Electronic Supporting Information

RSC Advances

Water Soluble β-Aminobisulfonate Building Blocks for pH and Cu^{2+} Indicators

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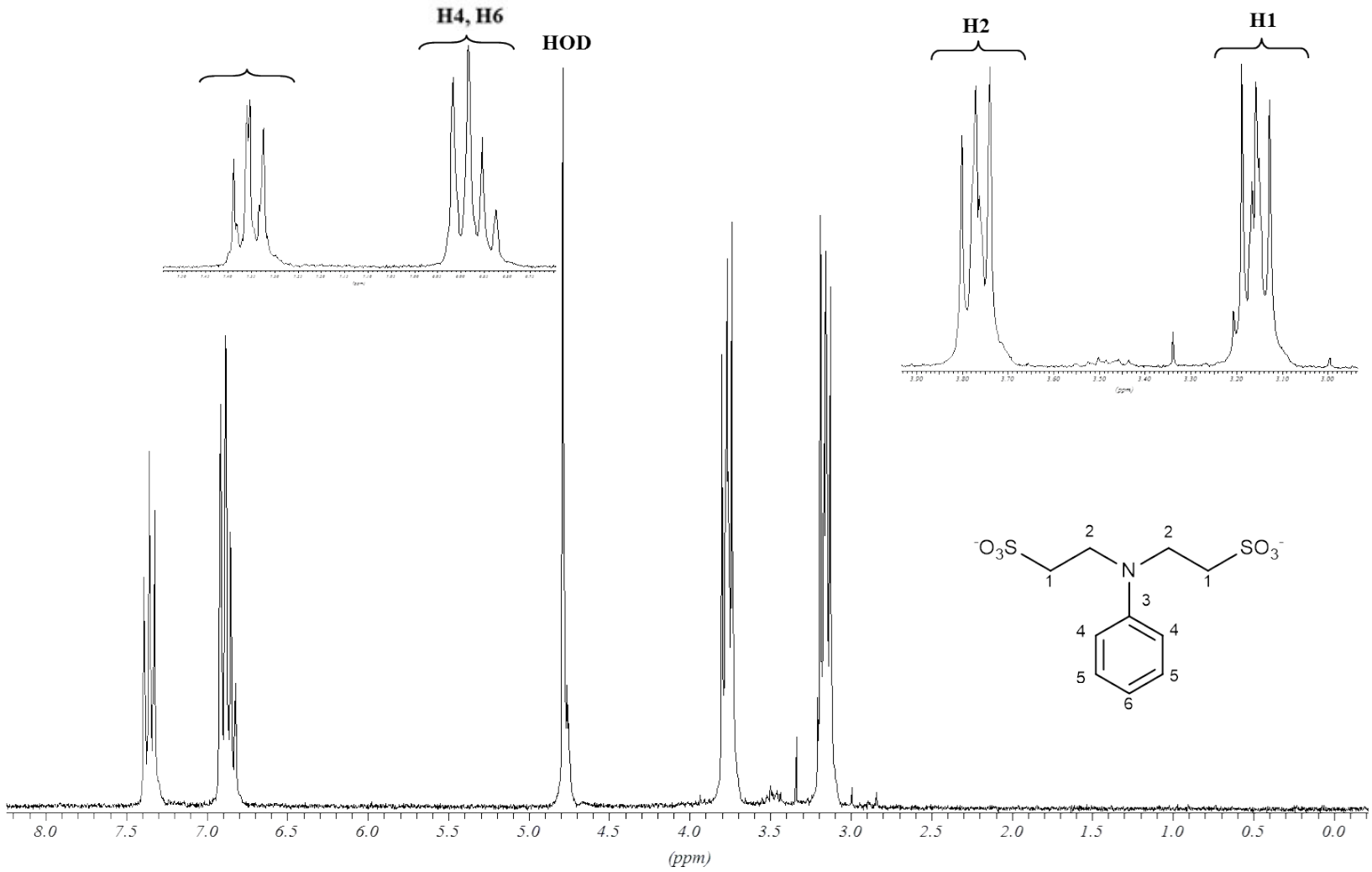

Figure S1: ^{1}H NMR spectrum of **1** at 250 MHz in D_2O.

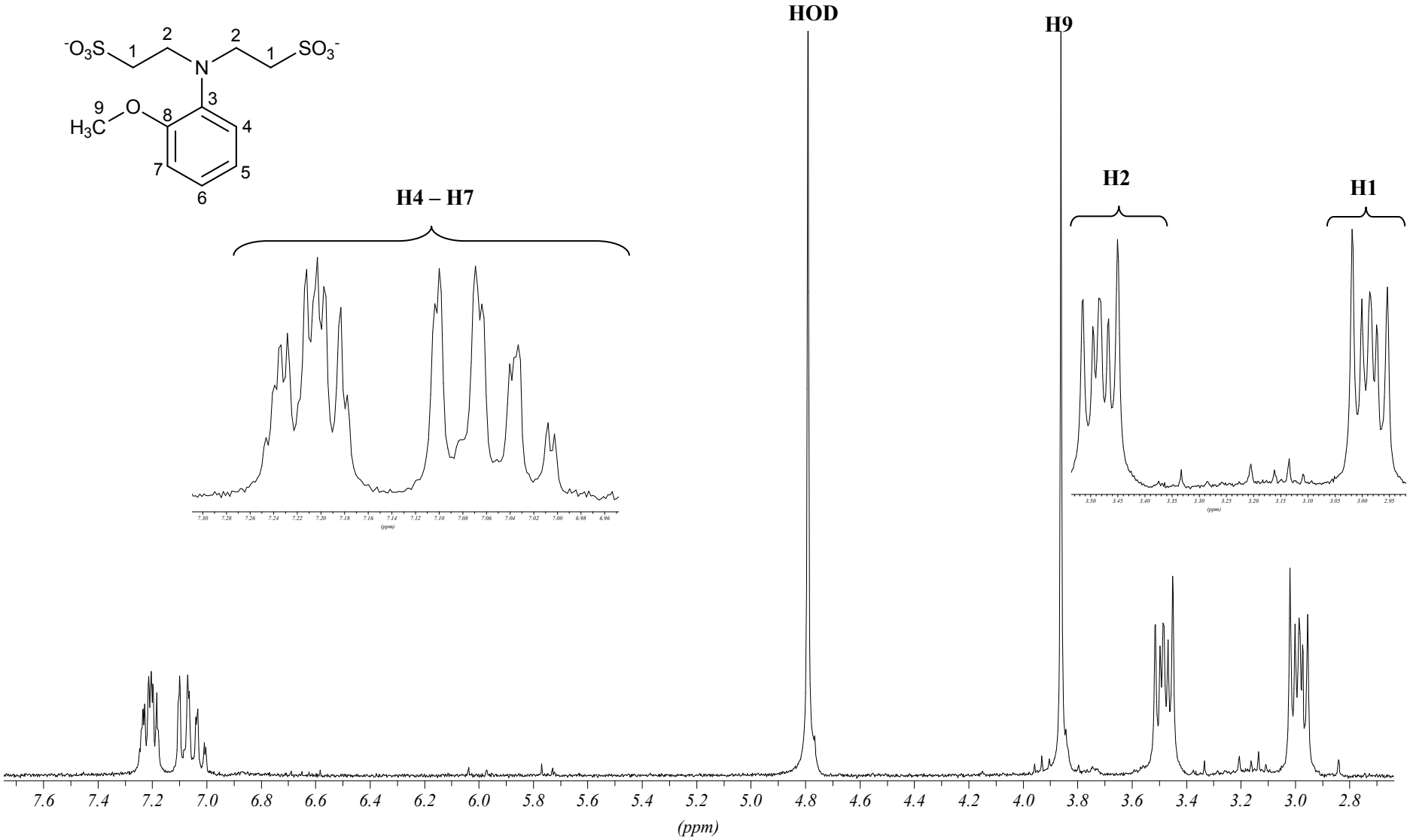

Figure S2: ^{1}H NMR spectrum of **2** in D_2O at 250 MHz.

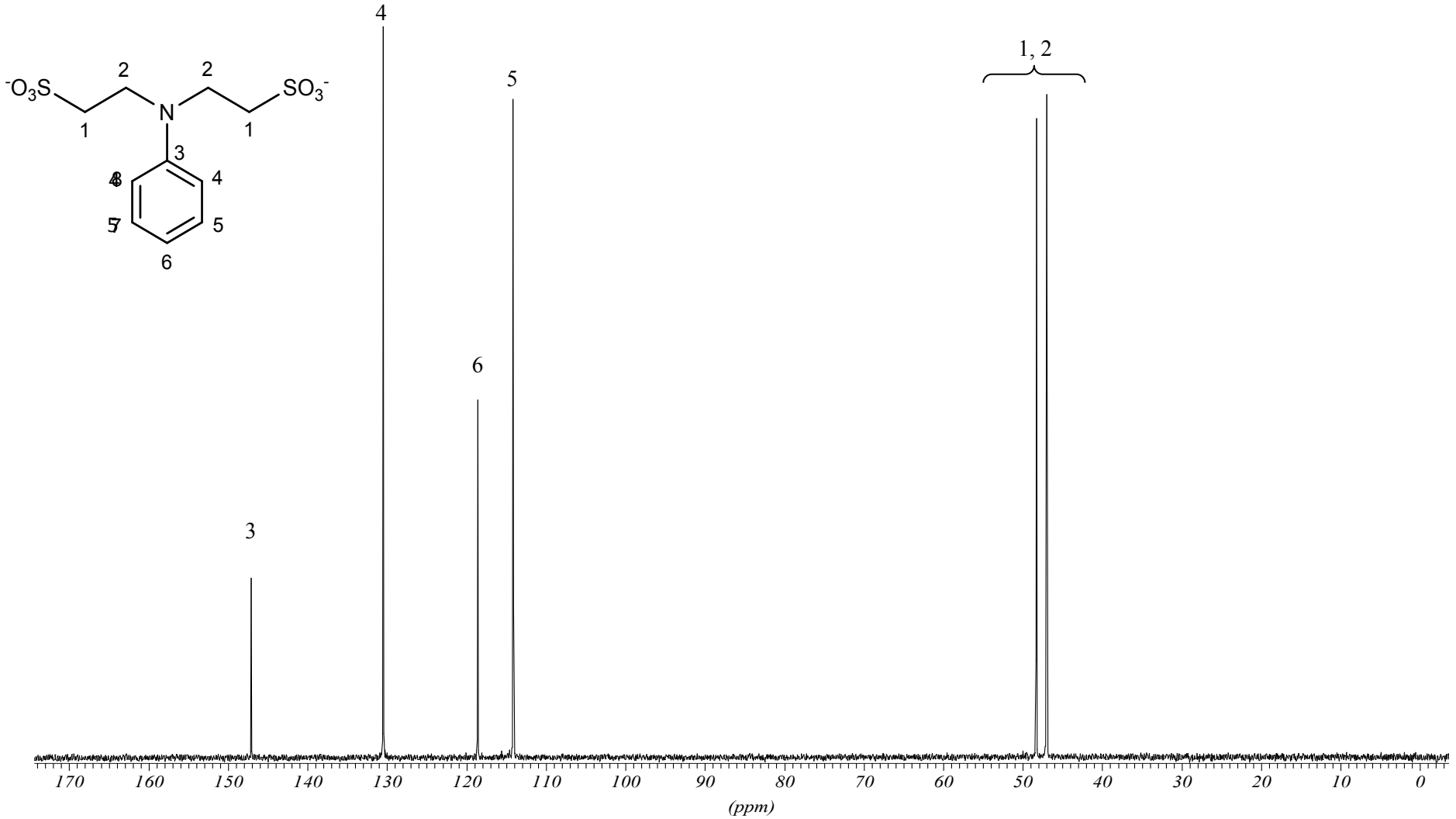

Figure S3: ^{13}C NMR of **1** in D_2O at 250 MHz. (1,4-dioxane standard run as a separate spectrum.)

