SUPPORTING INFORMATION

Synthesis of 1,1-[1-Naphthyloxy-2-thiophenyl]-2-methylaminomethylcyclopropanes and their Evaluation as Inhibitors of Serotonin, Norepinephrine and Dopamine Transporters

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- X-ray crystal structure of (±)-**12**
- X-ray crystal structure of (+)-**15**
- X-ray crystal structure of (-)-**15**
- X-ray crystal structure of (+)-**16**
- X-ray crystal structure of (-)-**16**

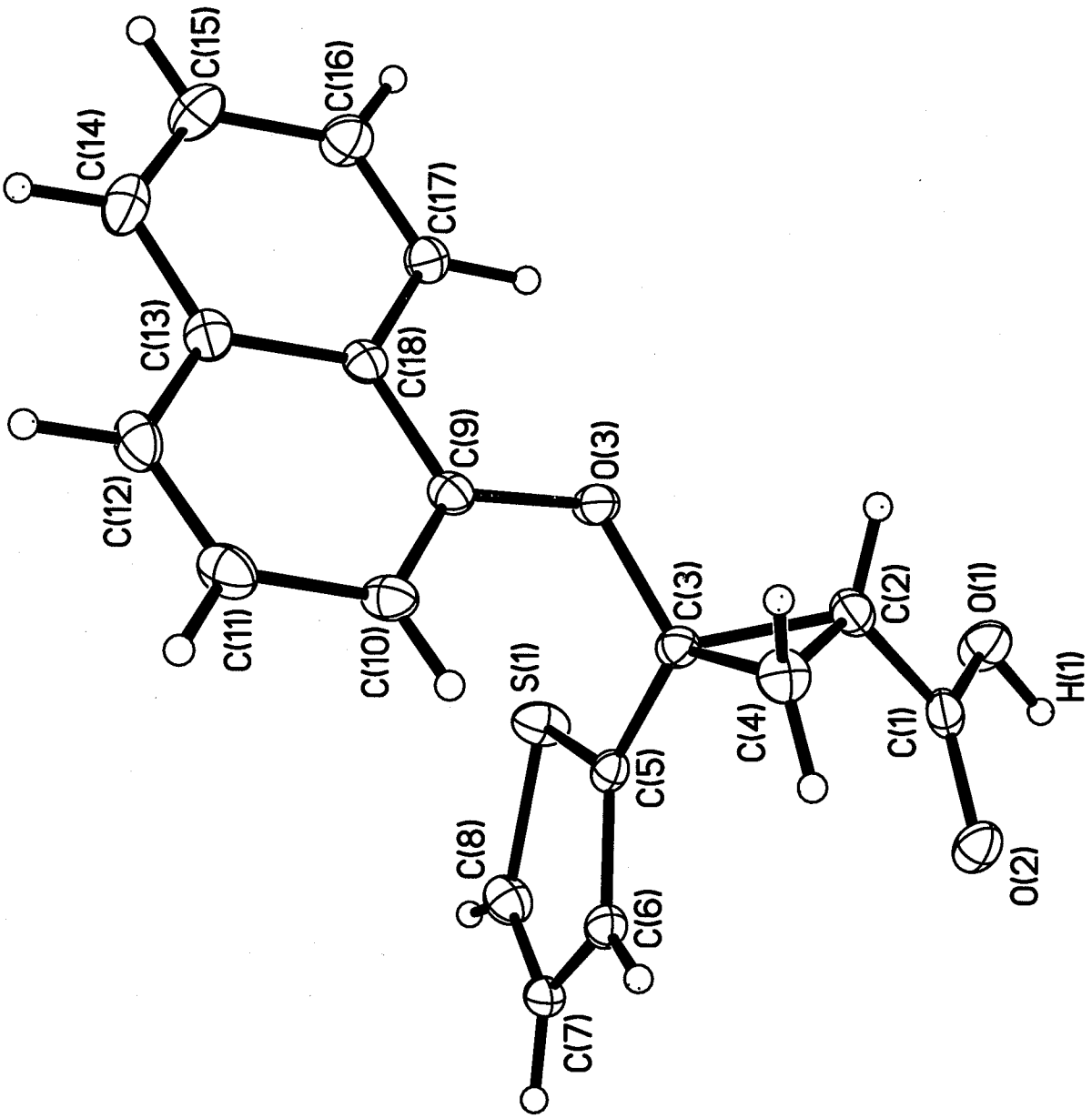

C(15)
C(16)
C(14)
C(17)
C(13)
C(18)
C(9)
O(3)
C(12)
C(11)
C(10)
C(3)
C(2)
O(1)
S(1)
C(4)
C(1)
H(1)
C(5)
C(8)
C(6)
O(2)
C(7)

Table 1. Crystal data and structure refinement for jw11.

Identification code	jw11	
Empirical formula	C18 H14 O3 S	
Formula weight	310.35	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.268(4) Å	a= 90°.
	b = 7.245(2) Å	b= 92.048(5)°.
	c = 17.100(5) Å	g = 90°.
Volume	1518.8(7) Å^3	
Z	4	
Density (calculated)	1.357 Mg/m^3	
Absorption coefficient	0.223 mm^{-1}	
F(000)	648	
Crystal size	0.30 x 0.11 x 0.06 mm^3	
Theta range for data collection	2.01 to 28.30°.	
Index ranges	-14<=h<=16, -9<=k<=9, -20<=l<=22	
Reflections collected	9164	
Independent reflections	3525 [R(int) = 0.0277]	
Completeness to theta = 28.30°	93.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.768	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3525 / 0 / 255	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1029	
R indices (all data)	R1 = 0.0676, wR2 = 0.1144	
Largest diff. peak and hole	0.363 and -0.239 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for jw11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1306(1)	7705(1)	2476(1)	35(1)
O(1)	-734(1)	4899(2)	899(1)	38(1)
O(2)	-216(1)	7220(2)	136(1)	34(1)
O(3)	-1012(1)	9123(2)	2543(1)	27(1)
C(1)	-687(2)	6653(3)	705(1)	28(1)
C(2)	-1255(2)	7862(3)	1253(1)	29(1)
C(3)	-570(2)	9129(3)	1791(1)	24(1)
C(4)	-1251(2)	9921(3)	1133(1)	32(1)
C(5)	632(2)	9087(2)	1798(1)	22(1)
C(6)	1343(2)	9861(3)	1299(1)	27(1)
C(7)	2441(2)	9332(3)	1478(1)	30(1)
C(8)	2542(2)	8176(3)	2090(1)	34(1)

C(9)	-898(1)	10700(3)	2992(1)	25(1)
C(10)	-609(2)	12395(3)	2717(1)	31(1)
C(11)	-537(2)	13897(3)	3241(1)	36(1)
C(12)	-741(2)	13687(3)	4011(1)	35(1)
C(13)	-1058(2)	11956(3)	4307(1)	29(1)
C(14)	-1308(2)	11675(3)	5099(1)	38(1)
C(15)	-1647(2)	10001(3)	5359(1)	43(1)
C(16)	-1751(2)	8507(3)	4841(1)	37(1)
C(17)	-1498(2)	8708(3)	4078(1)	29(1)
C(18)	-1150(1)	10430(3)	3790(1)	24(1)

Table 3. Bond lengths [Å] and angles [°] for j w11.

S(1)-C(8)	1.709(2)
S(1)-C(5)	1.7213(19)
O(1)-C(1)	1.315(2)
O(2)-C(1)	1.220(2)
O(3)-C(9)	1.381(2)
O(3)-C(3)	1.414(2)
C(1)-C(2)	1.476(3)
C(2)-C(4)	1.506(3)
C(2)-C(3)	1.529(3)
C(3)-C(5)	1.475(3)
C(3)-C(4)	1.491(3)
C(5)-C(6)	1.361(3)
C(6)-C(7)	1.423(3)
C(7)-C(8)	1.343(3)
C(9)-C(10)	1.366(3)
C(9)-C(18)	1.422(3)
C(10)-C(11)	1.410(3)
C(11)-C(12)	1.357(3)
C(12)-C(13)	1.412(3)
C(13)-C(14)	1.415(3)
C(13)-C(18)	1.418(3)
C(14)-C(15)	1.362(3)
C(15)-C(16)	1.401(3)
C(16)-C(17)	1.361(3)
C(17)-C(18)	1.413(3)
C(8)-S(1)-C(5)	92.03(10)
C(9)-O(3)-C(3)	117.99(14)
O(2)-C(1)-O(1)	123.56(19)
O(2)-C(1)-C(2)	123.63(18)
O(1)-C(1)-C(2)	112.80(18)
C(1)-C(2)-C(4)	119.87(18)
C(1)-C(2)-C(3)	118.46(16)

C(4)-C(2)-C(3)	58.87(13)
O(3)-C(3)-C(5)	114.12(16)
O(3)-C(3)-C(4)	117.66(16)
C(5)-C(3)-C(4)	123.16(16)
O(3)-C(3)-C(2)	108.97(15)
C(5)-C(3)-C(2)	121.35(16)
C(4)-C(3)-C(2)	59.80(13)
C(3)-C(4)-C(2)	61.33(13)
C(6)-C(5)-C(3)	130.48(18)
C(6)-C(5)-S(1)	110.99(15)
C(3)-C(5)-S(1)	118.26(13)
C(5)-C(6)-C(7)	112.18(19)
C(8)-C(7)-C(6)	113.27(19)
C(7)-C(8)-S(1)	111.53(17)
C(10)-C(9)-O(3)	125.06(18)
C(10)-C(9)-C(18)	121.43(18)
O(3)-C(9)-C(18)	113.48(16)
C(9)-C(10)-C(11)	119.1(2)
C(12)-C(11)-C(10)	121.3(2)
C(11)-C(12)-C(13)	120.64(19)
C(12)-C(13)-C(14)	122.87(19)
C(12)-C(13)-C(18)	119.06(19)
C(14)-C(13)-C(18)	118.07(19)
C(15)-C(14)-C(13)	121.3(2)
C(14)-C(15)-C(16)	120.2(2)
C(17)-C(16)-C(15)	120.3(2)
C(16)-C(17)-C(18)	120.7(2)
C(17)-C(18)-C(13)	119.30(18)
C(17)-C(18)-C(9)	122.29(17)
C(13)-C(18)-C(9)	118.41(17)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jw11. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	28(1)	40(1)	38(1)	17(1)	1(1)	2(1)
O(1)	59(1)	26(1)	31(1)	3(1)	9(1)	-6(1)
O(2)	52(1)	26(1)	25(1)	2(1)	4(1)	-4(1)
O(3)	31(1)	22(1)	29(1)	-3(1)	10(1)	-3(1)
C(1)	32(1)	27(1)	25(1)	1(1)	-8(1)	-8(1)
C(2)	25(1)	30(1)	30(1)	1(1)	-2(1)	-5(1)
C(3)	27(1)	21(1)	24(1)	0(1)	4(1)	-2(1)
C(4)	28(1)	32(1)	34(1)	2(1)	-2(1)	5(1)

C(5)	28(1)	19(1)	19(1)	-1(1)	1(1)	0(1)
C(6)	33(1)	25(1)	23(1)	0(1)	2(1)	-4(1)
C(7)	29(1)	32(1)	30(1)	-9(1)	9(1)	-8(1)
C(8)	25(1)	35(1)	42(1)	-2(1)	0(1)	2(1)
C(9)	20(1)	22(1)	32(1)	-2(1)	4(1)	1(1)
C(10)	32(1)	24(1)	38(1)	3(1)	11(1)	-1(1)
C(11)	34(1)	21(1)	53(2)	-1(1)	8(1)	-2(1)
C(12)	31(1)	24(1)	48(1)	-11(1)	0(1)	2(1)
C(13)	24(1)	27(1)	35(1)	-5(1)	-1(1)	5(1)
C(14)	43(1)	38(1)	34(1)	-11(1)	-1(1)	6(1)
C(15)	54(2)	48(2)	26(1)	-1(1)	5(1)	4(1)
C(16)	45(1)	33(1)	32(1)	4(1)	5(1)	-2(1)
C(17)	30(1)	25(1)	31(1)	-2(1)	3(1)	-2(1)
C(18)	17(1)	23(1)	31(1)	-2(1)	1(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for jw11.

