-S-C(16)-C(17)	91.81(18)
N(1)-S-C(16)-C(17)	-151.86(17)
C(21)-C(16)-C(17)-C(18)	1.5(3)
S-C(16)-C(17)-C(18)	-173.88(17)
C(16)-C(17)-C(18)-C(19)	-0.2(4)
C(17)-C(18)-C(19)-C(20)	-1.0(4)
C(17)-C(18)-C(19)-C(22)	178.6(2)
C(18)-C(19)-C(20)-C(21)	0.9(4)
C(22)-C(19)-C(20)-C(21)	-178.7(2)
C(17)-C(16)-C(21)-C(20)	-1.6(3)
S-C(16)-C(21)-C(20)	173.59(17)
C(19)-C(20)-C(21)-C(16)	0.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd23267 [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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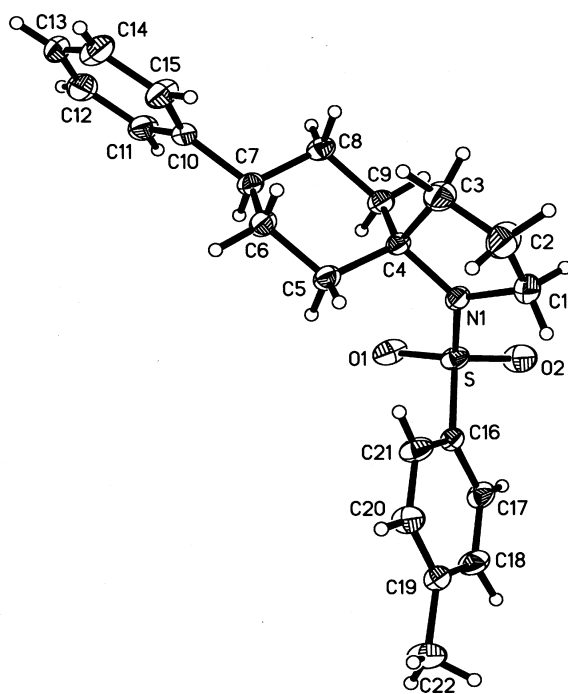


Figure 1. X-ray crystal structure of **5f**.