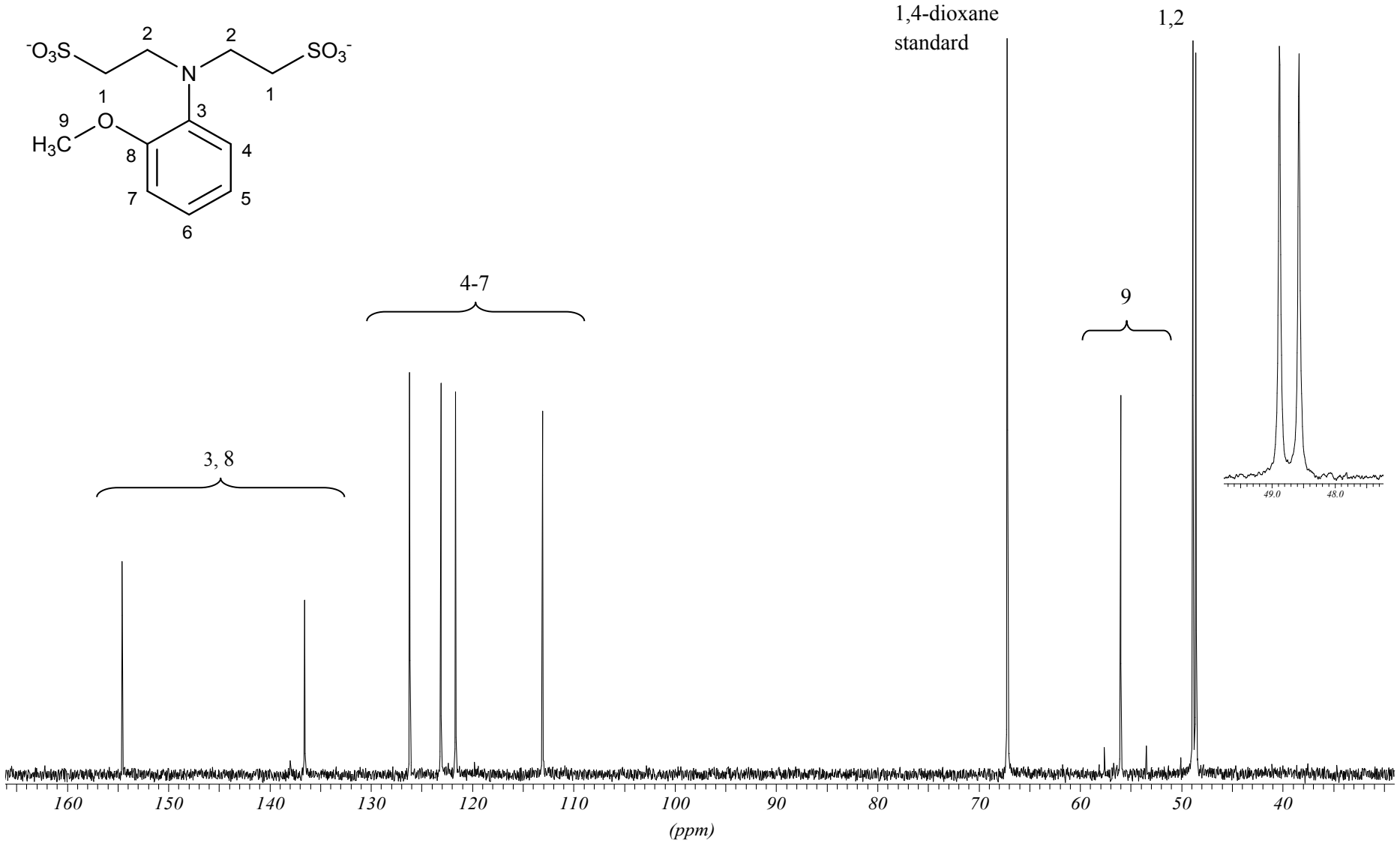

Figure S4: ^{13}C NMR spectrum of **2** in D_2O/1,4-dioxane at 250 MHz.

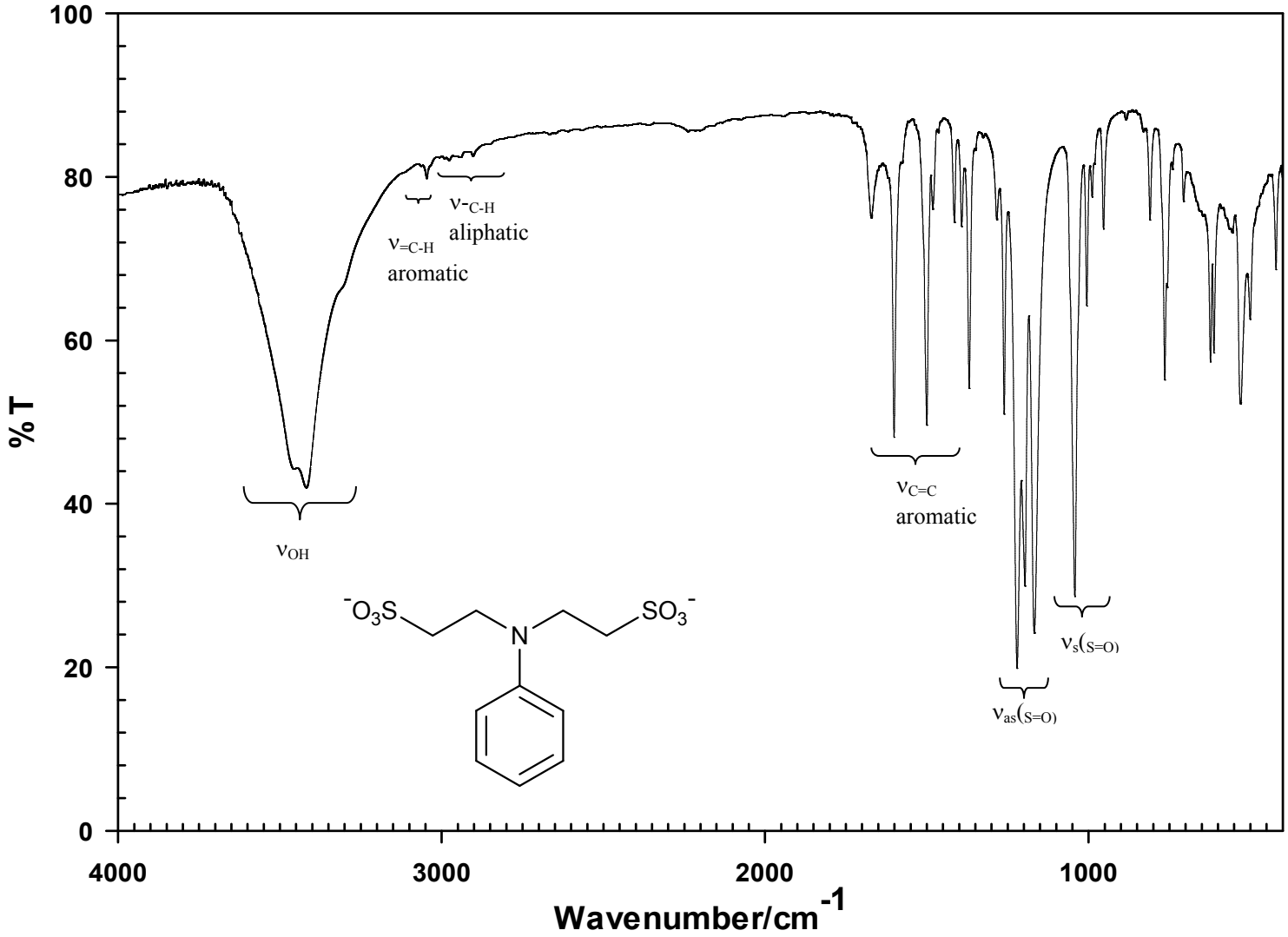

Figure S5: IR spectrum of **1** (KBr disc).