	x	y	z	U(eq)
H(1)	-380(30)	4210(40)	516(18)	90(11)
H(2)	-1848(19)	7310(30)	1485(13)	37(6)
H(4A)	-890(17)	10350(30)	675(13)	32(6)
H(4B)	-1899(19)	10540(30)	1259(13)	36(6)
H(6)	1123(19)	10670(30)	908(14)	41(6)
H(7)	3048(18)	9710(30)	1195(12)	34(6)
H(8)	3140(20)	7650(30)	2330(14)	46(7)
H(10)	-466(17)	12540(30)	2207(13)	32(6)
H(11)	-328(18)	15050(30)	3045(13)	36(6)
H(12)	-668(18)	14710(30)	4368(13)	41(6)
H(14)	-1220(20)	12680(30)	5448(15)	50(7)
H(15)	-1830(20)	9890(30)	5886(16)	52(7)
H(16)	-2006(19)	7330(30)	5007(14)	41(6)
H(17)	-1560(17)	7700(30)	3714(12)	29(6)

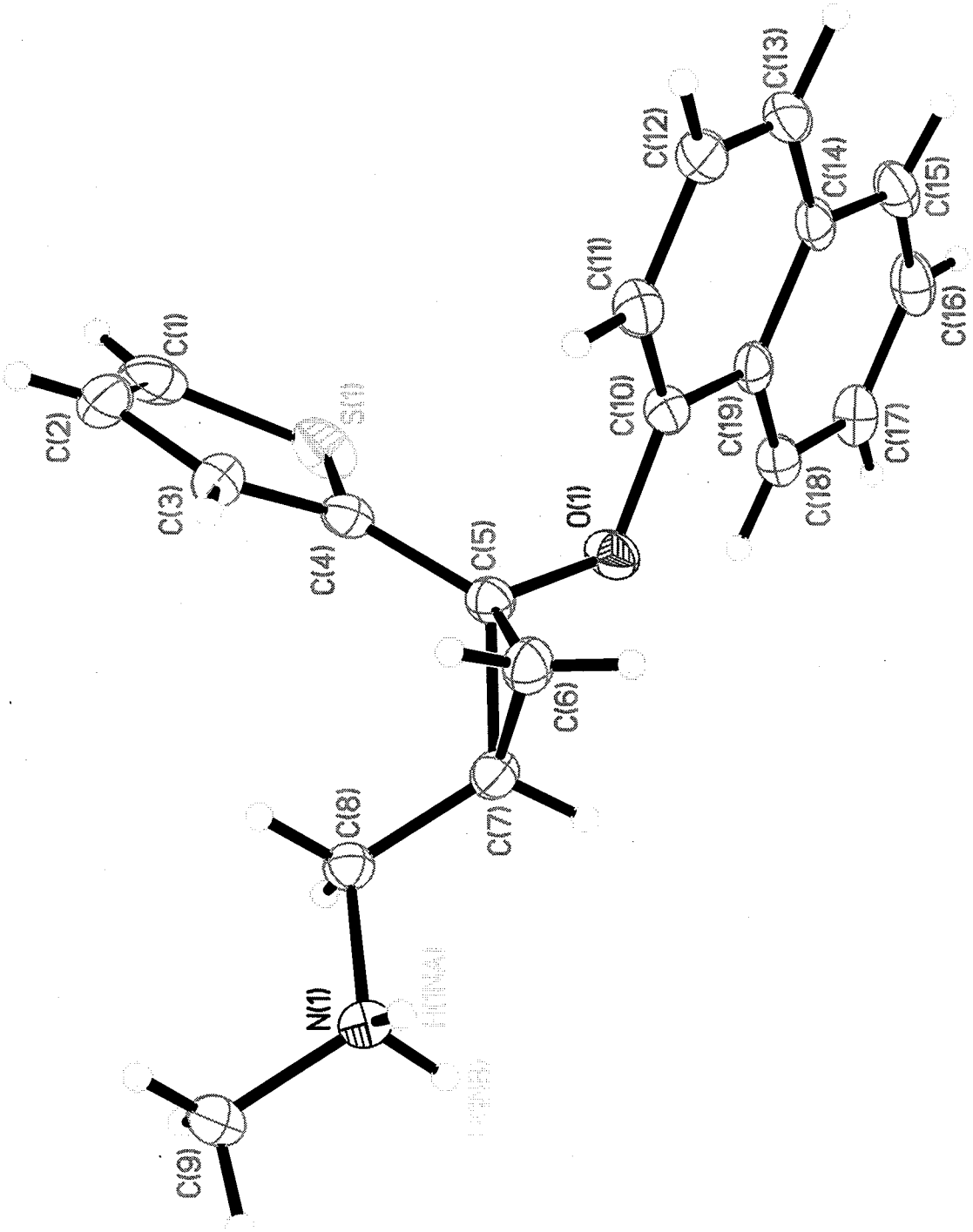
Table 6. Hydrogen bonds for jw11 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#1	0.94(3)	1.71(3)	2.645(2)	174(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

(+)-(1R,2S)-15 (JW 26)


C(13)
C(12)
C(14)
C(15)
C(11)
C(16)
C(10)
C(19)
C(17)
C(18)
O(1)
C(1)
C(2)
C(3)
C(4)
C(5)
C(6)
C(7)
C(8)
N(1)
C(9)

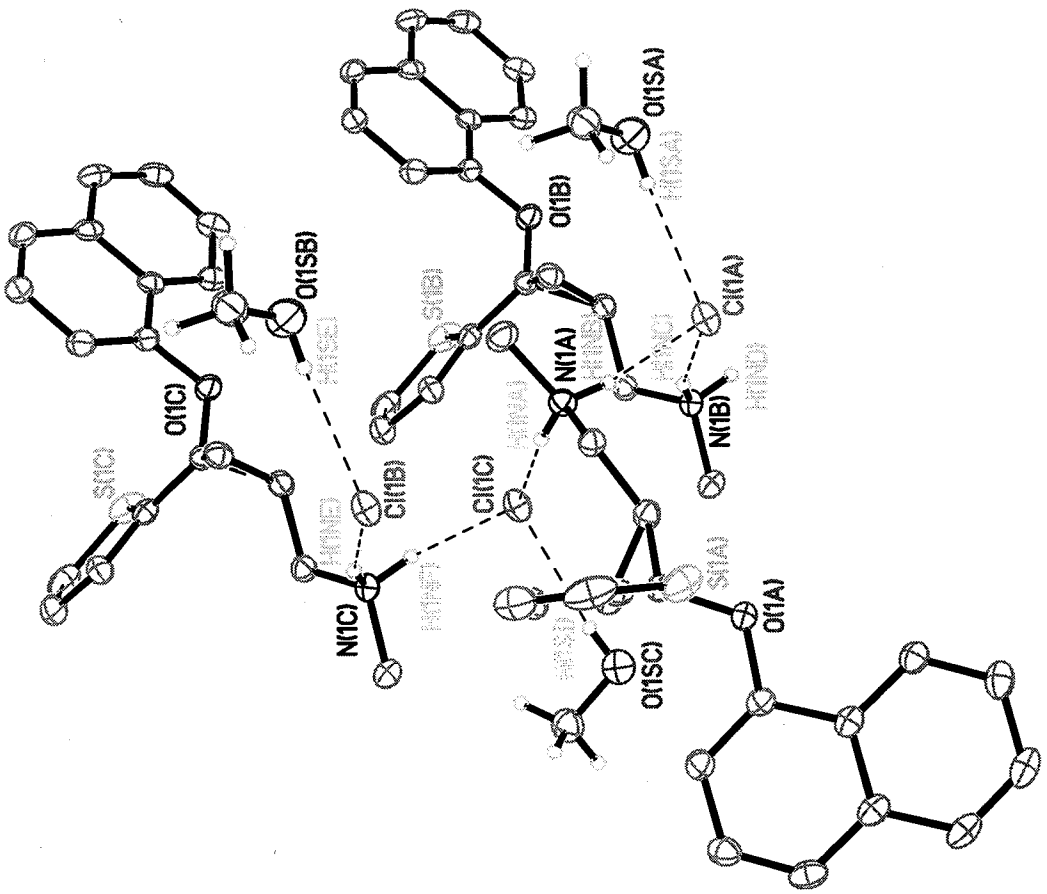

O(1SB)
O(1C)
Cl(1B)
Cl(1C)
N(1C)
O(1SA)
O(1B)
Cl(1A)
N(1A)
N(1B)
O(1SC)
O(1A)

Table 1. Crystal data and structure refinement for jw26.

Identification code	jw26	
Empirical formula	C20 H18 Cl N O S	
Formula weight	355.86	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 6.9481(4) Å	α= 90°.
	b = 8.9988(5) Å	β= 90°.
	c = 31.8427(17) Å	γ = 90°.
Volume	1990.95(19) $Å^3$	
Z	4	
Density (calculated)	1.187 Mg/m^3	
Absorption coefficient	0.302 mm^{-1}	
F(000)	744	
Crystal size	0.26 x 0.12 x 0.08 mm^3	
Theta range for data collection	2.35 to 27.00°.	
Index ranges	-8<=h<=8, -11<=k<=11, -40<=l<=40	
Reflections collected	22350	
Independent reflections	4343 [R(int) = 0.0267]	
Completeness to theta = 27.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9762 and 0.9256	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4343 / 0 / 322	
Goodness-of-fit on F^2	1.084	
Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.0931	
R indices (all data)	R1 = 0.0411, wR2 = 0.0965	
Absolute structure parameter	0.03(6)	
Largest diff. peak and hole	0.509 and -0.187 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jw26. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	2330(1)	8404(1)	405(1)	42(1)
S(1)	5496(1)	5547(1)	1957(1)	51(1)
O(1)	7894(2)	3973(2)	1318(1)	39(1)
N(1)	7901(2)	8358(2)	438(1)	33(1)
C(1)	3273(5)	6274(3)	2053(1)	60(1)
C(2)	2278(4)	6503(3)	1702(1)	52(1)
C(3)	3313(3)	6085(2)	1338(1)	37(1)
C(4)	5115(3)	5554(2)	1423(1)	31(1)
C(5)	6656(3)	5034(2)	1137(1)	31(1)
C(6)	6355(3)	4958(2)	668(1)	36(1)
C(7)	7755(3)	6074(2)	852(1)	34(1)
C(8)	7299(3)	7692(2)	846(1)	32(1)
C(9)	7328(4)	9928(3)	388(1)	47(1)
C(10)	7133(3)	2603(2)	1421(1)	32(1)
C(11)	5386(3)	2079(2)	1281(1)	38(1)
C(12)	4751(3)	665(2)	1411(1)	41(1)
C(13)	5825(4)	-188(2)	1671(1)	42(1)
C(14)	7642(3)	311(2)	1815(1)	35(1)
C(15)	8833(4)	-552(3)	2081(1)	44(1)
C(16)	10543(4)	-32(3)	2221(1)	47(1)
C(17)	11191(4)	1385(3)	2104(1)	44(1)
C(18)	10108(3)	2259(2)	1844(1)	36(1)
C(19)	8311(3)	1746(2)	1692(1)	32(1)
O(1S)	2751(3)	2031(3)	323(1)	64(1)
C(1S)	1264(4)	2698(3)	550(1)	56(1)

Table 3. Bond lengths [Å] and angles [°] for jw26.