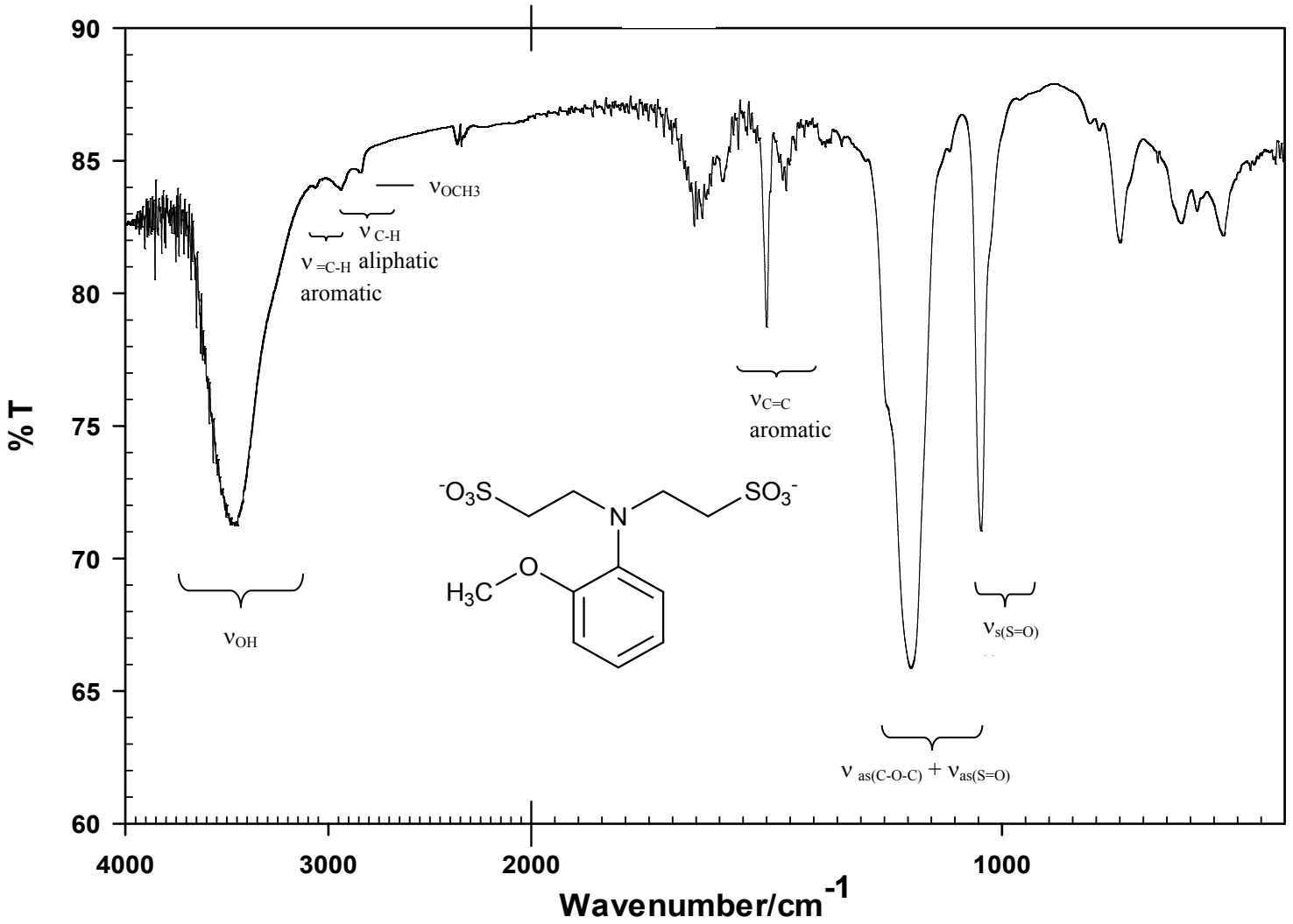

Figure S6: IR spectrum of **2** (KBr disc).

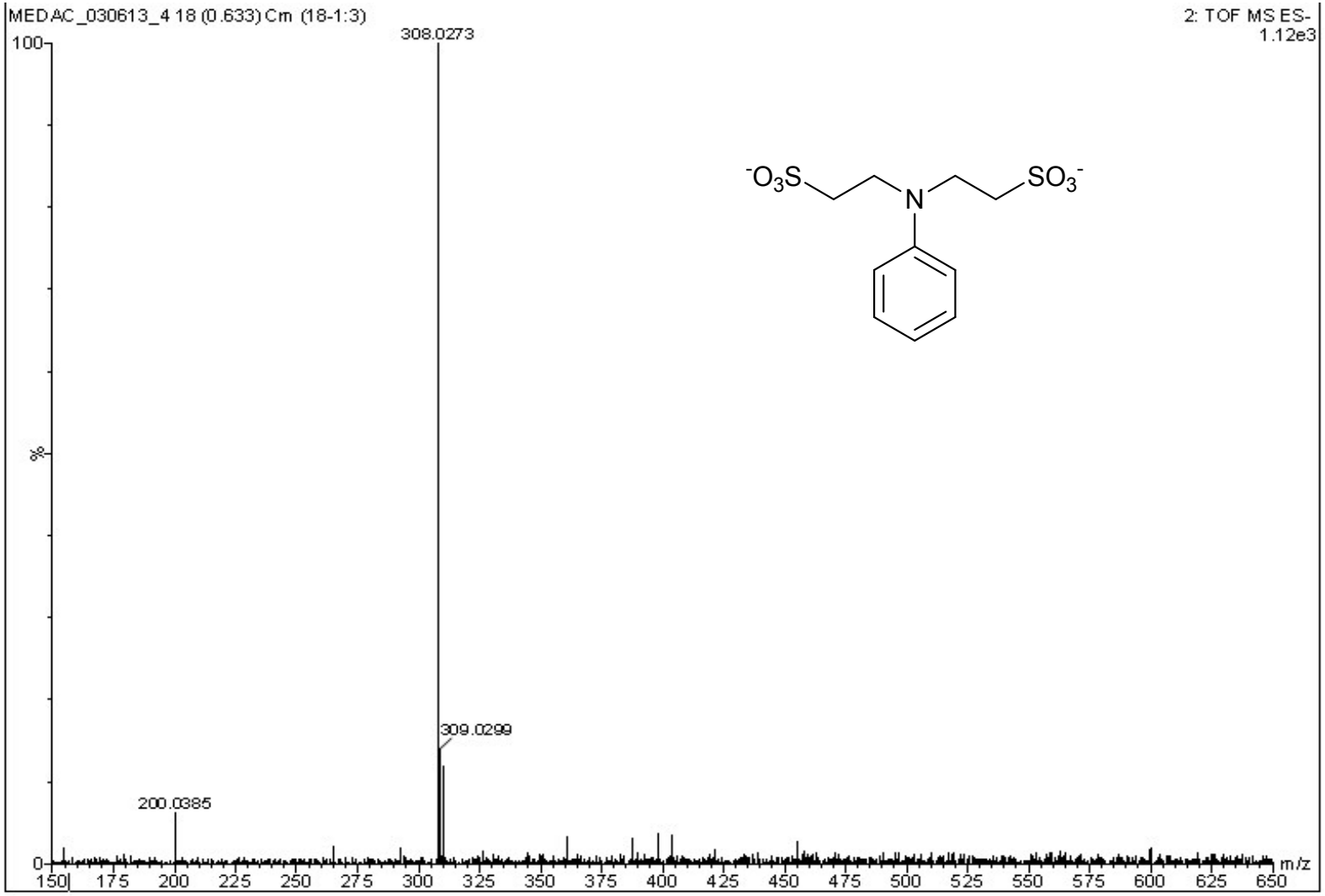

Figure S7: High-resolution mass spectrum of **1**.

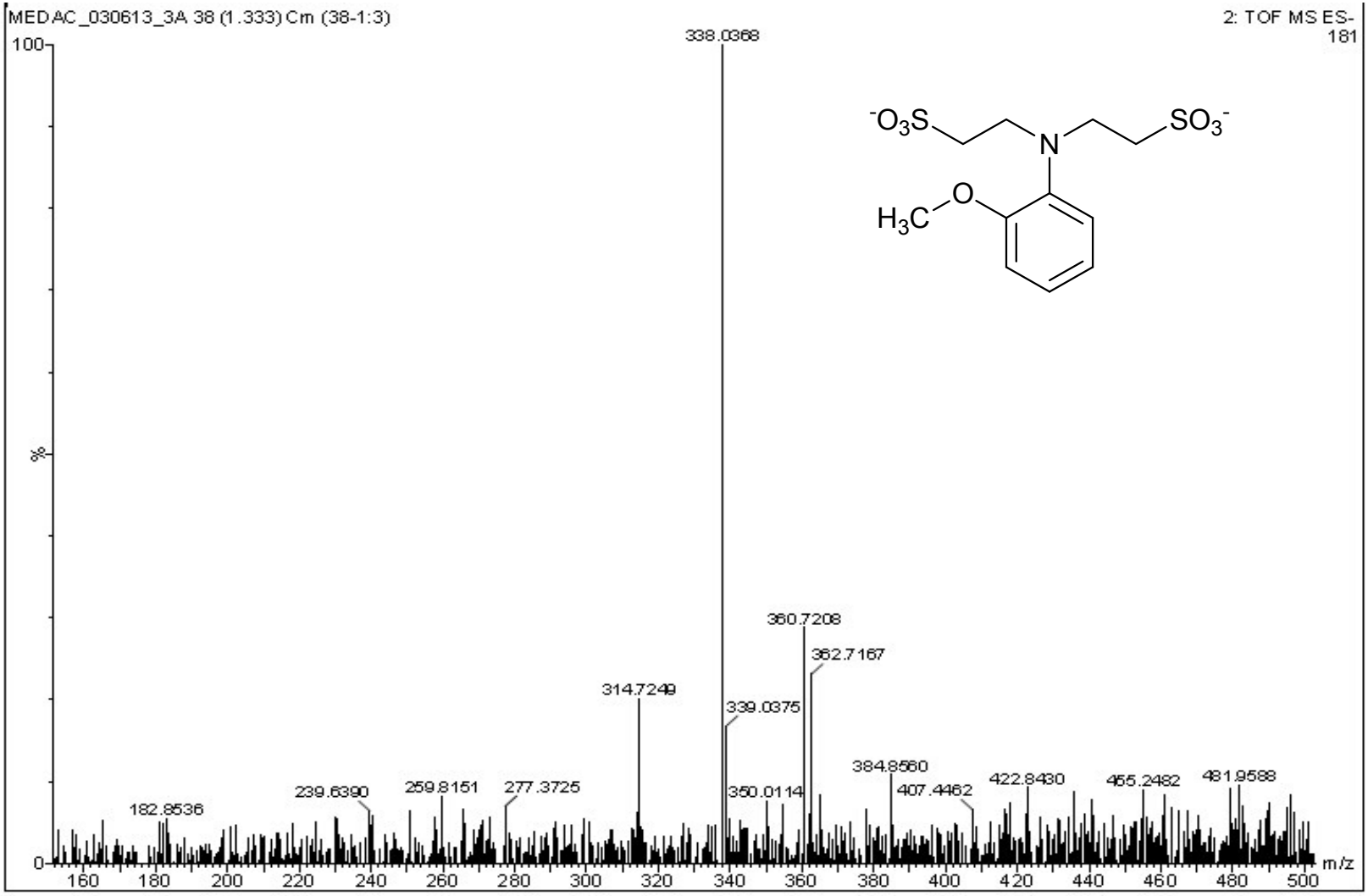

Figure S8: High-resolution mass spectrum of **2.**

X-Ray Crystallographic Data for 1

Table 1 Crystal data and structure refinement for 1.

Compound Name	phenyl *β*-aminobisulfonate
Empirical formula	$C_{10}H_{17}K_2NO_8S_2$
Formula weight / g·mol^{-1}	421.56
Temperature/K	150.01(10)
Crystal system	orthorhombic
Space group	*Pnma*
a/Å	8.2498(3)
b/Å	22.5592(7)
c/Å	8.7439(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1627.33(9)
Z	4
ρ_{calc}g/cm^3	1.721
μ/mm^{-1}	0.877
F(000)	872.0
Crystal size/mm^3	0.3155 × 0.188 × 0.1822
Radiation	MoK_α (λ = 0.71073)
2Θ range for data collection/°	6.79 to 57.556
Index ranges	$-11 \le h \le 10$, $-29 \le k \le 29$, $-11 \le l \le 10$
Reflections collected	24720
Independent reflections	2066 [R_{int} = 0.0354, R_{sigma} = 0.0180]
Data/restraints/parameters	2066/0/144
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0242, wR_2 = 0.0568
Final R indexes [all data]	R_1 = 0.0308, wR_2 = 0.0607
Largest diff. peak/hole / e Å^{-3}	0.36/-0.46

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
K1	1647.0(4)	4826.0(2)	8058.8(3)	16.53(9)
S1	300.1(4)	4028.6(2)	4948.1(4)	12.24(9)
N5	2585(2)	2500	3846.6(18)	14.7(3)
O1	-630.5(12)	4159.8(4)	6321.3(11)	17.5(2)
O91	1132.3(14)	4437.8(5)	10993.5(12)	21.0(2)
O90	672.4(12)	5899.2(4)	6449.1(11)	17.1(2)
O2	1818.6(12)	4353.0(4)	4876.8(11)	19.0(2)
C4	1710.3(17)	3051.6(6)	3596.3(16)	15.0(3)
C9	6949(3)	2500	6348(2)	19.6(4)
C7	4736.1(17)	3032.8(6)	5175.2(15)	16.3(3)
C3	805.2(18)	3266.5(6)	5026.1(15)	16.1(3)
C6	3983(2)	2500	4736(2)	13.4(4)
C8	6198.8(18)	3027.6(6)	5948.2(16)	19.3(3)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K1	17.06(16)	15.19(16)	17.34(16)	0.19(10)	-2.98(11)	0.47(11)
S1	12.26(17)	10.53(16)	13.94(17)	0.54(11)	-0.05(11)	0.68(11)
N5	17.2(8)	9.8(7)	17.2(8)	0	0.0(6)	0
O1	18.8(5)	16.6(5)	17.3(5)	-2.2(4)	2.9(4)	3.1(4)
O91	16.6(5)	23.6(6)	22.6(5)	6.1(4)	3.3(4)	3.2(4)
O90	15.7(5)	19.5(5)	16.0(5)	1.8(4)	-2.2(4)	2.8(4)
O2	16.1(5)	16.0(5)	24.7(5)	0.6(4)	-0.3(4)	-4.1(4)
C4	18.4(7)	12.1(6)	14.4(6)	1.3(5)	0.4(5)	1.5(5)
C9	15.6(10)	27.5(11)	15.8(9)	0	2.1(8)	0
C7	18.4(7)	12.9(7)	17.5(7)	0.2(5)	3.0(5)	0.1(5)
C3	18.4(7)	11.6(6)	18.3(7)	2.9(5)	3.3(5)	2.0(5)
C6	15.3(9)	12.4(9)	12.5(8)	0	4.4(7)	0
C8	21.7(7)	19.1(7)	17.0(7)	-1.2(5)	3.2(6)	-4.5(6)

Table 4 Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
K1	K1[1]	4.23906(19)	S1	C3	1.7704(14)
K1	K1[2]	4.4188(6)	N5	C4	1.4551(15)
K1	K1[3]	4.23911(19)	N5	C4[7]	1.4551(15)
K1	S1	3.4452(4)	N5	C6	1.391(3)
K1	O1	2.8455(10)	O1	K1[1]	2.7563(10)
K1	O1[3]	2.7563(10)	O91	K1[2]	2.9500(12)
K1	O91	2.7445(11)	O91	K1[5]	3.0621(11)
K1	O91[2]	2.9500(12)	O90	S1[6]	1.4707(10)
K1	O91[4]	3.0621(12)	O2	K1[4]	2.7495(10)
K1	O90	2.9136(10)	C4	C3	1.5348(19)
K1	O2	2.9833(10)	C9	C8[7]	1.3860(18)
K1	O2[5]	2.7494(10)	C9	C8	1.3861(18)
S1	O1	1.4556(10)	C7	C6	1.4066(17)
S1	O90[6]	1.4707(10)	C7	C8	1.383(2)
S1	O2	1.4522(10)	C6	C7[7]	1.4067(17)

[1]-1/2+X,+Y,3/2-Z; [2]-X,1-Y,2-Z; [3]1/2+X,+Y,3/2-Z; [4]1/2-X,1-Y,-1/2+Z; [5]1/2-X,1-Y,1/2+Z; [6]-X,1-Y,1-Z; [7]+X,1/2-Y,+Z

Table 5 Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
K1[1]	K1	K1[2]	65.082(7)	O90	K1	O91[4]	55.22(3)
K1[3]	K1	K1[2]	140.854(13)	O90	K1	O2	81.94(3)
K1[1]	K1	K1[3]	153.344(15)	O2[5]	K1	K1[1]	125.54(2)
S1	K1	K1[3]	97.576(11)	O2	K1	K1[2]	144.02(2)
S1	K1	K1[2]	120.063(12)	O2	K1	K1[3]	74.86(2)
S1	K1	K1[1]	60.274(9)	O2[5]	K1	K1[3]	71.66(2)
O1[3]	K1	K1[1]	146.95(2)	O2	K1	K1[1]	80.28(2)
O1	K1	K1[3]	121.29(2)	O2[5]	K1	K1[2]	73.70(2)
O1[3]	K1	K1[3]	41.62(2)	O2	K1	S1	24.80(2)
O1	K1	K1[2]	95.62(2)	O2[5]	K1	S1	163.08(2)
O1	K1	K1[1]	40.04(2)	O2[5]	K1	O1[3]	83.02(3)
O1[3]	K1	K1[2]	116.55(2)	O2[5]	K1	O1	165.57(3)
O1	K1	S1	24.46(2)	O2[5]	K1	O91[2]	79.41(3)
O1[3]	K1	S1	97.66(2)	O2	K1	O91[4]	67.39(3)
O1[3]	K1	O1	110.79(3)	O2[5]	K1	O91[4]	72.55(3)
O1	K1	O91[2]	86.22(3)	O2[5]	K1	O90	81.18(3)
O1[3]	K1	O91[4]	85.65(3)	O2[5]	K1	O2	139.32(2)
O1	K1	O91[4]	111.51(3)	O1	S1	K1	54.03(4)

O1[3]	K1	O91[2]	152.27(3)	O1	S1	O90[6]	112.03(6)
O1[3]	K1	O90	140.62(3)	O1	S1	C3	106.85(6)
O1	K1	O90	89.93(3)	O90[6]	S1	K1	140.71(4)
O1[3]	K1	O2	87.12(3)	O90[6]	S1	C3	105.54(6)
O1	K1	O2	49.04(3)	O2	S1	K1	59.50(4)
O91	K1	K1[3]	111.48(3)	O2	S1	O1	112.82(6)
O91	K1	K1[2]	40.82(2)	O2	S1	O90[6]	112.28(6)
O91[4]	K1	K1[3]	44.10(2)	O2	S1	C3	106.74(7)
O91[4]	K1	K1[2]	136.44(2)	C3	S1	K1	113.63(5)
O91[2]	K1	K1[1]	46.25(2)	C4	N5	C4[7]	117.55(16)
O91[2]	K1	K1[2]	37.45(2)	C6	N5	C4[7]	119.70(8)
O91[2]	K1	K1[3]	145.19(2)	C6	N5	C4	119.70(8)
O91	K1	K1[1]	93.73(3)	K1[1]	O1	K1	98.34(3)
O91[4]	K1	K1[1]	116.50(2)	S1	O1	K1	101.51(5)
O91	K1	S1	121.44(3)	S1	O1	K1[1]	134.66(6)
O91[2]	K1	S1	105.37(2)	K1	O91	K1[5]	106.60(4)
O91[4]	K1	S1	90.61(2)	K1[2]	O91	K1[5]	89.65(3)
O91	K1	O1[3]	76.60(3)	K1	O91	K1[2]	101.73(3)
O91	K1	O1	103.21(3)	S1[6]	O90	K1	130.08(5)
O91	K1	O91[4]	144.80(3)	K1[4]	O2	K1	108.67(3)
O91	K1	O91[2]	78.27(3)	S1	O2	K1	95.70(5)
O91[2]	K1	O91[4]	108.99(4)	S1	O2	K1[4]	139.60(6)
O91	K1	O90	132.39(3)	N5	C4	C3	112.88(12)
O91[2]	K1	O2	120.02(3)	C8[7]	C9	C8	118.34(19)
O91	K1	O2[5]	75.26(3)	C8	C7	C6	120.78(14)
O91	K1	O2	139.93(3)	C4	C3	S1	112.94(9)
O90	K1	K1[1]	67.67(2)	N5	C6	C7[7]	121.26(9)
O90	K1	K1[2]	93.08(2)	N5	C6	C7	121.27(9)
O90	K1	K1[3]	99.04(2)	C7	C6	C7[7]	117.41(18)
O90	K1	S1	87.91(2)	C7	C8	C9	121.31(14)
O90	K1	O91[2]	56.86(3)				

[1]-1/2+X,+Y,3/2-Z; [2]-X,1-Y,2-Z; [3]1/2+X,+Y,3/2-Z; [4]1/2-X,1-Y,-1/2+Z; [5]1/2-X,1-Y,1/2+Z; [6]-X,1-Y,1-Z; [7]+X,1/2-Y,+Z

Table 6 Hydrogen Bonds for 1.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O91	H91A	O90[1]	0.82(2)	1.97(2)	2.7723(15)	167.1(19)
O91	H91B	O90[2]	0.79(2)	2.04(2)	2.7919(15)	157(2)

[1]1/2-X,1-Y,1/2+Z; [2]-X,1-Y,2-Z

Table 7 Torsion Angles for 1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
K1	S1	O1	K1[1]	114.17(8)	C4[4]	N5	C4	C3	87.99(17)
K1	S1	O2	K1[2]	-127.85(10)	C4	N5	C6	C7[4]	171.25(14)
K1	S1	C3	C4	-125.91(9)	C4[4]	N5	C6	C7[4]	11.5(2)
N5	C4	C3	S1	160.85(10)	C4[4]	N5	C6	C7	-171.25(14)
O1	S1	O2	K1	9.10(6)	C4	N5	C6	C7	-11.5(2)
O1	S1	O2	K1[2]	-118.75(9)	C3	S1	O1	K1	107.31(6)
O1	S1	C3	C4	176.59(10)	C3	S1	O1	K1[1]	-138.52(8)
O90[3]	S1	O1	K1[1]	-23.40(10)	C3	S1	O2	K1[2]	124.18(9)
O90[3]	S1	O1	K1	-137.56(5)	C3	S1	O2	K1	-107.97(5)
O90[3]	S1	O2	K1	136.84(5)	C6	N5	C4	C3	-72.20(18)
O90[3]	S1	O2	K1[2]	8.99(11)	C6	C7	C8	C9	-1.6(2)
O90[3]	S1	C3	C4	57.18(12)	C8[4]	C9	C8	C7	0.2(3)
O2	S1	O1	K1	-9.69(6)	C8	C7	C6	N5	-174.48(15)
O2	S1	O1	K1[1]	104.48(8)	C8	C7	C6	C7[4]	2.9(3)
O2	S1	C3	C4	-62.45(12)					

[1]-1/2+X,+Y,3/2-Z; [2]1/2-X,1-Y,-1/2+Z; [3]-X,1-Y,1-Z; [4]+X,1/2-Y,+Z

Table 8 Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for 1.