S(1)-C(1)	1.705(3)
S(1)-C(4)	1.7201(18)
O(1)-C(10)	1.381(2)
O(1)-C(5)	1.408(2)
N(1)-C(9)	1.476(3)
N(1)-C(8)	1.490(2)
N(1)-H(1NA)	0.90(3)
N(1)-H(1NB)	0.94(3)
C(1)-C(2)	1.329(4)
C(1)-H(1)	0.98(3)
C(2)-C(3)	1.416(3)
C(2)-H(2)	0.84(3)
C(3)-C(4)	1.367(3)
C(3)-H(3)	0.84(3)
C(4)-C(5)	1.481(3)
C(5)-C(6)	1.511(3)
C(5)-C(7)	1.513(3)
C(6)-C(7)	1.516(3)
C(6)-H(6A)	0.88(2)
C(6)-H(6B)	0.91(2)
C(7)-C(8)	1.490(3)
C(7)-H(7)	0.94(3)
C(8)-H(8A)	1.00(3)
C(8)-H(8B)	0.97(2)
C(9)-H(9A)	0.93(3)
C(9)-H(9B)	0.93(3)
C(9)-H(9C)	0.94(3)
C(10)-C(11)	1.377(3)
C(10)-C(19)	1.417(3)
C(11)-C(12)	1.409(3)
C(11)-H(11)	0.96(2)
C(12)-C(13)	1.354(3)
C(12)-H(12)	0.87(2)
C(13)-C(14)	1.416(3)

C(13)-H(13)	0.97(3)
C(14)-C(15)	1.416(3)
C(14)-C(19)	1.427(3)
C(15)-C(16)	1.352(4)
C(15)-H(15)	0.90(3)
C(16)-C(17)	1.402(4)
C(16)-H(16)	0.92(3)
C(17)-C(18)	1.367(3)
C(17)-H(17)	0.94(3)
C(18)-C(19)	1.417(3)
C(18)-H(18)	0.92(3)
O(1S)-C(1S)	1.397(3)
O(1S)-H(1S)	0.84(4)
C(1S)-H(1SA)	1.03(4)
C(1S)-H(1SB)	1.01(3)
C(1S)-H(1SC)	1.07(3)

C(1)-S(1)-C(4)	92.10(12)
C(10)-O(1)-C(5)	117.99(15)
C(9)-N(1)-C(8)	113.79(17)
C(9)-N(1)-H(1NA)	108.7(18)
C(8)-N(1)-H(1NA)	110.7(18)
C(9)-N(1)-H(1NB)	110.9(16)
C(8)-N(1)-H(1NB)	106.9(15)
H(1NA)-N(1)-H(1NB)	106(2)
C(2)-C(1)-S(1)	112.34(18)
C(2)-C(1)-H(1)	125.9(18)
S(1)-C(1)-H(1)	121.7(18)
C(1)-C(2)-C(3)	112.5(2)
C(1)-C(2)-H(2)	129(2)
C(3)-C(2)-H(2)	119(2)
C(4)-C(3)-C(2)	113.3(2)
C(4)-C(3)-H(3)	120.5(18)
C(2)-C(3)-H(3)	126.1(18)
C(3)-C(4)-C(5)	130.59(17)
C(3)-C(4)-S(1)	109.76(15)

C(5)-C(4)-S(1)	119.65(15)
O(1)-C(5)-C(4)	113.92(15)
O(1)-C(5)-C(6)	117.21(17)
C(4)-C(5)-C(6)	121.46(17)
O(1)-C(5)-C(7)	110.92(16)
C(4)-C(5)-C(7)	122.64(17)
C(6)-C(5)-C(7)	60.19(13)
C(5)-C(6)-C(7)	59.97(13)
C(5)-C(6)-H(6A)	116.1(14)
C(7)-C(6)-H(6A)	113.4(15)
C(5)-C(6)-H(6B)	116.0(13)
C(7)-C(6)-H(6B)	118.6(13)
H(6A)-C(6)-H(6B)	119(2)
C(8)-C(7)-C(5)	120.32(17)
C(8)-C(7)-C(6)	120.41(18)
C(5)-C(7)-C(6)	59.85(13)
C(8)-C(7)-H(7)	118.4(15)
C(5)-C(7)-H(7)	112.4(15)
C(6)-C(7)-H(7)	112.0(15)
N(1)-C(8)-C(7)	110.14(16)
N(1)-C(8)-H(8A)	104.2(14)
C(7)-C(8)-H(8A)	113.7(15)
N(1)-C(8)-H(8B)	104.4(12)
C(7)-C(8)-H(8B)	112.7(13)
H(8A)-C(8)-H(8B)	110.9(19)
N(1)-C(9)-H(9A)	110.0(19)
N(1)-C(9)-H(9B)	109.1(18)
H(9A)-C(9)-H(9B)	112(3)
N(1)-C(9)-H(9C)	107.4(17)
H(9A)-C(9)-H(9C)	109(2)
H(9B)-C(9)-H(9C)	109(2)
C(11)-C(10)-O(1)	124.46(18)
C(11)-C(10)-C(19)	121.32(18)
O(1)-C(10)-C(19)	114.22(17)
C(10)-C(11)-C(12)	119.4(2)
C(10)-C(11)-H(11)	118.4(14)

C(12)-C(11)-H(11)	122.1(14)
C(13)-C(12)-C(11)	121.2(2)
C(13)-C(12)-H(12)	118.4(16)
C(11)-C(12)-H(12)	120.3(16)
C(12)-C(13)-C(14)	120.64(19)
C(12)-C(13)-H(13)	119.9(15)
C(14)-C(13)-H(13)	119.3(15)
C(13)-C(14)-C(15)	122.7(2)
C(13)-C(14)-C(19)	119.29(18)
C(15)-C(14)-C(19)	118.0(2)
C(16)-C(15)-C(14)	121.4(2)
C(16)-C(15)-H(15)	117.4(15)
C(14)-C(15)-H(15)	121.0(15)
C(15)-C(16)-C(17)	120.6(2)
C(15)-C(16)-H(16)	120.4(16)
C(17)-C(16)-H(16)	118.9(16)
C(18)-C(17)-C(16)	120.5(2)
C(18)-C(17)-H(17)	120.1(16)
C(16)-C(17)-H(17)	119.4(16)
C(17)-C(18)-C(19)	120.3(2)
C(17)-C(18)-H(18)	120.4(15)
C(19)-C(18)-H(18)	119.2(15)
C(18)-C(19)-C(10)	122.66(18)
C(18)-C(19)-C(14)	119.24(18)
C(10)-C(19)-C(14)	118.10(19)
C(1S)-O(1S)-H(1S)	104(2)
O(1S)-C(1S)-H(1SA)	112(2)
O(1S)-C(1S)-H(1SB)	107.2(18)
H(1SA)-C(1S)-H(1SB)	113(3)
O(1S)-C(1S)-H(1SC)	99.8(17)
H(1SA)-C(1S)-H(1SC)	114(3)
H(1SB)-C(1S)-H(1SC)	110(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jw26. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	33(1)	57(1)	35(1)	-1(1)	-2(1)	0(1)
S(1)	85(1)	40(1)	29(1)	4(1)	-5(1)	1(1)
O(1)	31(1)	33(1)	51(1)	11(1)	-8(1)	0(1)
N(1)	32(1)	34(1)	31(1)	2(1)	3(1)	-3(1)
C(1)	98(2)	38(1)	45(1)	-2(1)	37(1)	-12(1)
C(2)	48(1)	43(1)	64(2)	-5(1)	24(1)	-2(1)
C(3)	34(1)	41(1)	38(1)	-2(1)	2(1)	0(1)
C(4)	40(1)	27(1)	26(1)	2(1)	1(1)	-5(1)
C(5)	30(1)	30(1)	33(1)	5(1)	-2(1)	0(1)
C(6)	39(1)	37(1)	31(1)	-2(1)	4(1)	5(1)
C(7)	30(1)	37(1)	35(1)	4(1)	4(1)	3(1)
C(8)	31(1)	34(1)	31(1)	4(1)	1(1)	0(1)
C(9)	45(1)	36(1)	59(1)	14(1)	7(1)	-1(1)
C(10)	34(1)	28(1)	34(1)	1(1)	2(1)	2(1)
C(11)	38(1)	35(1)	43(1)	-2(1)	-3(1)	4(1)
C(12)	38(1)	35(1)	49(1)	-8(1)	4(1)	-3(1)
C(13)	53(1)	28(1)	44(1)	-6(1)	14(1)	-2(1)
C(14)	47(1)	27(1)	29(1)	-4(1)	7(1)	9(1)
C(15)	67(2)	30(1)	36(1)	3(1)	6(1)	11(1)
C(16)	65(2)	43(1)	33(1)	2(1)	-3(1)	22(1)
C(17)	47(1)	47(1)	37(1)	-6(1)	-4(1)	14(1)
C(18)	42(1)	34(1)	33(1)	-2(1)	0(1)	6(1)
C(19)	38(1)	30(1)	27(1)	-4(1)	4(1)	9(1)
O(1S)	62(1)	59(1)	71(1)	5(1)	13(1)	2(1)
C(1S)	47(1)	56(2)	65(2)	-7(1)	-1(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jw26.

	x	y	z	U(eq)
H(1NA)	7420(40)	7830(30)	221(9)	58(8)
H(1NB)	9240(40)	8260(30)	420(7)	43(6)
H(1)	2830(40)	6490(30)	2340(10)	71(8)
H(2)	1170(50)	6860(40)	1675(9)	67(9)
H(3)	2940(40)	6180(30)	1087(9)	48(7)
H(6A)	6920(30)	4220(30)	538(7)	32(5)
H(6B)	5200(30)	5290(20)	573(6)	23(5)
H(7)	9050(40)	5780(30)	814(7)	46(7)
H(8A)	8010(40)	8280(30)	1060(8)	49(7)
H(8B)	5930(30)	7890(20)	861(6)	27(5)
H(9A)	6000(50)	9990(30)	352(9)	62(8)
H(9B)	7750(40)	10470(30)	620(9)	58(8)
H(9C)	7940(40)	10290(30)	146(8)	53(7)
H(11)	4660(30)	2680(30)	1089(7)	38(6)
H(12)	3640(40)	330(30)	1330(7)	39(6)
H(13)	5400(40)	-1180(30)	1744(8)	47(6)
H(15)	8520(30)	-1490(30)	2146(7)	39(6)
H(16)	11270(40)	-580(30)	2404(7)	45(6)
H(17)	12400(40)	1710(30)	2196(8)	46(7)
H(18)	10520(30)	3200(30)	1772(7)	41(6)
H(1S)	2560(50)	1120(40)	353(11)	76(10)
H(1SA)	850(60)	2060(40)	800(12)	102(12)
H(1SB)	1730(50)	3720(40)	635(10)	74(9)
H(1SC)	210(50)	2800(40)	308(10)	79(10)

Table 6. Torsion angles [°] for jw26.

C(4)-S(1)-C(1)-C(2)	0.4(2)
S(1)-C(1)-C(2)-C(3)	0.1(3)
C(1)-C(2)-C(3)-C(4)	-0.7(3)
C(2)-C(3)-C(4)-C(5)	-178.6(2)
C(2)-C(3)-C(4)-S(1)	1.0(2)
C(1)-S(1)-C(4)-C(3)	-0.83(17)
C(1)-S(1)-C(4)-C(5)	178.84(16)
C(10)-O(1)-C(5)-C(4)	65.7(2)
C(10)-O(1)-C(5)-C(6)	-84.7(2)
C(10)-O(1)-C(5)-C(7)	-151.03(16)
C(3)-C(4)-C(5)-O(1)	-152.2(2)
S(1)-C(4)-C(5)-O(1)	28.3(2)
C(3)-C(4)-C(5)-C(6)	-3.1(3)
S(1)-C(4)-C(5)-C(6)	177.32(15)
C(3)-C(4)-C(5)-C(7)	69.4(3)
S(1)-C(4)-C(5)-C(7)	-110.16(18)
O(1)-C(5)-C(6)-C(7)	-99.67(18)
C(4)-C(5)-C(6)-C(7)	112.2(2)
O(1)-C(5)-C(7)-C(8)	-140.03(18)
C(4)-C(5)-C(7)-C(8)	-0.5(3)
C(6)-C(5)-C(7)-C(8)	109.8(2)
O(1)-C(5)-C(7)-C(6)	110.20(18)
C(4)-C(5)-C(7)-C(6)	-110.3(2)
C(5)-C(6)-C(7)-C(8)	-109.6(2)
C(9)-N(1)-C(8)-C(7)	174.22(19)
C(5)-C(7)-C(8)-N(1)	-156.15(17)
C(6)-C(7)-C(8)-N(1)	-85.5(2)
C(5)-O(1)-C(10)-C(11)	14.8(3)
C(5)-O(1)-C(10)-C(19)	-164.97(16)
O(1)-C(10)-C(11)-C(12)	-179.51(18)
C(19)-C(10)-C(11)-C(12)	0.2(3)
C(10)-C(11)-C(12)-C(13)	0.2(3)
C(11)-C(12)-C(13)-C(14)	-1.3(3)
C(12)-C(13)-C(14)-C(15)	-178.75(19)