Atom	*X*	*y*	*z*	U(eq)
H4A	954(19)	2979(7)	2783(18)	15(4)
H8	6690(20)	3400(8)	6230(20)	25(4)
H7	4260(20)	3396(8)	4945(18)	21(4)
H4B	2490(20)	3352(7)	3230(17)	17(4)
H9	7980(30)	2500	6840(30)	19(6)
H3A	1480(20)	3219(8)	5940(20)	28(5)
H3B	-200(20)	3058(8)	5186(18)	22(4)
H91A	2030(30)	4288(9)	11070(20)	32(5)
H91B	630(30)	4253(10)	11600(30)	39(6)

X-Ray Crystallographic Data for 2

Table 9 Crystal data and structure refinement for 2.

Identification code	2
Empirical formula	$C_{44}H_{72}BrK_9N_4O_{37}S_8$
Formula weight/g mol^{-1}	1937.34
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.9837(3)
b/Å	13.1145(2)
c/Å	32.7662(6)
α/°	90
β/°	102.8278(19)
γ/°	90
Volume/Å^3	7534.9(2)
Z	4
ρ_{calc}g/cm^3	1.708
μ/mm^{-1}	8.075
F(000)	3976.0
Crystal size/mm^3	0.342 × 0.265 × 0.101
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.04 to 132.686
Index ranges	$-18 \leq h \leq 20$, $-15 \leq k \leq 15$, $-38 \leq l \leq 36$
Reflections collected	103432
Independent reflections	13155 [R_{int} = 0.1612, R_{sigma} = 0.0670]
Data/restraints/parameters	13155/0/946
Goodness-of-fit on F^2	1.536
Final R indexes [I>=2σ (I)]	R_1 = 0.1480, wR_2 = 0.3662
Final R indexes [all data]	R_1 = 0.1636, wR_2 = 0.3843
Largest diff. peak/hole / e Å^{-3}	4.27/-1.37

Table 10 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
K3	9825.6(11)	1538.9(14)	3768.1(7)	32.6(5)
S90	4269.6(11)	8665.0(15)	3720.4(6)	20.3(5)
S69	6800.1(11)	238.3(14)	3750.5(6)	20.3(5)
K6	7318.9(11)	7388.6(14)	3701.6(6)	28.0(5)
S48	9342.0(11)	-1117.1(16)	3729.9(7)	23.9(5)
S84	5859.7(11)	3909.8(15)	4291.8(6)	20.2(4)
S42	10894.0(12)	3976.0(17)	4285.0(8)	29.9(5)
S27	11794.7(11)	114.8(17)	3668.6(6)	24.6(5)
S21	13412.5(12)	4899.8(17)	4289.0(7)	27.6(5)
S017	8424.9(12)	5273.9(16)	4102.5(7)	28.1(5)
O38	11777(3)	6166(4)	3116.1(19)	23.5(12)
O17	14238(3)	2854(4)	3055.2(19)	24.6(13)
O86	5316(3)	3075(4)	4272.9(18)	22.3(12)
O66	7872(4)	5817(5)	4286(2)	28.1(13)
O80	6744(3)	6002(5)	3074.1(18)	23.4(12)
O24	12909(3)	5785(4)	4279.2(19)	24.4(13)
O59	9267(3)	2863(5)	3098.9(19)	24.7(13)
O45	10339(4)	3189(5)	4289(2)	29.9(14)
O85	6622(3)	3544(5)	4286(2)	26.3(13)
N31	10729(4)	6539(5)	3570(2)	16.5(13)
N10	13193(4)	2454(5)	3513(2)	19.2(14)
O91	4138(3)	9625(5)	3498.3(19)	26.3(13)
O70	6641(3)	-720(4)	3521.2(19)	23.7(12)
C53	7971(5)	2758(6)	3133(3)	20.2(16)
C74	5448(5)	6113(6)	3113(3)	19.1(16)
N73	5719(4)	6407(5)	3540(2)	15.9(13)
O29	11161(4)	747(6)	3722(3)	42.8(18)
O71	6133(3)	923(5)	3699(2)	29.1(14)
O92	3597(3)	7999(5)	3652(2)	28.1(13)
C11	12945(5)	2803(6)	3095(3)	23.0(17)
O87	5874(4)	4593(5)	4645.8(17)	26.4(13)
C79	5989(5)	5862(6)	2875(3)	19.4(16)
N52	8242(4)	2474(5)	3563(2)	18.1(14)
O72	7138(4)	81(5)	4195.4(19)	27.9(13)
O65	9121(4)	5037(6)	4403(2)	39.8(17)
C36	10806(6)	5625(7)	2505(3)	29(2)

O30	11568(4)	-725(5)	3386(2)	33.7(15)
O22	14179(4)	5187(6)	4298(2)	41.4(18)
O50	9146(4)	-242(5)	3459(2)	35.4(16)
C32	10469(5)	6213(6)	3145(3)	18.7(16)
C33	9707(5)	6061(6)	2956(3)	24.2(18)
C13	11958(5)	3277(7)	2490(3)	28.2(19)
C37	11034(5)	5991(6)	2910(2)	18.7(16)
C57	8280(5)	3350(7)	2491(3)	26.8(19)
O93	4584(4)	8798(5)	4168(2)	35.0(15)
O49	8689(4)	-1696(5)	3772(3)	43.4(19)
C82	6072(4)	5573(7)	3812(3)	20.9(17)
C56	7523(6)	3424(7)	2305(3)	28.3(19)
C58	8514(5)	3001(6)	2896(3)	23.1(17)
C75	4671(5)	6020(6)	2921(3)	23.3(17)
C76	4444(5)	5731(6)	2505(3)	25.6(18)
C34	9498(5)	5723(6)	2538(3)	26.4(19)
C88	5169(5)	6979(6)	3730(3)	21.4(17)
C55	6976(5)	3164(6)	2525(3)	25.7(19)
O44	10973(4)	4605(6)	4674(2)	40.6(17)
C16	13496(5)	3038(6)	2860(3)	22.5(17)
C78	5734(6)	5524(7)	2462(3)	26.8(19)
C40	11066(4)	5708(6)	3849(3)	18.9(16)
C54	7206(5)	2854(6)	2943(3)	23.4(17)
C15	13267(5)	3420(6)	2453(3)	25.0(18)
O23	13376(4)	4177(6)	4624(2)	36.0(15)
C14	12505(6)	3540(7)	2270(3)	32(2)
C19	13555(5)	3265(7)	3798(3)	21.8(17)
C18	14814(5)	3071(7)	2832(3)	28.8(19)
C61	8579(5)	3330(7)	3829(3)	23.5(17)
C62	7998(5)	4119(6)	3906(3)	23.4(17)
O43	11630(5)	3652(7)	4242(3)	60(3)
C67	7698(5)	1914(6)	3758(3)	23.0(17)
C83	5531(5)	4676(6)	3840(3)	21.9(17)
C12	12177(5)	2944(6)	2897(3)	24.6(18)
C20	13041(5)	4197(7)	3829(3)	27.9(19)
C35	10050(6)	5502(7)	2322(3)	30(2)
C77	4989(5)	5459(6)	2278(3)	26.6(18)
C47	9944(5)	-1890(6)	3503(3)	20.8(17)
O28	12247(4)	-303(7)	4067(2)	45.9(19)
C89	4978(5)	8021(6)	3519(3)	20.1(16)

C60	9833(5)	3104(7)	2869(3)	28.6(19)
C41	10506(5)	4838(7)	3882(3)	24.6(18)
C81	7309(5)	5805(7)	2833(3)	25.0(18)
C46	10170(5)	-2869(6)	3748(2)	19.3(16)
C39	12353(5)	5920(7)	2900(3)	26.1(18)
C25	12633(5)	1863(7)	3687(3)	26.0(18)
C26	12428(5)	879(6)	3452(3)	24.3(17)
O64	8568(4)	5812(6)	3737(2)	39.1(16)
C68	7494(5)	884(6)	3545(2)	17.5(15)
O51	9810(5)	-803(7)	4138(3)	54(2)
K8	5179.5(11)	6295.9(15)	4957.6(6)	27.8(5)
K9	4739.6(10)	11499.2(14)	3713.5(6)	25.8(4)
K4	9799.1(14)	3777(2)	5037.7(8)	49.4(6)
K2	12247(5)	7558(10)	3858(10)	25(2)
K5	7542.0(11)	4766.5(16)	4967.1(6)	28.9(5)
K1	11172.7(15)	-85(2)	4577.0(7)	46.1(6)
K7	6527.0(12)	1546.3(15)	4659.8(6)	33.1(5)
Br1	8308.6(7)	2448.4(9)	5140.0(4)	35.1(4)
O102	11014(4)	2592(6)	5334(3)	47(2)
O104	3854(4)	7487(5)	4662(2)	32.3(15)
O105	6957(6)	8043(7)	4438(3)	62(2)
O100	11309(5)	22(8)	5398(3)	59(2)
O101	9966(7)	1243(7)	4621(4)	74(3)
O103	5699(5)	8220(8)	4862(3)	68(3)
O106	4998(6)	10764(7)	4503(3)	66(3)
O107	11918(7)	1892(9)	4776(4)	89(4)
O108	13168(10)	190(12)	4818(4)	135(7)
Br1A	8061(6)	2165(8)	5279(3)	35.1(4)
K2A	12259(19)	7490(30)	3765(14)	25(2)

Table 11 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K3	22.2(10)	16.8(10)	56.2(12)	-5.3(8)	3.1(8)	4.9(7)
S90	17(1)	13.2(9)	31.3(10)	-0.1(7)	6.9(8)	2.7(7)
S69	15.8(10)	11.8(9)	33.9(10)	-1.2(7)	6.7(8)	-0.2(7)
K6	22.7(10)	14.2(9)	47.0(11)	2.9(7)	7.5(8)	0.0(7)
S48	17(1)	18.5(10)	37.0(11)	-0.3(8)	8.0(8)	5.4(8)
S84	14.4(10)	15.4(10)	29.9(10)	1.9(7)	3.3(7)	1.5(7)
S42	15.5(10)	21.7(11)	51.3(13)	14.5(9)	4.9(9)	1.0(8)

S27	14.3(10)	28.7(11)	31.4(10)	0.5(8)	6.5(8)	-2.8(8)
S21	18.6(11)	22.0(11)	40.9(12)	-10.9(9)	3.7(8)	0.9(8)
S017	19.2(11)	15(1)	47.7(12)	-4.4(8)	2.0(9)	-1.6(8)
O38	16(3)	20(3)	37(3)	1(2)	11(2)	1(2)
O17	19(3)	19(3)	38(3)	-1(2)	9(2)	1(2)
O86	17(3)	15(3)	34(3)	1(2)	4(2)	-4(2)
O66	28(3)	14(3)	42(3)	-2(2)	9(3)	3(2)
O80	14(3)	26(3)	32(3)	0(2)	8(2)	5(2)
O24	14(3)	17(3)	41(3)	-5(2)	4(2)	3(2)
O59	15(3)	23(3)	37(3)	1(2)	9(2)	-1(2)
O45	23(3)	20(3)	46(4)	6(3)	6(3)	-8(3)
O85	10(3)	26(3)	45(3)	9(3)	9(2)	4(2)
N31	8(3)	18(3)	25(3)	1(3)	6(2)	-1(2)
N10	15(3)	12(3)	31(3)	-3(3)	6(3)	-1(3)
O91	23(3)	17(3)	41(3)	5(2)	11(2)	12(2)
O70	20(3)	11(3)	40(3)	-7(2)	6(2)	-5(2)
C53	22(4)	10(4)	28(4)	-3(3)	6(3)	-1(3)
C74	19(4)	8(4)	31(4)	5(3)	7(3)	3(3)
N73	11(3)	13(3)	25(3)	2(2)	6(2)	5(2)
O29	20(3)	44(4)	68(5)	-19(4)	19(3)	-4(3)
O71	17(3)	22(3)	49(4)	-1(3)	9(3)	5(2)
O92	15(3)	22(3)	49(4)	5(3)	11(3)	2(2)
C11	21(4)	17(4)	31(4)	-5(3)	5(3)	1(3)
O87	28(3)	28(3)	23(3)	-5(2)	5(2)	1(3)
C79	16(4)	13(4)	28(4)	1(3)	4(3)	1(3)
N52	11(3)	17(3)	26(3)	-3(3)	5(3)	-7(3)
O72	28(3)	21(3)	37(3)	4(2)	12(3)	-6(2)
O65	29(4)	35(4)	50(4)	-10(3)	-5(3)	3(3)
C36	42(6)	14(4)	37(5)	2(3)	21(4)	3(4)
O30	32(4)	22(3)	52(4)	-4(3)	19(3)	-8(3)
O22	20(3)	39(4)	64(5)	-21(3)	6(3)	6(3)
O50	30(4)	14(3)	67(4)	9(3)	19(3)	10(3)
C32	20(4)	10(4)	28(4)	2(3)	10(3)	5(3)
C33	16(4)	19(4)	38(5)	0(3)	7(3)	3(3)
C13	21(4)	21(4)	39(5)	-7(4)	-2(4)	4(4)
C37	18(4)	12(4)	28(4)	4(3)	8(3)	2(3)
C57	31(5)	18(4)	35(5)	0(3)	15(4)	0(4)
O93	36(4)	30(4)	39(4)	-6(3)	8(3)	1(3)
O49	28(4)	25(4)	86(6)	15(3)	31(4)	5(3)
C82	7(4)	27(5)	29(4)	0(3)	4(3)	2(3)

C56	40(5)	16(4)	28(4)	-2(3)	4(4)	-7(4)
C58	21(4)	11(4)	40(5)	-5(3)	14(3)	-6(3)
C75	21(4)	10(4)	40(5)	4(3)	9(3)	-4(3)
C76	24(5)	12(4)	37(5)	6(3)	0(3)	-6(3)
C34	23(4)	15(4)	36(5)	2(3)	-4(4)	-4(3)
C88	25(4)	11(4)	31(4)	-2(3)	11(3)	-1(3)
C55	19(4)	15(4)	38(5)	-3(3)	-5(3)	7(3)
O44	44(4)	43(4)	31(3)	1(3)	2(3)	-13(3)
C16	26(5)	11(4)	31(4)	-2(3)	6(3)	-3(3)
C78	35(5)	19(4)	28(4)	1(3)	11(4)	-1(4)
C40	10(4)	13(4)	34(4)	0(3)	5(3)	0(3)
C54	20(4)	15(4)	35(4)	-5(3)	4(3)	-1(3)
C15	33(5)	15(4)	29(4)	2(3)	11(4)	0(3)
O23	38(4)	38(4)	30(3)	0(3)	3(3)	10(3)
C14	50(6)	12(4)	30(5)	-6(3)	-2(4)	0(4)
C19	15(4)	23(4)	28(4)	-5(3)	4(3)	1(3)
C18	23(5)	22(5)	46(5)	-10(4)	16(4)	-2(4)
C61	17(4)	20(4)	34(4)	-3(3)	7(3)	1(3)
C62	22(4)	12(4)	38(5)	-6(3)	9(3)	-5(3)
O43	30(4)	44(5)	109(7)	39(5)	21(4)	14(3)
C67	30(5)	8(4)	32(4)	-3(3)	9(3)	-7(3)
C83	22(4)	12(4)	29(4)	2(3)	1(3)	1(3)
C12	21(4)	16(4)	36(4)	-1(3)	6(3)	1(3)
C20	30(5)	28(5)	23(4)	-3(3)	1(3)	14(4)
C35	39(6)	17(4)	30(4)	-2(3)	1(4)	0(4)
C77	35(5)	10(4)	32(4)	1(3)	2(4)	-2(3)
C47	14(4)	10(4)	39(4)	-2(3)	8(3)	2(3)
O28	39(4)	59(5)	37(4)	9(3)	3(3)	-6(4)
C89	16(4)	8(4)	38(4)	1(3)	10(3)	5(3)
C60	16(4)	28(5)	47(5)	-8(4)	20(4)	-5(4)
C41	16(4)	18(4)	38(5)	6(3)	1(3)	-4(3)
C81	18(4)	17(4)	44(5)	5(3)	15(4)	2(3)
C46	22(4)	9(4)	28(4)	2(3)	7(3)	-1(3)
C39	21(4)	21(4)	40(5)	7(4)	16(4)	0(3)
C25	30(5)	16(4)	32(4)	-4(3)	8(4)	3(3)
C26	24(4)	14(4)	36(4)	1(3)	10(3)	-1(3)
O64	33(4)	39(4)	49(4)	8(3)	18(3)	-2(3)
C68	16(4)	6(4)	31(4)	1(3)	6(3)	-4(3)
O51	51(5)	51(5)	57(5)	-24(4)	4(4)	22(4)
K8	23.7(10)	25.7(10)	33.2(10)	1.2(7)	4.8(7)	6.0(7)

K9	18.8(9)	17.4(9)	40(1)	-1.9(7)	4.0(7)	3.2(7)
K4	34.4(13)	66.0(17)	47.2(13)	4.9(11)	7.7(10)	3.7(11)
K2	16.5(10)	16.5(17)	43(7)	0(3)	8(2)	-0.8(10)
K5	22.2(10)	28.7(10)	34.1(10)	-2.2(7)	3.0(7)	-0.3(7)
K1	47.2(14)	50.0(14)	42.2(12)	0(1)	12.1(10)	2.9(11)
K7	39.3(12)	24.2(10)	34.7(10)	-0.3(7)	5.5(8)	4.5(8)
Br1	31.6(7)	22.3(6)	48.0(7)	0.1(5)	1.2(5)	2.7(5)
O102	32(4)	39(4)	66(5)	-32(4)	3(3)	4(3)
O104	44(4)	19(3)	33(3)	-3(2)	7(3)	-13(3)
O105	76(6)	43(5)	81(6)	25(4)	46(5)	21(4)
O100	56(5)	69(6)	48(5)	-8(4)	5(4)	-3(4)
O101	85(7)	42(5)	96(7)	-1(5)	26(6)	-1(5)
O103	43(5)	61(6)	87(6)	34(5)	-11(4)	-11(4)
O106	102(8)	40(5)	51(5)	-3(4)	6(5)	-27(5)
O107	68(7)	73(8)	113(9)	13(7)	-9(6)	0(6)
O108	192(16)	119(12)	59(7)	37(7)	-48(8)	-82(12)
Br1A	31.6(7)	22.3(6)	48.0(7)	0.1(5)	1.2(5)	2.7(5)
K2A	16.5(10)	16.5(17)	43(7)	0(3)	8(2)	-0.8(10)

Table 12 Bond Lengths for 2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
K3	O59	2.802(6)	O71	$K9^{4}$	2.628(6)
K3	O45	2.783(7)	O71	K7	3.178(7)
K3	O29	2.651(7)	O92	$K2^{6}$	2.723(18)
K3	N52	3.036(7)	O92	$K2A^{6}$	2.60(4)
K3	O50	2.725(7)	C11	C16	1.416(13)
K3	O101	2.777(12)	C11	C12	1.402(13)
S90	O91	1.447(6)	O87	K8	2.856(6)
S90	O92	1.469(6)	O87	$K8^{2}$	2.781(6)
S90	O93	1.460(7)	O87	K5	2.959(6)
S90	C89	1.773(8)	C79	C78	1.402(12)
S69	O70	1.460(6)	N52	C61	1.468(11)
S69	O71	1.478(6)	N52	C67	1.477(10)
S69	O72	1.464(7)	O72	K7	2.821(7)
S69	C68	1.762(8)	O65	K4	2.723(8)
S69	K7	3.565(3)	O65	$K4^{3}$	2.823(7)
K6	O66	2.838(6)	C36	C37	1.384(13)
K6	O80	2.767(6)	C36	C35	1.367(15)
K6	$O70^{1}$	2.769(6)	O30	$K2^{4}$	2.849(13)
K6	$O49^{1}$	2.704(7)	O30	$K2A^{4}$	2.81(3)