C(12)-C(13)-C(14)-C(19)	1.9(3)
C(13)-C(14)-C(15)-C(16)	-178.4(2)
C(19)-C(14)-C(15)-C(16)	0.9(3)
C(14)-C(15)-C(16)-C(17)	-0.2(3)
C(15)-C(16)-C(17)-C(18)	-0.5(3)
C(16)-C(17)-C(18)-C(19)	0.4(3)
C(17)-C(18)-C(19)-C(10)	-179.83(19)
C(17)-C(18)-C(19)-C(14)	0.3(3)
C(11)-C(10)-C(19)-C(18)	-179.46(18)
O(1)-C(10)-C(19)-C(18)	0.3(3)
C(11)-C(10)-C(19)-C(14)	0.4(3)
O(1)-C(10)-C(19)-C(14)	-179.81(16)
C(13)-C(14)-C(19)-C(18)	178.44(18)
C(15)-C(14)-C(19)-C(18)	-1.0(3)
C(13)-C(14)-C(19)-C(10)	-1.5(3)
C(15)-C(14)-C(19)-C(10)	179.15(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for jw26 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1NA)...Cl(1)#1	0.90(3)	2.28(3)	3.1425(18)	159(3)
N(1)-H(1NB)...Cl(1)#2	0.94(3)	2.15(3)	3.0793(17)	171(2)
O(1S)-H(1S)...Cl(1)#3	0.84(4)	2.46(4)	3.288(2)	174(3)

Symmetry transformations used to generate equivalent atoms:

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

(-)-(1S,2R)-15

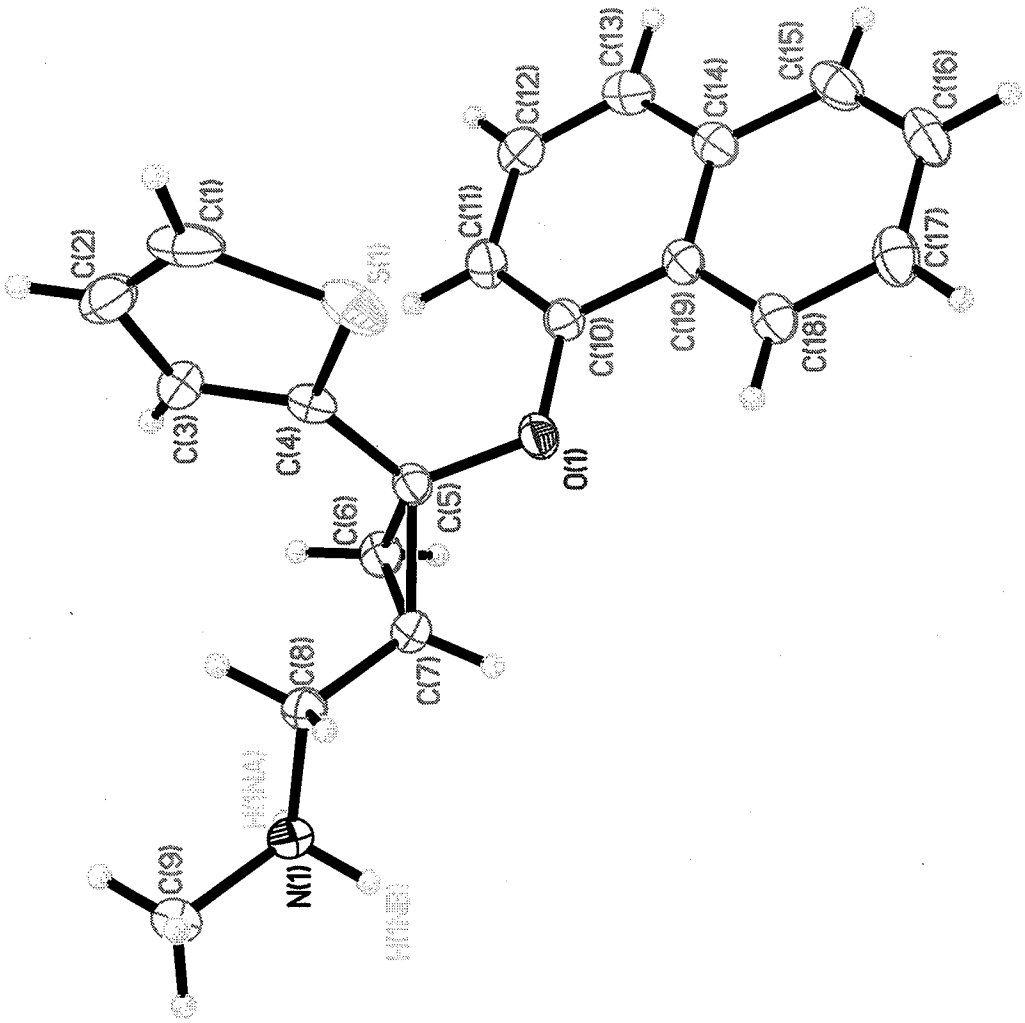

C(13)
C(12)
C(14)
C(15)
C(16)
C(1)
C(11)
C(17)
C(2)
S(1)
C(10)
C(19)
C(18)
C(3)
C(4)
O(1)
C(5)
C(6)
C(8)
C(7)
H(1NA)
C(9)
N(1)
H(1NB)

Table 1. Crystal data and structure refinement for jw27.

Identification code	jw27	
Empirical formula	C20 H24 Cl N O2 S	
Formula weight	377.91	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 6.9491(5) Å	a= 90°.
	b = 9.0000(7) Å	b= 90°.
	c = 31.877(2) Å	g = 90°.
Volume	1993.6(3) $Å^3$	
Z	4	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	0.309 mm^{-1}	
F(000)	800	
Crystal size	0.38 x 0.17 x 0.14 mm^3	
Theta range for data collection	1.28 to 26.99°.	
Index ranges	-8<=h<=8, -11<=k<=11, -40<=l<=40	
Reflections collected	22446	
Independent reflections	4349 [R(int) = 0.0238]	
Completeness to theta = 26.99°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9580 and 0.8916	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4349 / 6 / 322	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.1005	
R indices (all data)	R1 = 0.0412, wR2 = 0.1021	
Absolute structure parameter	0.02(6)	
Largest diff. peak and hole	0.621 and -0.171 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jw27. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	2333(1)	3401(1)	9595(1)	44(1)
S(1)	5499(1)	10548(1)	8043(1)	54(1)
O(1)	7897(2)	8972(2)	8682(1)	41(1)
O(2)	2753(3)	7032(3)	9678(1)	67(1)
N(1)	7904(2)	13358(2)	9562(1)	34(1)
C(1)	3272(5)	11273(3)	7947(1)	63(1)
C(2)	2283(4)	11508(3)	8299(1)	56(1)
C(3)	3303(3)	11082(2)	8660(1)	38(1)
C(4)	5122(3)	10554(2)	8577(1)	33(1)
C(5)	6659(3)	10031(2)	8864(1)	32(1)

C(6)	6355(3)	9955(2)	9330(1)	37(1)
C(7)	7755(3)	11072(2)	9148(1)	35(1)
C(8)	7298(3)	12692(2)	9154(1)	34(1)
C(9)	7323(4)	14924(3)	9613(1)	48(1)
C(10)	7139(3)	7603(2)	8578(1)	34(1)
C(11)	5387(3)	7077(2)	8719(1)	41(1)
C(12)	4750(3)	5667(2)	8589(1)	43(1)
C(13)	5827(4)	4813(2)	8329(1)	43(1)
C(14)	7644(3)	5315(2)	8186(1)	37(1)
C(15)	8836(4)	4450(3)	7919(1)	47(1)
C(16)	10549(4)	4968(3)	7780(1)	49(1)
C(17)	11193(4)	6386(3)	7896(1)	46(1)
C(18)	10113(3)	7257(2)	8156(1)	38(1)
C(19)	8314(3)	6747(2)	8308(1)	33(1)
C(20)	1272(4)	7691(3)	9451(1)	58(1)

Table 3. Bond lengths [Å] and angles [°] for jw 27.

S(1)-C(1)	1.708(3)
S(1)-C(4)	1.7195(18)
O(1)-C(10)	1.381(2)
O(1)-C(5)	1.408(2)
O(2)-C(20)	1.390(4)
O(2)-H(2O)	0.82(4)
N(1)-C(9)	1.475(3)
N(1)-C(8)	1.491(3)
N(1)-H(1NA)	0.89(3)
N(1)-H(1NB)	0.91(3)
C(1)-C(2)	1.333(4)
C(1)-H(1)	0.98(3)
C(2)-C(3)	1.405(3)
C(2)-H(2)	0.91(4)
C(3)-C(4)	1.376(3)
C(3)-H(3)	0.77(3)
C(4)-C(5)	1.483(3)
C(5)-C(6)	1.504(3)
C(5)-C(7)	1.509(3)
C(6)-C(7)	1.515(3)
C(6)-H(6A)	0.86(3)
C(6)-H(6B)	0.94(2)
C(7)-C(8)	1.492(3)
C(7)-H(7)	0.92(3)
C(8)-H(8A)	0.98(3)
C(8)-H(8B)	0.99(2)
C(9)-H(9A)	0.93(3)
C(9)-H(9B)	0.96(3)

C(9)-H(9C)	0.90(3)
C(10)-C(11)	1.381(3)
C(10)-C(19)	1.416(3)
C(11)-C(12)	1.407(3)
C(11)-H(11)	0.93(2)
C(12)-C(13)	1.356(3)
C(12)-H(12)	0.87(3)
C(13)-C(14)	1.416(3)
C(13)-H(13)	0.97(3)
C(14)-C(15)	1.419(3)
C(14)-C(19)	1.424(3)
C(15)-C(16)	1.353(4)
C(15)-H(15)	0.88(3)
C(16)-C(17)	1.402(4)
C(16)-H(16)	0.93(3)
C(17)-C(18)	1.365(3)
C(17)-H(17)	0.93(3)
C(18)-C(19)	1.417(3)
C(18)-H(18)	0.93(3)
C(20)-H(20C)	1.021(16)
C(20)-H(20B)	0.969(17)
C(20)-H(20A)	0.983(16)

C(1)-S(1)-C(4)	92.26(12)
C(10)-O(1)-C(5)	117.97(15)
C(20)-O(2)-H(2O)	101(3)
C(9)-N(1)-C(8)	113.78(18)
C(9)-N(1)-H(1NA)	110.1(19)
C(8)-N(1)-H(1NA)	109.2(19)
C(9)-N(1)-H(1NB)	111.5(18)
C(8)-N(1)-H(1NB)	107.0(17)
H(1NA)-N(1)-H(1NB)	105(3)
C(2)-C(1)-S(1)	112.04(19)
C(2)-C(1)-H(1)	126(2)
S(1)-C(1)-H(1)	121(2)
C(1)-C(2)-C(3)	112.7(3)
C(1)-C(2)-H(2)	131(2)
C(3)-C(2)-H(2)	117(2)
C(4)-C(3)-C(2)	113.5(2)
C(4)-C(3)-H(3)	121(2)
C(2)-C(3)-H(3)	126(2)
C(3)-C(4)-C(5)	130.66(17)
C(3)-C(4)-S(1)	109.40(15)
C(5)-C(4)-S(1)	119.94(15)
O(1)-C(5)-C(4)	113.67(16)
O(1)-C(5)-C(6)	117.45(17)

C(4)-C(5)-C(6)	121.59(17)
O(1)-C(5)-C(7)	110.96(16)
C(4)-C(5)-C(7)	122.48(17)
C(6)-C(5)-C(7)	60.38(13)
C(5)-C(6)-C(7)	59.97(13)
C(5)-C(6)-H(6A)	116.3(16)
C(7)-C(6)-H(6A)	115.0(17)
C(5)-C(6)-H(6B)	116.5(12)
C(7)-C(6)-H(6B)	117.4(12)
H(6A)-C(6)-H(6B)	119(2)
C(8)-C(7)-C(5)	120.53(17)
C(8)-C(7)-C(6)	120.40(18)
C(5)-C(7)-C(6)	59.65(13)
C(8)-C(7)-H(7)	118.8(17)
C(5)-C(7)-H(7)	112.6(16)
C(6)-C(7)-H(7)	111.0(16)
N(1)-C(8)-C(7)	110.24(16)
N(1)-C(8)-H(8A)	105.0(17)
C(7)-C(8)-H(8A)	112.2(17)
N(1)-C(8)-H(8B)	105.5(12)
C(7)-C(8)-H(8B)	111.7(13)
H(8A)-C(8)-H(8B)	112(2)
N(1)-C(9)-H(9A)	110(2)
N(1)-C(9)-H(9B)	108.6(18)
H(9A)-C(9)-H(9B)	113(3)
N(1)-C(9)-H(9C)	108(2)
H(9A)-C(9)-H(9C)	107(3)
H(9B)-C(9)-H(9C)	110(3)
O(1)-C(10)-C(11)	124.37(18)
O(1)-C(10)-C(19)	114.34(17)
C(11)-C(10)-C(19)	121.30(19)
C(10)-C(11)-C(12)	119.4(2)
C(10)-C(11)-H(11)	118.9(15)
C(12)-C(11)-H(11)	121.7(15)
C(13)-C(12)-C(11)	121.2(2)
C(13)-C(12)-H(12)	118.3(17)
C(11)-C(12)-H(12)	120.5(17)
C(12)-C(13)-C(14)	120.6(2)
C(12)-C(13)-H(13)	120.5(16)
C(14)-C(13)-H(13)	118.8(16)
C(13)-C(14)-C(15)	122.6(2)
C(13)-C(14)-C(19)	119.47(18)
C(15)-C(14)-C(19)	117.9(2)
C(16)-C(15)-C(14)	121.4(2)
C(16)-C(15)-H(15)	116.9(17)
C(14)-C(15)-H(15)	121.5(17)