K6	O64	3.036(8)
K6	O105	2.770(9)
S48	O50	1.445(7)
S48	O49	1.430(7)
S48	C47	1.763(8)
S48	O51	1.473(8)
S84	O86	1.460(6)
S84	O85	1.457(6)
S84	O87	1.461(6)
S84	C83	1.778(8)
S84	K8[2]	3.414(3)
S84	K5	3.513(3)
S84	K7	3.444(3)
S42	O45	1.438(6)
S42	O44	1.497(8)
S42	O43	1.428(8)
S42	C41	1.760(9)
S42	K4	3.491(3)
S42	K5[3]	3.684(3)
S27	O29	1.451(7)
S27	O30	1.438(7)
S27	O28	1.481(8)
S27	C26	1.778(9)
S27	K2[4]	3.473(11)
S27	K1	3.414(3)
S27	K2A[4]	3.54(3)
S21	O24	1.468(6)
S21	O22	1.423(8)
S21	O23	1.464(7)
S21	C20	1.768(9)
S21	K8[3]	3.491(3)
S21	K5[3]	3.307(3)
S017	O66	1.457(7)
S017	O65	1.444(7)
S017	C62	1.755(8)
S017	O64	1.461(7)
S017	K5	3.604(3)
O38	C37	1.377(10)
O38	C39	1.416(10)
O38	K2	3.01(3)
O22	K8[3]	3.132(9)
O22	K8[7]	2.880(7)
C32	C33	1.387(12)
C32	C37	1.434(11)
C33	C34	1.408(13)
C13	C14	1.386(15)
C13	C12	1.373(13)
C57	C56	1.366(14)
C57	C58	1.379(13)
O49	K6[4]	2.705(7)
C82	C83	1.541(11)
C56	C55	1.386(14)
C75	C76	1.385(13)
C76	C77	1.402(14)
C34	C35	1.373(14)
C88	C89	1.535(11)
C55	C54	1.400(13)
O44	K4[3]	2.812(8)
O44	K4	2.858(8)
O44	K5[3]	2.794(7)
C16	C15	1.397(12)
C78	C77	1.345(14)
C40	C41	1.543(11)
C40	K2	3.220(12)
C40	K2A	3.23(3)
C15	C14	1.376(14)
O23	K8[3]	2.726(7)
O23	K5[3]	2.723(7)
C19	C20	1.549(12)
C19	K9[5]	3.200(8)
C61	C62	1.531(12)
O43	K5[3]	3.395(12)
C67	C68	1.527(11)
C47	C46	1.522(11)
O28	K2[4]	2.89(2)
O28	K1	2.836(8)
O28	K2A[4]	3.06(4)
C46	N31[4]	1.488(10)
C39	K2A	3.54(5)
C25	C26	1.504(12)

O38	K2A	2.73(4)	O51	K1	2.719(9)
O17	C16	1.367(11)	K8	O87[2]	2.781(6)
O17	C18	1.423(11)	K8	O22[6]	2.880(7)
O17	K9[5]	2.786(6)	K8	O23[3]	2.726(7)
O86	K8[2]	2.971(6)	K8	O104	2.835(7)
O86	K9[4]	2.804(6)	K8	O103	2.734(9)
O86	K7	3.024(6)	K9	O17[8]	2.786(6)
O66	K5	2.797(7)	K9	O71[1]	2.628(6)
O80	C79	1.382(10)	K9	O106	2.704(9)
O80	C81	1.444(10)	K4	O65[3]	2.823(7)
O24	K2	2.829(12)	K4	O44[3]	2.812(8)
O24	K5[3]	2.858(6)	K4	O102	2.681(8)
O24	K2A	2.89(4)	K2	O92[7]	2.723(18)
O59	C58	1.382(11)	K2	O30[1]	2.849(13)
O59	C60	1.429(10)	K2	O28[1]	2.89(2)
O45	K4	2.936(7)	K5	O24[3]	2.858(6)
O85	K5	2.941(7)	K5	O44[3]	2.794(7)
O85	K7	2.914(6)	K5	O23[3]	2.723(7)
N31	C32	1.433(11)	K1	O100	2.650(8)
N31	C40	1.465(10)	K1	O101	2.811(11)
N31	C46[1]	1.488(10)	K1	O107	2.925(13)
N31	K2	2.998(13)	K7	O104[2]	2.773(7)
N31	K2A	2.96(3)	K7	O106[4]	2.873(11)
N10	C11	1.418(11)	K7	O108[9]	2.828(13)
N10	C19	1.470(10)	Br1	K2[3]	3.64(3)
N10	C25	1.482(11)	Br1	K1[9]	3.309(3)
N10	K9[5]	2.987(7)	O104	K7[2]	2.773(7)
O91	K9	2.715(7)	O106	K7[1]	2.873(11)
O70	K6[4]	2.769(6)	O108	K7[9]	2.828(13)
C53	N52	1.433(11)	Br1A	K1[9]	3.044(9)
C53	C58	1.412(12)	Br1A	K2A[3]	3.34(5)
C53	C54	1.385(12)	K2A	S27[1]	3.54(3)
C74	N73	1.429(11)	K2A	O92[7]	2.60(4)
C74	C79	1.414(12)	K2A	O30[1]	2.81(3)
C74	C75	1.406(12)	K2A	O28[1]	3.06(4)
N73	C82	1.463(10)	K2A	K1[1]	4.83(4)
N73	C88	1.485(10)	K2A	Br1A[3]	3.34(5)
O29	K1	3.002(9)			

[1]+X,1+Y,+Z; [2]1-X,1-Y,1-Z; [3]2-X,1-Y,1-Z; [4]+X,-1+Y,+Z; [5]1+X,-1+Y,+Z; [6]-1+X,+Y,+Z; [7]1+X,+Y,+Z; [8]-1+X,1+Y,+Z; [9]2-X,-Y,1-Z

Table 13 Bond Angles for 2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O59	K3	N52	54.60(17)	C33	C32	C37	118.6(8)
O45	K3	O59	90.60(19)	C32	C33	C34	120.2(8)
O45	K3	N52	89.38(19)	C12	C13	C14	120.0(8)
O29	K3	O59	111.7(2)	O38	C37	C36	125.3(8)
O29	K3	O45	99.1(2)	O38	C37	C32	115.4(7)
O29	K3	N52	164.3(2)	C36	C37	C32	119.4(8)
O29	K3	O50	88.9(2)	C56	C57	C58	120.9(8)
O29	K3	O101	97.0(3)	S48	O49	K6[4]	168.3(5)
O50	K3	O59	100.8(2)	N73	C82	K6	67.2(4)
O50	K3	O45	162.7(2)	N73	C82	C83	114.4(6)
O50	K3	N52	86.71(19)	C83	C82	K6	175.0(6)
O50	K3	O101	100.8(3)	C57	C56	C55	120.2(8)
O101	K3	O59	144.2(3)	O59	C58	C53	115.4(8)
O101	K3	O45	63.1(3)	C57	C58	O59	124.3(8)
O101	K3	N52	98.7(3)	C57	C58	C53	120.3(8)
O91	S90	O92	113.8(4)	C76	C75	C74	120.7(8)
O91	S90	O93	112.6(4)	C75	C76	C77	120.3(8)
O91	S90	C89	106.2(4)	C35	C34	C33	120.0(8)
O92	S90	C89	107.1(4)	N73	C88	C89	111.4(6)
O93	S90	O92	110.3(4)	C56	C55	C54	119.4(8)
O93	S90	C89	106.3(4)	S42	O44	K4	101.9(3)
O70	S69	O71	113.7(4)	S42	O44	K4[3]	137.8(4)
O70	S69	O72	112.4(4)	S42	O44	K5[3]	114.9(4)
O70	S69	C68	107.0(4)	K4[3]	O44	K4	71.4(2)
O70	S69	K7	142.8(3)	K5[3]	O44	K4[3]	97.6(2)
O71	S69	C68	106.9(4)	K5[3]	O44	K4	131.4(3)
O71	S69	K7	62.9(3)	O17	C16	C11	115.8(7)
O72	S69	O71	110.3(4)	O17	C16	C15	124.0(8)
O72	S69	C68	106.0(4)	C15	C16	C11	120.2(8)
O72	S69	K7	48.7(3)	C77	C78	C79	122.2(8)
C68	S69	K7	109.2(3)	N31	C40	C41	114.0(6)
O66	K6	O64	48.26(18)	N31	C40	K2	68.1(5)
O80	K6	O66	92.38(18)	N31	C40	K2A	66.4(7)
O80	K6	O70[1]	110.83(18)	C41	C40	K2	175.4(8)
O80	K6	O64	74.47(19)	C41	C40	K2A	178.6(10)
O80	K6	O105	136.8(3)	C53	C54	C55	121.0(8)
O70[1]	K6	O66	150.01(19)	C14	C15	C16	120.7(9)
O70[1]	K6	O64	154.83(19)	S21	O23	K8[3]	109.1(4)