C(15)-C(16)-C(17)	120.5(2)
C(15)-C(16)-H(16)	119.7(17)
C(17)-C(16)-H(16)	119.8(17)
C(18)-C(17)-C(16)	120.5(2)
C(18)-C(17)-H(17)	118.0(17)
C(16)-C(17)-H(17)	121.4(17)
C(17)-C(18)-C(19)	120.4(2)
C(17)-C(18)-H(18)	120.1(16)
C(19)-C(18)-H(18)	119.4(15)
C(18)-C(19)-C(10)	122.69(18)
C(18)-C(19)-C(14)	119.25(19)
C(10)-C(19)-C(14)	118.06(19)
O(2)-C(20)-H(20C)	102.0(13)
O(2)-C(20)-H(20B)	110.5(16)
H(20C)-C(20)-H(20B)	116(3)
O(2)-C(20)-H(20A)	107.7(14)
H(20C)-C(20)-H(20A)	105(3)
H(20B)-C(20)-H(20A)	115(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jw27. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	34(1)	61(1)	36(1)	1(1)	2(1)	-1(1)
S(1)	89(1)	41(1)	30(1)	-4(1)	6(1)	1(1)
O(1)	32(1)	35(1)	54(1)	-12(1)	9(1)	0(1)
O(2)	64(1)	64(1)	75(1)	-5(1)	-14(1)	0(1)
N(1)	33(1)	35(1)	33(1)	-2(1)	-3(1)	-3(1)
C(1)	104(2)	39(1)	47(1)	2(1)	-38(2)	-12(1)
C(2)	53(1)	47(1)	67(2)	4(1)	-25(1)	-4(1)
C(3)	33(1)	44(1)	37(1)	3(1)	-1(1)	1(1)
C(4)	43(1)	29(1)	27(1)	-2(1)	0(1)	-5(1)
C(5)	31(1)	31(1)	34(1)	-4(1)	3(1)	1(1)
C(6)	41(1)	39(1)	32(1)	3(1)	-2(1)	4(1)
C(7)	31(1)	38(1)	37(1)	-3(1)	-3(1)	3(1)
C(8)	34(1)	37(1)	32(1)	-3(1)	-2(1)	0(1)
C(9)	47(1)	39(1)	59(1)	-13(1)	-8(1)	0(1)
C(10)	35(1)	30(1)	36(1)	-1(1)	-2(1)	2(1)
C(11)	39(1)	37(1)	46(1)	1(1)	4(1)	4(1)
C(12)	41(1)	37(1)	50(1)	8(1)	-4(1)	-3(1)
C(13)	56(1)	28(1)	45(1)	6(1)	-12(1)	-2(1)
C(14)	50(1)	30(1)	30(1)	4(1)	-7(1)	10(1)
C(15)	70(2)	32(1)	37(1)	-2(1)	-5(1)	12(1)

C(16)	67(2)	45(1)	36(1)	-2(1)	5(1)	23(1)
C(17)	50(1)	49(1)	39(1)	6(1)	5(1)	14(1)
C(18)	42(1)	36(1)	35(1)	3(1)	1(1)	6(1)
C(19)	39(1)	31(1)	29(1)	5(1)	-4(1)	9(1)
C(20)	48(1)	57(2)	70(2)	6(1)	1(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jw27.

	x	y	z	U(eq)
H(1NA)	7430(40)	12810(30)	9772(9)	58(8)
H(1NB)	9210(40)	13250(30)	9580(8)	50(7)
H(2O)	2520(60)	6150(50)	9642(12)	87(12)
H(1)	2850(50)	11510(40)	7661(10)	72(9)
H(2)	1090(50)	11900(40)	8340(10)	79(10)
H(3)	2950(40)	11160(30)	8888(9)	49(8)
H(6A)	6880(40)	9220(30)	9458(7)	37(6)
H(6B)	5180(30)	10320(20)	9431(6)	20(4)
H(7)	9010(40)	10770(30)	9189(8)	48(7)
H(8A)	8010(40)	13240(30)	8941(9)	56(7)
H(8B)	5900(30)	12870(20)	9134(6)	28(5)
H(9A)	5980(50)	14990(40)	9626(9)	65(9)
H(9B)	7940(50)	15320(30)	9858(9)	62(8)
H(9C)	7700(50)	15430(30)	9382(10)	62(9)
H(11)	4650(40)	7670(30)	8899(7)	36(6)
H(12)	3630(40)	5330(30)	8669(7)	40(6)
H(13)	5400(40)	3820(30)	8251(8)	51(7)
H(15)	8530(40)	3530(30)	7852(7)	44(6)
H(16)	11280(40)	4390(30)	7597(8)	47(7)
H(17)	12390(40)	6740(30)	7811(8)	51(7)
H(18)	10530(40)	8200(30)	8227(7)	42(6)
H(20C)	260(30)	7860(40)	9678(7)	79(10)
H(20B)	890(40)	7060(30)	9218(8)	91(11)
H(20A)	1700(40)	8690(20)	9371(8)	64(8)

Table 6. Torsion angles [°] for jw27.

C(4)-S(1)-C(1)-C(2)	-0.1(2)
S(1)-C(1)-C(2)-C(3)	-0.9(3)
C(1)-C(2)-C(3)-C(4)	1.7(3)
C(2)-C(3)-C(4)-C(5)	178.4(2)
C(2)-C(3)-C(4)-S(1)	-1.7(2)
C(1)-S(1)-C(4)-C(3)	1.04(17)
C(1)-S(1)-C(4)-C(5)	-179.09(17)
C(10)-O(1)-C(5)-C(4)	-66.0(2)

C(10)-O(1)-C(5)-C(6)	84.7(2)
C(10)-O(1)-C(5)-C(7)	151.27(17)
C(3)-C(4)-C(5)-O(1)	151.9(2)
S(1)-C(4)-C(5)-O(1)	-27.9(2)
C(3)-C(4)-C(5)-C(6)	2.6(3)
S(1)-C(4)-C(5)-C(6)	-177.28(15)
C(3)-C(4)-C(5)-C(7)	-70.2(3)
S(1)-C(4)-C(5)-C(7)	109.96(19)
O(1)-C(5)-C(6)-C(7)	99.69(19)
C(4)-C(5)-C(6)-C(7)	-112.1(2)
O(1)-C(5)-C(7)-C(8)	139.92(19)
C(4)-C(5)-C(7)-C(8)	1.0(3)
C(6)-C(5)-C(7)-C(8)	-109.6(2)
O(1)-C(5)-C(7)-C(6)	-110.49(19)
C(4)-C(5)-C(7)-C(6)	110.6(2)
C(5)-C(6)-C(7)-C(8)	109.8(2)
C(9)-N(1)-C(8)-C(7)	-174.00(19)
C(5)-C(7)-C(8)-N(1)	156.09(18)
C(6)-C(7)-C(8)-N(1)	85.6(2)
C(5)-O(1)-C(10)-C(11)	-14.8(3)
C(5)-O(1)-C(10)-C(19)	165.14(17)
O(1)-C(10)-C(11)-C(12)	179.43(19)
C(19)-C(10)-C(11)-C(12)	-0.5(3)
C(10)-C(11)-C(12)-C(13)	0.2(3)
C(11)-C(12)-C(13)-C(14)	1.0(3)
C(12)-C(13)-C(14)-C(15)	178.9(2)
C(12)-C(13)-C(14)-C(19)	-1.8(3)
C(13)-C(14)-C(15)-C(16)	178.6(2)
C(19)-C(14)-C(15)-C(16)	-0.7(3)
C(14)-C(15)-C(16)-C(17)	-0.1(3)
C(15)-C(16)-C(17)-C(18)	0.8(3)
C(16)-C(17)-C(18)-C(19)	-0.7(3)
C(17)-C(18)-C(19)-C(10)	179.9(2)
C(17)-C(18)-C(19)-C(14)	-0.1(3)
O(1)-C(10)-C(19)-C(18)	-0.3(3)
C(11)-C(10)-C(19)-C(18)	179.68(19)
O(1)-C(10)-C(19)-C(14)	179.71(16)
C(11)-C(10)-C(19)-C(14)	-0.4(3)
C(13)-C(14)-C(19)-C(18)	-178.53(18)
C(15)-C(14)-C(19)-C(18)	0.8(3)
C(13)-C(14)-C(19)-C(10)	1.5(3)
C(15)-C(14)-C(19)-C(10)	-179.18(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for jw27 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...Cl(1)	0.82(4)	2.48(4)	3.292(3)	170(4)
N(1)-H(1NA)...Cl(1)#1	0.89(3)	2.30(3)	3.1448(18)	159(3)
N(1)-H(1NB)...Cl(1)#2	0.91(3)	2.18(3)	3.0800(18)	170(3)

Symmetry transformations used to generate equivalent atoms:

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

#1 - (9S, 23) - 16 (JWZ0)

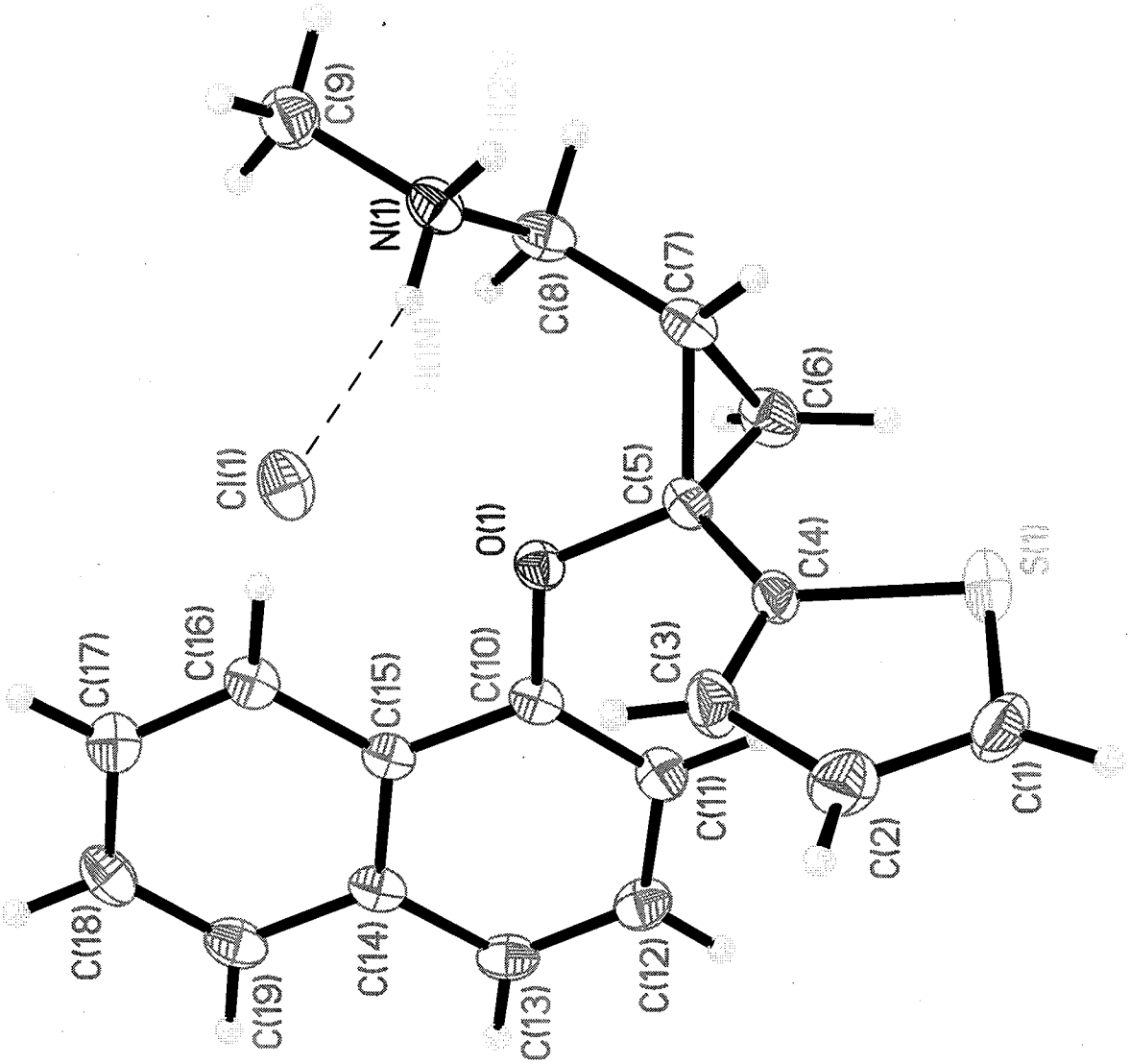


Table 1. Crystal data and structure refinement for jw20.

Identification code	jw20	
Empirical formula	C19 H20 Cl N O S	
Formula weight	345.87	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.2407(6) Å	α= 90°.
	b = 6.7846(4) Å	β= 104.3170(10)°.
	c = 14.9432(10) Å	γ = 90°.
Volume	907.76(10) Å^3	
Z	2	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.329 mm^{-1}	
F(000)	364	
Crystal size	0.25 x 0.16 x 0.12 mm^3	
Theta range for data collection	1.41 to 26.99°.	
Index ranges	-11<=h<=11, -8<=k<=8, -19<=l<=18	
Reflections collected	10237	
Independent reflections	3942 [R(int) = 0.0174]	
Completeness to theta = 26.99°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9616 and 0.9223	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3942 / 1 / 288	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0735	
R indices (all data)	R1 = 0.0317, wR2 = 0.0751	
Absolute structure parameter	0.04(5)	
Largest diff. peak and hole	0.218 and -0.152 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jw20. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4042(1)	5633(1)	5554(1)	38(1)
S(1)	10398(1)	4110(1)	6708(1)	59(1)
O(1)	6701(1)	4485(2)	7641(1)	31(1)
N(1)	4674(2)	1315(3)	6157(1)	36(1)
C(1)	10525(2)	6179(4)	6081(2)	53(1)
C(2)	9323(3)	7301(4)	5980(2)	50(1)
C(3)	8222(2)	6496(3)	6392(1)	41(1)
C(4)	8656(2)	4753(3)	6824(1)	32(1)
C(5)	7816(2)	3478(3)	7321(1)	32(1)
C(6)	8495(2)	1685(3)	7865(1)	44(1)
C(7)	7331(2)	1435(3)	6963(1)	35(1)
C(8)	5822(2)	675(3)	6981(1)	37(1)
C(9)	3163(2)	592(4)	6151(2)	48(1)
C(10)	7139(2)	5777(3)	8367(1)	30(1)
C(11)	8587(2)	6071(3)	8848(1)	35(1)
C(12)	8913(2)	7457(3)	9582(1)	40(1)
C(13)	7806(2)	8488(3)	9816(1)	39(1)
C(14)	6289(2)	8230(3)	9321(1)	33(1)
C(15)	5941(2)	6833(2)	8586(1)	29(1)
C(16)	4427(2)	6566(3)	8101(1)	34(1)
C(17)	3328(2)	7643(3)	8329(1)	40(1)
C(18)	3671(2)	9031(3)	9054(1)	46(1)
C(19)	5105(2)	9304(3)	9532(1)	42(1)

Table 3. Bond lengths [Å] and angles [°] for jw20.

S(1)-C(1)	1.708(3)
S(1)-C(4)	1.7174(17)
O(1)-C(10)	1.3759(19)
O(1)-C(5)	1.415(2)
N(1)-C(8)	1.478(2)
N(1)-C(9)	1.478(3)
N(1)-H(1N)	0.87(3)
N(1)-H(2N)	0.83(2)
C(1)-C(2)	1.324(3)
C(1)-H(1)	0.93(2)
C(2)-C(3)	1.422(3)
C(2)-H(2)	0.84(3)
C(3)-C(4)	1.360(3)
C(3)-H(3)	0.79(2)
C(4)-C(5)	1.479(2)
C(5)-C(6)	1.510(2)
C(5)-C(7)	1.513(2)
C(6)-C(7)	1.511(3)
C(6)-H(6A)	1.01(2)
C(6)-H(6B)	0.91(2)
C(7)-C(8)	1.493(3)
C(7)-H(7)	0.91(2)
C(8)-H(8A)	0.95(2)
C(8)-H(8B)	0.99(2)
C(9)-H(9A)	0.97(3)
C(9)-H(9B)	0.91(3)
C(9)-H(9C)	0.97(2)
C(10)-C(11)	1.367(2)
C(10)-C(15)	1.423(2)
C(11)-C(12)	1.420(3)
C(11)-H(11)	0.94(2)
C(12)-C(13)	1.354(3)
C(12)-H(12)	0.91(2)
C(13)-C(14)	1.425(3)

C(13)-H(13)	0.94(2)
C(14)-C(19)	1.414(3)
C(14)-C(15)	1.426(2)
C(15)-C(16)	1.419(2)
C(16)-C(17)	1.361(3)
C(16)-H(16)	0.95(2)
C(17)-C(18)	1.410(3)
C(17)-H(17)	0.93(2)
C(18)-C(19)	1.354(3)
C(18)-H(18)	0.91(2)
C(19)-H(19)	0.96(2)

C(1)-S(1)-C(4)	92.28(10)
C(10)-O(1)-C(5)	118.53(12)
C(8)-N(1)-C(9)	112.97(16)
C(8)-N(1)-H(1N)	108.6(15)
C(9)-N(1)-H(1N)	109.9(15)
C(8)-N(1)-H(2N)	105.0(14)
C(9)-N(1)-H(2N)	114.2(15)
H(1N)-N(1)-H(2N)	106(2)
C(2)-C(1)-S(1)	111.46(16)
C(2)-C(1)-H(1)	128.3(16)
S(1)-C(1)-H(1)	120.3(15)
C(1)-C(2)-C(3)	113.5(2)
C(1)-C(2)-H(2)	125.8(17)
C(3)-C(2)-H(2)	120.6(17)
C(4)-C(3)-C(2)	112.44(19)
C(4)-C(3)-H(3)	121.8(18)
C(2)-C(3)-H(3)	125.5(18)
C(3)-C(4)-C(5)	128.13(16)
C(3)-C(4)-S(1)	110.27(14)
C(5)-C(4)-S(1)	121.59(13)
O(1)-C(5)-C(4)	113.81(14)
O(1)-C(5)-C(6)	116.59(15)
C(4)-C(5)-C(6)	122.75(16)
O(1)-C(5)-C(7)	112.66(15)

C(4)-C(5)-C(7)	120.33(14)
C(6)-C(5)-C(7)	59.99(12)
C(5)-C(6)-C(7)	60.08(11)
C(5)-C(6)-H(6A)	117.6(14)
C(7)-C(6)-H(6A)	118.1(13)
C(5)-C(6)-H(6B)	117.9(15)
C(7)-C(6)-H(6B)	118.3(15)
H(6A)-C(6)-H(6B)	114(2)
C(8)-C(7)-C(6)	119.01(16)
C(8)-C(7)-C(5)	120.42(16)
C(6)-C(7)-C(5)	59.94(12)
C(8)-C(7)-H(7)	116.5(13)
C(6)-C(7)-H(7)	116.1(13)
C(5)-C(7)-H(7)	112.8(14)
N(1)-C(8)-C(7)	111.39(15)
N(1)-C(8)-H(8A)	108.7(12)
C(7)-C(8)-H(8A)	112.7(12)
N(1)-C(8)-H(8B)	108.7(11)
C(7)-C(8)-H(8B)	108.7(11)
H(8A)-C(8)-H(8B)	106.5(17)
N(1)-C(9)-H(9A)	109.9(15)
N(1)-C(9)-H(9B)	109.8(16)
H(9A)-C(9)-H(9B)	112(2)
N(1)-C(9)-H(9C)	105.9(13)
H(9A)-C(9)-H(9C)	114(2)
H(9B)-C(9)-H(9C)	106(2)
C(11)-C(10)-O(1)	124.48(15)
C(11)-C(10)-C(15)	121.43(15)
O(1)-C(10)-C(15)	114.09(14)
C(10)-C(11)-C(12)	119.70(17)
C(10)-C(11)-H(11)	120.0(12)
C(12)-C(11)-H(11)	120.3(12)
C(13)-C(12)-C(11)	120.80(17)
C(13)-C(12)-H(12)	118.3(16)
C(11)-C(12)-H(12)	120.8(15)
C(12)-C(13)-C(14)	120.75(16)

C(12)-C(13)-H(13)	121.3(12)
C(14)-C(13)-H(13)	118.0(12)
C(19)-C(14)-C(13)	122.50(16)
C(19)-C(14)-C(15)	118.36(17)
C(13)-C(14)-C(15)	119.15(16)
C(16)-C(15)-C(10)	122.86(15)
C(16)-C(15)-C(14)	118.98(16)
C(10)-C(15)-C(14)	118.15(15)
C(17)-C(16)-C(15)	120.37(17)
C(17)-C(16)-H(16)	121.6(11)
C(15)-C(16)-H(16)	118.1(11)
C(16)-C(17)-C(18)	120.74(18)
C(16)-C(17)-H(17)	121.1(13)
C(18)-C(17)-H(17)	118.2(13)
C(19)-C(18)-C(17)	120.07(18)
C(19)-C(18)-H(18)	122.6(13)
C(17)-C(18)-H(18)	117.2(13)
C(18)-C(19)-C(14)	121.49(17)
C(18)-C(19)-H(19)	119.5(12)
C(14)-C(19)-H(19)	119.0(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jw20. 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)	40(1)	43(1)	35(1)	8(1)	17(1)	10(1)
S(1)	34(1)	59(1)	88(1)	-5(1)	23(1)	10(1)
O(1)	33(1)	34(1)	26(1)	-6(1)	8(1)	2(1)
N(1)	45(1)	34(1)	33(1)	1(1)	19(1)	4(1)
C(1)	38(1)	67(2)	61(1)	-22(1)	25(1)	-19(1)
C(2)	56(1)	46(1)	54(1)	2(1)	26(1)	-9(1)
C(3)	38(1)	43(1)	50(1)	4(1)	23(1)	6(1)
C(4)	27(1)	36(1)	32(1)	-9(1)	8(1)	3(1)
C(5)	33(1)	33(1)	29(1)	-2(1)	6(1)	6(1)
C(6)	49(1)	39(1)	41(1)	5(1)	3(1)	10(1)
C(7)	45(1)	28(1)	33(1)	0(1)	12(1)	6(1)
C(8)	54(1)	28(1)	32(1)	2(1)	15(1)	-2(1)
C(9)	46(1)	43(1)	58(1)	-1(1)	19(1)	1(1)
C(10)	41(1)	28(1)	21(1)	1(1)	9(1)	1(1)
C(11)	36(1)	39(1)	29(1)	0(1)	5(1)	4(1)
C(12)	41(1)	42(1)	32(1)	-1(1)	0(1)	-5(1)
C(13)	53(1)	34(1)	28(1)	-6(1)	5(1)	-7(1)
C(14)	49(1)	27(1)	26(1)	1(1)	13(1)	-1(1)
C(15)	39(1)	27(1)	23(1)	4(1)	10(1)	0(1)
C(16)	41(1)	35(1)	26(1)	1(1)	11(1)	0(1)
C(17)	39(1)	48(1)	33(1)	2(1)	10(1)	3(1)
C(18)	54(1)	44(1)	45(1)	-3(1)	21(1)	13(1)
C(19)	59(1)	35(1)	35(1)	-6(1)	17(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jw20.

	x	y	z	U(eq)
H(1N)	4670(20)	2600(40)	6134(15)	48(6)
H(2N)	4990(20)	940(30)	5710(15)	39(5)
H(1)	11370(30)	6410(40)	5869(16)	58(7)
H(2)	9190(30)	8400(40)	5709(18)	62(8)
H(3)	7410(30)	6930(40)	6344(16)	54(7)
H(6A)	9570(30)	1360(40)	7878(15)	50(6)
H(6B)	8230(30)	1420(40)	8402(17)	53(6)
H(7)	7680(20)	1100(30)	6465(14)	40(5)
H(8A)	5520(20)	1070(30)	7515(14)	40(5)
H(8B)	5850(20)	-790(40)	6992(12)	36(5)
H(9A)	2880(30)	1050(40)	6703(17)	61(7)
H(9B)	3140(30)	-740(50)	6105(17)	61(7)
H(9C)	2510(30)	1070(40)	5578(16)	50(6)
H(11)	9360(20)	5380(30)	8684(12)	34(5)
H(12)	9870(30)	7640(40)	9924(17)	49(6)
H(13)	8010(20)	9370(30)	10319(14)	44(5)
H(16)	4210(20)	5620(30)	7614(13)	32(4)
H(17)	2330(20)	7510(30)	8000(14)	41(5)
H(18)	2900(20)	9770(30)	9155(14)	44(6)
H(19)	5330(20)	10280(30)	10012(15)	41(5)

Table 6. Torsion angles [°] for jw20.

C(4)-S(1)-C(1)-C(2)	0.87(18)
S(1)-C(1)-C(2)-C(3)	-1.4(3)
C(1)-C(2)-C(3)-C(4)	1.4(3)
C(2)-C(3)-C(4)-C(5)	-179.49(18)
C(2)-C(3)-C(4)-S(1)	-0.7(2)
C(1)-S(1)-C(4)-C(3)	-0.06(15)
C(1)-S(1)-C(4)-C(5)	178.81(14)
C(10)-O(1)-C(5)-C(4)	-71.25(18)
C(10)-O(1)-C(5)-C(6)	80.65(19)
C(10)-O(1)-C(5)-C(7)	147.25(14)
C(3)-C(4)-C(5)-O(1)	-22.9(2)
S(1)-C(4)-C(5)-O(1)	158.40(11)
C(3)-C(4)-C(5)-C(6)	-172.90(18)
S(1)-C(4)-C(5)-C(6)	8.4(2)
C(3)-C(4)-C(5)-C(7)	115.3(2)
S(1)-C(4)-C(5)-C(7)	-63.3(2)
O(1)-C(5)-C(6)-C(7)	102.03(17)
C(4)-C(5)-C(6)-C(7)	-108.78(18)
C(5)-C(6)-C(7)-C(8)	-110.37(19)
O(1)-C(5)-C(7)-C(8)	-0.6(2)
C(4)-C(5)-C(7)-C(8)	-139.26(17)
C(6)-C(5)-C(7)-C(8)	108.05(19)
O(1)-C(5)-C(7)-C(6)	-108.61(17)
C(4)-C(5)-C(7)-C(6)	112.69(18)
C(9)-N(1)-C(8)-C(7)	-179.92(17)
C(6)-C(7)-C(8)-N(1)	155.16(17)
C(5)-C(7)-C(8)-N(1)	85.0(2)
C(5)-O(1)-C(10)-C(11)	-4.4(2)
C(5)-O(1)-C(10)-C(15)	175.10(13)
O(1)-C(10)-C(11)-C(12)	179.45(16)
C(15)-C(10)-C(11)-C(12)	-0.1(3)
C(10)-C(11)-C(12)-C(13)	0.3(3)
C(11)-C(12)-C(13)-C(14)	-1.1(3)
C(12)-C(13)-C(14)-C(19)	-178.78(18)

C(12)-C(13)-C(14)-C(15)	1.5(3)
C(11)-C(10)-C(15)-C(16)	179.91(16)
O(1)-C(10)-C(15)-C(16)	0.4(2)
C(11)-C(10)-C(15)-C(14)	0.5(2)
O(1)-C(10)-C(15)-C(14)	-179.04(13)
C(19)-C(14)-C(15)-C(16)	-0.3(2)
C(13)-C(14)-C(15)-C(16)	179.37(16)
C(19)-C(14)-C(15)-C(10)	179.07(16)
C(13)-C(14)-C(15)-C(10)	-1.2(2)
C(10)-C(15)-C(16)-C(17)	-178.80(16)
C(14)-C(15)-C(16)-C(17)	0.6(2)
C(15)-C(16)-C(17)-C(18)	-0.3(3)
C(16)-C(17)-C(18)-C(19)	-0.1(3)
C(17)-C(18)-C(19)-C(14)	0.4(3)
C(13)-C(14)-C(19)-C(18)	-179.85(19)
C(15)-C(14)-C(19)-C(18)	-0.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for jw20 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(2N)...Cl(1)#1	0.83(2)	2.29(2)	3.1079(16)	167(2)
N(1)-H(1N)...Cl(1)	0.87(3)	2.26(3)	3.0782(18)	158(2)

Symmetry transformations used to generate equivalent atoms:

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

(-)-(1R, 2R)-16 (JW 25)

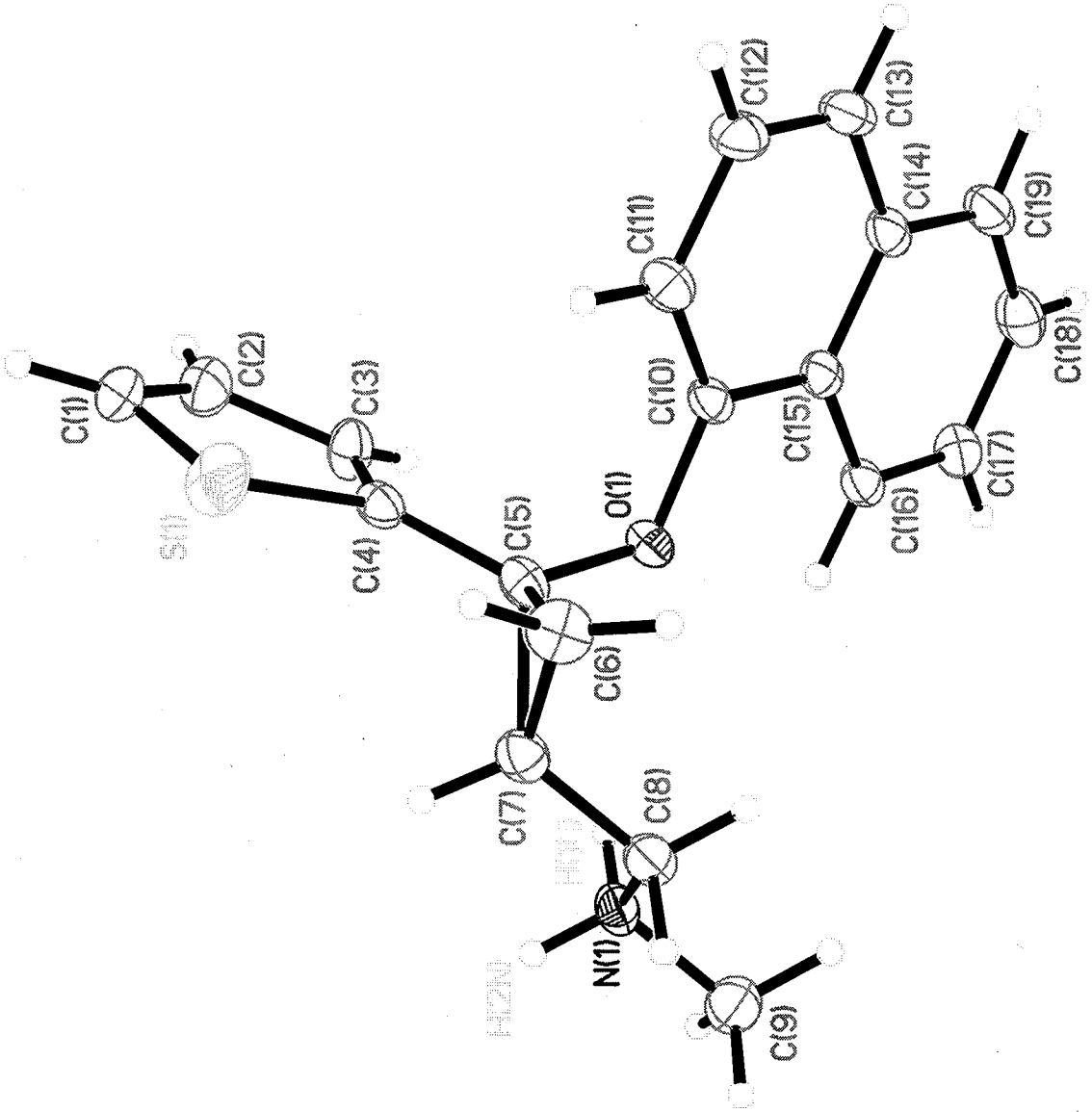

C(12)
C(13)
C(14)
C(19)
C(11)
C(18)
C(2)
C(3)
C(1)
C(10)
C(15)
C(17)
O(1)
S(1)
C(4)
C(5)
C(16)
C(6)
C(7)
C(8)
N(1)
C(9)

Table 1. Crystal data and structure refinement for jw25.

Identification code	jw25	
Empirical formula	C19 H20 Cl N O S	
Formula weight	345.87	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.2343(11) Å	α= 90°.
	b = 6.7831(8) Å	β= 104.353(2)°.
	c = 14.9383(18) Å	γ = 90°.
Volume	906.49(19) $Å^3$	
Z	2	
Density (calculated)	1.267 Mg/m^3	
Absorption coefficient	0.329 mm^{-1}	
F(000)	364	
Crystal size	0.36 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.41 to 27.00°.	
Index ranges	-11<=h<=11, -8<=k<=8, -19<=l<=19	
Reflections collected	10218	
Independent reflections	3938 [R(int) = 0.0298]	
Completeness to theta = 27.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9741 and 0.8906	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3938 / 1 / 288	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0780	
R indices (all data)	R1 = 0.0452, wR2 = 0.0830	
Absolute structure parameter	0.04(5)	
Largest diff. peak and hole	0.267 and -0.155 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jw25. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	4602(1)	298(1)	8293(1)	60(1)
Cl(1)	959(1)	-1222(1)	9446(1)	39(1)
O(1)	8297(2)	-79(2)	7359(1)	31(1)
N(1)	10325(2)	3102(3)	8842(1)	36(1)
C(1)	4480(3)	-1769(4)	8919(2)	55(1)
C(2)	5677(3)	-2890(5)	9021(2)	49(1)
C(3)	6772(3)	-2087(4)	8608(2)	41(1)
C(4)	6341(2)	-344(3)	8177(1)	31(1)
C(5)	7185(2)	933(3)	7681(1)	32(1)
C(6)	6505(3)	2718(4)	7134(2)	44(1)
C(7)	7664(3)	2972(3)	8038(2)	36(1)
C(8)	9174(3)	3731(4)	8019(2)	38(1)
C(9)	11836(3)	3827(5)	8847(2)	48(1)
C(10)	7858(2)	-1366(3)	6633(1)	29(1)
C(11)	6415(2)	-1664(3)	6151(1)	36(1)
C(12)	6096(3)	-3048(4)	5421(2)	40(1)
C(13)	7196(3)	-4074(3)	5186(2)	40(1)
C(14)	8713(3)	-3814(3)	5680(1)	34(1)
C(15)	9058(2)	-2422(3)	6412(1)	29(1)
C(16)	10572(2)	-2159(3)	6900(2)	33(1)
C(17)	11670(3)	-3234(4)	6672(2)	40(1)
C(18)	11334(3)	-4617(4)	5948(2)	47(1)
C(19)	9897(3)	-4892(4)	5469(2)	42(1)

Table 3. Bond lengths [Å] and angles [°] for jw25.

S(1)-C(1)	1.703(3)
S(1)-C(4)	1.713(2)
O(1)-C(10)	1.373(2)
O(1)-C(5)	1.414(2)
N(1)-C(8)	1.475(3)
N(1)-C(9)	1.477(3)
N(1)-H(1N)	0.86(3)
N(1)-H(2N)	0.86(3)
C(1)-C(2)	1.319(4)
C(1)-H(1)	0.91(3)
C(2)-C(3)	1.417(3)
C(2)-H(2)	0.90(3)
C(3)-C(4)	1.358(3)
C(3)-H(3)	0.78(3)
C(4)-C(5)	1.481(3)
C(5)-C(6)	1.508(3)
C(5)-C(7)	1.509(3)
C(6)-C(7)	1.510(3)
C(6)-H(6A)	1.00(2)
C(6)-H(6B)	0.93(3)
C(7)-C(8)	1.493(3)
C(7)-H(7)	0.93(2)
C(8)-H(8A)	0.95(2)
C(8)-H(8B)	0.93(2)
C(9)-H(9A)	1.00(3)
C(9)-H(9B)	0.93(4)
C(9)-H(9C)	0.95(3)
C(10)-C(11)	1.363(3)
C(10)-C(15)	1.426(3)
C(11)-C(12)	1.413(3)
C(11)-H(11)	0.95(2)
C(12)-C(13)	1.348(3)
C(12)-H(12)	0.87(3)
C(13)-C(14)	1.424(3)

C(13)-H(13)	0.93(2)
C(14)-C(19)	1.414(3)
C(14)-C(15)	1.419(3)
C(15)-C(16)	1.419(3)
C(16)-C(17)	1.359(3)
C(16)-H(16)	0.96(2)
C(17)-C(18)	1.406(4)
C(17)-H(17)	0.93(2)
C(18)-C(19)	1.355(3)
C(18)-H(18)	0.92(3)
C(19)-H(19)	0.93(3)

C(1)-S(1)-C(4)	92.17(13)
C(10)-O(1)-C(5)	118.68(15)
C(8)-N(1)-C(9)	113.1(2)
C(8)-N(1)-H(1N)	109.4(15)
C(9)-N(1)-H(1N)	109.3(15)
C(8)-N(1)-H(2N)	106.2(17)
C(9)-N(1)-H(2N)	112.0(18)
H(1N)-N(1)-H(2N)	106(3)
C(2)-C(1)-S(1)	111.7(2)
C(2)-C(1)-H(1)	128.1(18)
S(1)-C(1)-H(1)	120.1(18)
C(1)-C(2)-C(3)	113.3(3)
C(1)-C(2)-H(2)	129.5(17)
C(3)-C(2)-H(2)	117.2(17)
C(4)-C(3)-C(2)	112.6(2)
C(4)-C(3)-H(3)	122(2)
C(2)-C(3)-H(3)	125(2)
C(3)-C(4)-C(5)	128.1(2)
C(3)-C(4)-S(1)	110.19(18)
C(5)-C(4)-S(1)	121.68(16)
O(1)-C(5)-C(4)	113.76(17)
O(1)-C(5)-C(6)	116.45(19)
C(4)-C(5)-C(6)	122.68(19)
O(1)-C(5)-C(7)	113.03(18)

C(4)-C(5)-C(7)	120.28(18)
C(6)-C(5)-C(7)	60.08(15)
C(5)-C(6)-C(7)	59.98(14)
C(5)-C(6)-H(6A)	117.1(14)
C(7)-C(6)-H(6A)	118.7(13)
C(5)-C(6)-H(6B)	117.2(17)
C(7)-C(6)-H(6B)	116.4(17)
H(6A)-C(6)-H(6B)	116(2)
C(8)-C(7)-C(6)	118.7(2)
C(8)-C(7)-C(5)	120.1(2)
C(6)-C(7)-C(5)	59.94(15)
C(8)-C(7)-H(7)	116.4(16)
C(6)-C(7)-H(7)	116.4(15)
C(5)-C(7)-H(7)	113.3(16)
N(1)-C(8)-C(7)	111.59(19)
N(1)-C(8)-H(8A)	108.8(12)
C(7)-C(8)-H(8A)	110.0(12)
N(1)-C(8)-H(8B)	107.0(13)
C(7)-C(8)-H(8B)	112.2(12)
H(8A)-C(8)-H(8B)	107.0(18)
N(1)-C(9)-H(9A)	110.4(16)
N(1)-C(9)-H(9B)	108.5(17)
H(9A)-C(9)-H(9B)	110(3)
N(1)-C(9)-H(9C)	105.1(15)
H(9A)-C(9)-H(9C)	114(2)
H(9B)-C(9)-H(9C)	109(3)
C(11)-C(10)-O(1)	124.80(19)
C(11)-C(10)-C(15)	121.09(19)
O(1)-C(10)-C(15)	114.11(17)
C(10)-C(11)-C(12)	119.8(2)
C(10)-C(11)-H(11)	119.9(13)
C(12)-C(11)-H(11)	120.2(13)
C(13)-C(12)-C(11)	121.1(2)
C(13)-C(12)-H(12)	119.7(18)
C(11)-C(12)-H(12)	119.1(18)
C(12)-C(13)-C(14)	120.6(2)

C(12)-C(13)-H(13)	120.5(14)
C(14)-C(13)-H(13)	118.9(14)
C(19)-C(14)-C(13)	122.4(2)
C(19)-C(14)-C(15)	118.5(2)
C(13)-C(14)-C(15)	119.1(2)
C(16)-C(15)-C(14)	118.94(19)
C(16)-C(15)-C(10)	122.75(19)
C(14)-C(15)-C(10)	118.30(19)
C(17)-C(16)-C(15)	120.3(2)
C(17)-C(16)-H(16)	122.2(12)
C(15)-C(16)-H(16)	117.5(12)
C(16)-C(17)-C(18)	121.0(2)
C(16)-C(17)-H(17)	121.1(15)
C(18)-C(17)-H(17)	117.9(15)
C(19)-C(18)-C(17)	119.9(2)
C(19)-C(18)-H(18)	121.0(16)
C(17)-C(18)-H(18)	119.0(15)
C(18)-C(19)-C(14)	121.4(2)
C(18)-C(19)-H(19)	120.5(14)
C(14)-C(19)-H(19)	118.1(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jw25. 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)	34(1)	60(1)	89(1)	-5(1)	23(1)	9(1)
Cl(1)	41(1)	44(1)	35(1)	8(1)	17(1)	10(1)
O(1)	32(1)	34(1)	25(1)	-5(1)	6(1)	3(1)
N(1)	46(1)	32(1)	34(1)	0(1)	20(1)	4(1)
C(1)	39(1)	69(2)	62(2)	-24(1)	25(1)	-20(1)
C(2)	55(2)	45(2)	54(2)	0(1)	26(1)	-6(1)
C(3)	37(1)	43(1)	48(1)	5(1)	21(1)	7(1)
C(4)	28(1)	35(1)	31(1)	-8(1)	7(1)	4(1)
C(5)	33(1)	35(1)	28(1)	-3(1)	7(1)	7(1)
C(6)	46(2)	40(1)	43(1)	5(1)	4(1)	8(1)
C(7)	44(1)	29(1)	35(1)	0(1)	12(1)	4(1)
C(8)	55(1)	28(1)	32(1)	2(1)	15(1)	1(1)
C(9)	47(1)	44(2)	57(2)	0(2)	18(1)	-1(1)
C(10)	40(1)	27(1)	21(1)	0(1)	8(1)	-1(1)
C(11)	38(1)	39(1)	28(1)	1(1)	4(1)	4(1)
C(12)	40(1)	45(1)	31(1)	-2(1)	0(1)	-6(1)
C(13)	54(2)	34(1)	29(1)	-6(1)	6(1)	-6(1)
C(14)	49(1)	29(1)	26(1)	2(1)	13(1)	-2(1)
C(15)	37(1)	27(1)	23(1)	4(1)	9(1)	0(1)
C(16)	41(1)	34(1)	26(1)	0(1)	10(1)	0(1)
C(17)	37(1)	48(2)	35(1)	1(1)	11(1)	3(1)
C(18)	54(2)	44(2)	47(1)	-2(1)	23(1)	12(1)
C(19)	59(2)	35(1)	34(1)	-6(1)	16(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jw25.

	x	y	z	U(eq)
H(1N)	10340(20)	1840(40)	8873(14)	29(6)
H(2N)	10030(30)	3510(50)	9310(18)	51(7)
H(1)	3670(30)	-1970(40)	9148(18)	59(8)
H(2)	5870(30)	-4070(50)	9295(19)	59(9)
H(3)	7570(30)	-2520(40)	8655(18)	50(8)
H(6A)	5430(30)	3020(40)	7113(16)	41(6)
H(6B)	6810(30)	3000(40)	6600(20)	57(8)
H(7)	7310(30)	3330(40)	8548(17)	45(7)
H(8A)	9160(20)	5130(40)	7992(13)	24(5)
H(8B)	9480(20)	3280(30)	7503(14)	27(5)
H(9A)	12140(30)	3360(50)	8281(19)	62(8)
H(9B)	11830(30)	5200(50)	8865(19)	60(8)
H(9C)	12470(30)	3350(40)	9410(18)	48(7)
H(11)	5630(20)	-1010(40)	6332(13)	31(6)
H(12)	5170(30)	-3210(40)	5111(19)	47(7)
H(13)	6970(20)	-4970(40)	4698(16)	43(7)
H(16)	10780(20)	-1200(40)	7387(15)	31(5)
H(17)	12670(30)	-3080(40)	6991(15)	36(6)
H(18)	12090(30)	-5400(40)	5842(16)	49(7)
H(19)	9660(20)	-5830(40)	5003(16)	39(6)

Table 6. Torsion angles [°] for jw25.

C(4)-S(1)-C(1)-C(2)	-0.8(2)
S(1)-C(1)-C(2)-C(3)	1.3(3)
C(1)-C(2)-C(3)-C(4)	-1.3(3)
C(2)-C(3)-C(4)-C(5)	179.3(2)
C(2)-C(3)-C(4)-S(1)	0.6(3)
C(1)-S(1)-C(4)-C(3)	0.11(19)
C(1)-S(1)-C(4)-C(5)	-178.69(18)
C(10)-O(1)-C(5)-C(4)	71.2(2)
C(10)-O(1)-C(5)-C(6)	-80.2(2)
C(10)-O(1)-C(5)-C(7)	-147.04(17)
C(3)-C(4)-C(5)-O(1)	23.2(3)
S(1)-C(4)-C(5)-O(1)	-158.28(14)
C(3)-C(4)-C(5)-C(6)	172.6(2)
S(1)-C(4)-C(5)-C(6)	-8.9(3)
C(3)-C(4)-C(5)-C(7)	-115.6(3)
S(1)-C(4)-C(5)-C(7)	63.0(2)
O(1)-C(5)-C(6)-C(7)	-102.6(2)
C(4)-C(5)-C(6)-C(7)	108.8(2)
C(5)-C(6)-C(7)-C(8)	110.2(2)
O(1)-C(5)-C(7)-C(8)	0.5(3)
C(4)-C(5)-C(7)-C(8)	139.5(2)
C(6)-C(5)-C(7)-C(8)	-107.8(2)
O(1)-C(5)-C(7)-C(6)	108.3(2)
C(4)-C(5)-C(7)-C(6)	-112.7(2)
C(9)-N(1)-C(8)-C(7)	-180.0(2)
C(6)-C(7)-C(8)-N(1)	-155.1(2)
C(5)-C(7)-C(8)-N(1)	-85.1(3)
C(5)-O(1)-C(10)-C(11)	4.4(3)
C(5)-O(1)-C(10)-C(15)	-175.25(17)
O(1)-C(10)-C(11)-C(12)	-179.3(2)
C(15)-C(10)-C(11)-C(12)	0.3(3)
C(10)-C(11)-C(12)-C(13)	-0.5(3)
C(11)-C(12)-C(13)-C(14)	1.1(4)
C(12)-C(13)-C(14)-C(19)	178.5(2)

C(12)-C(13)-C(14)-C(15)	-1.4(3)
C(19)-C(14)-C(15)-C(16)	0.3(3)
C(13)-C(14)-C(15)-C(16)	-179.7(2)
C(19)-C(14)-C(15)-C(10)	-178.8(2)
C(13)-C(14)-C(15)-C(10)	1.1(3)
C(11)-C(10)-C(15)-C(16)	-179.74(19)
O(1)-C(10)-C(15)-C(16)	-0.1(3)
C(11)-C(10)-C(15)-C(14)	-0.6(3)
O(1)-C(10)-C(15)-C(14)	178.98(17)
C(14)-C(15)-C(16)-C(17)	-0.4(3)
C(10)-C(15)-C(16)-C(17)	178.7(2)
C(15)-C(16)-C(17)-C(18)	0.3(4)
C(16)-C(17)-C(18)-C(19)	-0.2(4)
C(17)-C(18)-C(19)-C(14)	0.1(4)
C(13)-C(14)-C(19)-C(18)	179.9(2)
C(15)-C(14)-C(19)-C(18)	-0.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for jw25 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...Cl(1)#1	0.86(3)	2.27(3)	3.082(2)	159.3(19)
N(1)-H(2N)...Cl(1)#2	0.86(3)	2.27(3)	3.109(2)	165(3)

Symmetry transformations used to generate equivalent atoms:

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