O70[1]	K6	O105	74.4(2)	S21	O23	K5[3]	100.0(3)
O49[1]	K6	O66	95.1(2)	K5[3]	O23	K8[3]	118.9(2)
O49[1]	K6	O80	122.6(2)	C15	C14	C13	119.9(9)
O49[1]	K6	O70[1]	88.29(19)	N10	C19	C20	115.2(7)
O49[1]	K6	O64	69.3(2)	N10	C19	K9[5]	68.3(4)
O49[1]	K6	O105	100.0(3)	C20	C19	K9[5]	174.2(6)
O105	K6	O66	75.7(2)	N52	C61	K3	67.3(4)
O105	K6	O64	119.5(2)	N52	C61	C62	114.0(7)
O50	S48	K3	43.5(3)	C62	C61	K3	173.7(6)
O50	S48	C47	106.6(4)	C61	C62	S017	112.6(6)
O50	S48	O51	110.4(5)	S42	O43	K5[3]	90.1(5)
O49	S48	K3	135.2(3)	N52	C67	C68	110.9(7)
O49	S48	O50	112.8(4)	C82	C83	S84	112.6(6)
O49	S48	C47	109.3(4)	C13	C12	C11	122.1(8)
O49	S48	O51	112.1(5)	C19	C20	S21	110.4(6)
C47	S48	K3	114.0(3)	C36	C35	C34	120.8(8)
O51	S48	K3	67.1(4)	C78	C77	C76	119.3(8)
O51	S48	C47	105.3(4)	C46	C47	S48	112.3(6)
O86	S84	O87	112.8(4)	S27	O28	K2[4]	100.3(6)
O86	S84	C83	107.0(4)	S27	O28	K1	99.7(4)
O86	S84	K8[2]	60.2(2)	S27	O28	K2A[4]	96.2(8)
O86	S84	K5	137.9(2)	K1	O28	K2[4]	105.9(5)
O86	S84	K7	61.2(2)	K1	O28	K2A[4]	109.9(8)
O85	S84	O86	112.1(4)	C88	C89	S90	111.4(6)
O85	S84	O87	111.2(4)	C40	C41	S42	111.8(6)
O85	S84	C83	108.3(4)	O80	C81	K6	47.8(4)
O85	S84	K8[2]	130.6(3)	N31[4]	C46	C47	110.9(6)
O85	S84	K5	55.4(3)	O38	C39	K2A	45.3(7)
O85	S84	K7	56.8(2)	N10	C25	C26	111.3(7)
O87	S84	C83	105.0(4)	C25	C26	S27	112.7(6)
O87	S84	K8[2]	52.6(3)	S017	O64	K6	95.6(3)
O87	S84	K5	56.1(3)	C67	C68	S69	111.6(6)
O87	S84	K7	109.3(3)	S48	O51	K3	88.6(4)
C83	S84	K8[2]	120.7(3)	S48	O51	K1	147.5(5)
C83	S84	K5	115.1(3)	K1	O51	K3	78.0(2)
C83	S84	K7	145.7(3)	O87[2]	K8	O87	103.71(16)
K8[2]	S84	K5	95.98(7)	O87[2]	K8	O22[6]	76.2(2)
K8[2]	S84	K7	83.15(6)	O87	K8	O22[6]	65.60(18)
K7	S84	K5	83.27(6)	O87[2]	K8	O104	77.39(19)
O45	S42	O44	108.8(4)	O23[3]	K8	O87[2]	110.0(2)

O45	S42	C41	107.9(4)	O23^{3}	K8	O87	63.76(19)
O45	S42	K4	55.9(3)	O23^{3}	K8	O22^{6}	129.0(2)
O45	S42	K5^{3}	138.1(3)	O23^{3}	K8	O104	158.8(2)
O44	S42	C41	103.4(4)	O23^{3}	K8	O103	87.5(3)
O44	S42	K4	53.2(3)	O104	K8	O87	135.24(18)
O44	S42	K5^{3}	43.4(3)	O104	K8	O22^{6}	71.57(19)
O43	S42	O45	116.6(5)	O103	K8	O87^{2}	136.6(3)
O43	S42	O44	109.5(6)	O103	K8	O87	119.5(3)
O43	S42	C41	109.8(5)	O103	K8	O22^{6}	123.5(3)
O43	S42	K4	136.9(4)	O103	K8	O104	74.7(2)
O43	S42	K5^{3}	67.1(5)	O91	K9	O17^{8}	109.54(19)
C41	S42	K4	112.7(3)	O71^{1}	K9	O17^{8}	108.4(2)
C41	S42	K5^{3}	109.2(3)	O71^{1}	K9	O91	93.52(19)
K4	S42	K5^{3}	91.75(8)	O71^{1}	K9	O106	87.3(3)
O29	S27	O28	113.5(5)	O106	K9	O17^{8}	157.8(3)
O29	S27	C26	108.4(4)	O106	K9	O91	84.2(2)
O29	S27	K2^{4}	133.5(5)	O65^{3}	K4	O45	112.3(2)
O29	S27	K1	61.4(3)	O65	K4	O45	72.3(2)
O29	S27	K2A^{4}	136.1(7)	O65	K4	O65^{3}	106.8(2)
O30	S27	O29	113.4(4)	O65	K4	O44^{3}	68.2(2)
O30	S27	O28	107.8(5)	O65^{3}	K4	O44	66.2(2)
O30	S27	C26	106.9(4)	O65	K4	O44	72.4(2)
O30	S27	K2^{4}	53.0(6)	O44^{3}	K4	O45	139.4(2)
O30	S27	K1	113.7(3)	O44	K4	O45	48.63(19)
O30	S27	K2A^{4}	48.8(8)	O44^{3}	K4	O65^{3}	71.7(2)
O28	S27	C26	106.5(4)	O44^{3}	K4	O44	108.6(2)
O28	S27	K2^{4}	54.9(6)	O102	K4	O45	75.9(2)
O28	S27	K1	55.0(3)	O102	K4	O65^{3}	72.3(2)
O28	S27	K2A^{4}	59.2(8)	O102	K4	O65	145.0(3)
C26	S27	K2^{4}	118.0(4)	O102	K4	O44^{3}	137.6(2)
C26	S27	K1	138.9(3)	O102	K4	O44	75.7(3)
C26	S27	K2A^{4}	115.1(7)	O24	K2	O38	84.7(5)
K1	S27	K2^{4}	83.1(5)	O24	K2	N31	92.4(3)
K1	S27	K2A^{4}	87.9(7)	O24	K2	O30^{1}	176.4(13)
O24	S21	C20	106.2(4)	O24	K2	O28^{1}	134.8(11)
O24	S21	K8^{3}	135.9(3)	N31	K2	O38	53.3(4)
O24	S21	K5^{3}	59.5(3)	O92^{7}	K2	O38	92.0(10)
O22	S21	O24	112.4(4)	O92^{7}	K2	O24	89.6(4)
O22	S21	O23	111.1(5)	O92^{7}	K2	N31	144.7(13)
O22	S21	C20	109.7(4)	O92^{7}	K2	O30^{1}	89.8(5)

O22	S21	K8[3]	63.7(3)	O92[7]	K2	O28[1]	84.2(3)
O22	S21	K5[3]	127.5(3)	O30[1]	K2	O38	91.8(8)
O23	S21	O24	113.4(4)	O30[1]	K2	N31	86.0(4)
O23	S21	C20	103.4(4)	O30[1]	K2	O28[1]	48.6(3)
O23	S21	K8[3]	47.5(3)	O28[1]	K2	O38	140.1(8)
O23	S21	K5[3]	54.2(3)	O28[1]	K2	N31	117.4(5)
C20	S21	K8[3]	116.5(3)	O66	K5	O24[3]	164.90(18)
C20	S21	K5[3]	122.6(3)	O66	K5	O85	81.15(18)
K5[3]	S21	K8[3]	87.25(7)	O66	K5	O87	97.59(18)
K6	S017	K5	97.39(7)	O24[3]	K5	O85	107.35(18)
O66	S017	K6	51.9(3)	O24[3]	K5	O87	80.11(17)
O66	S017	C62	106.9(4)	O85	K5	O87	48.16(16)
O66	S017	O64	111.2(4)	O44[3]	K5	O66	80.7(2)
O66	S017	K5	46.0(3)	O44[3]	K5	O24[3]	97.99(19)
O65	S017	K6	139.6(3)	O44[3]	K5	O85	143.6(2)
O65	S017	O66	113.0(4)	O44[3]	K5	O87	166.3(2)
O65	S017	C62	107.9(4)	O23[3]	K5	O66	113.6(2)
O65	S017	O64	112.3(5)	O23[3]	K5	O24[3]	52.03(18)
O65	S017	K5	83.7(3)	O23[3]	K5	O85	110.5(2)
C62	S017	K6	112.4(3)	O23[3]	K5	O87	62.41(19)
C62	S017	K5	84.1(3)	O23[3]	K5	O44[3]	105.7(2)
O64	S017	K6	59.8(3)	O28	K1	O29	49.6(2)
O64	S017	C62	104.9(4)	O28	K1	O107	83.2(4)
O64	S017	K5	157.2(3)	O51	K1	O29	79.3(2)
C37	O38	C39	117.0(7)	O51	K1	O28	107.8(2)
C37	O38	K2	124.5(5)	O51	K1	O101	68.1(3)
C37	O38	K2A	126.4(9)	O51	K1	O107	137.7(3)
C39	O38	K2	115.9(6)	O100	K1	O29	155.2(3)
C39	O38	K2A	113.2(9)	O100	K1	O28	133.0(3)
C16	O17	C18	118.1(7)	O100	K1	O51	115.1(3)
C16	O17	K9[5]	126.1(5)	O100	K1	O101	79.2(3)
C18	O17	K9[5]	112.2(5)	O100	K1	O107	78.0(4)
S84	O86	K8[2]	94.6(3)	O101	K1	O29	88.7(3)
S84	O86	K9[4]	136.7(3)	O101	K1	O28	136.7(3)
S84	O86	K7	93.8(3)	O101	K1	O107	76.1(3)
K8[2]	O86	K7	98.75(17)	O107	K1	O29	78.1(3)
K9[4]	O86	K8[2]	128.5(2)	O85	K7	O86	48.06(16)
K9[4]	O86	K7	84.99(16)	O72	K7	O86	123.79(18)
S017	O66	K6	104.2(3)	O72	K7	O85	108.64(18)
S017	O66	K5	111.9(3)	O72	K7	O106[4]	97.6(2)

K5	O66	K6	142.3(2)	O72	K7	O108[9]	74.4(4)
C79	O80	K6	127.2(5)	O104[2]	K7	O86	75.50(19)
C79	O80	C81	117.1(6)	O104[2]	K7	O85	88.49(18)
C81	O80	K6	109.4(5)	O104[2]	K7	O72	159.8(2)
S21	O24	K2	148.4(7)	O104[2]	K7	O106[4]	84.8(2)
S21	O24	K5[3]	94.2(3)	O104[2]	K7	O108[9]	86.2(4)
S21	O24	K2A	142.5(10)	O106[4]	K7	O86	65.8(2)
K2	O24	K5[3]	117.4(7)	O106[4]	K7	O85	112.9(2)
K5[3]	O24	K2A	123.0(9)	O108[9]	K7	O86	144.3(4)
C58	O59	K3	126.9(5)	O108[9]	K7	O85	163.1(3)
C58	O59	C60	117.0(7)	O108[9]	K7	O106[4]	82.5(4)
C60	O59	K3	112.0(5)	K4	Br1	K2[3]	119.2(2)
K3	O45	K4	126.2(2)	K4	Br1	K5	79.30(7)
S42	O45	K3	133.6(4)	K4	Br1	K1[9]	109.92(7)
S42	O45	K4	100.2(3)	K4	Br1	K7	146.49(7)
S84	O85	K5	100.5(3)	K5	Br1	K2[3]	88.26(18)
S84	O85	K7	98.4(3)	K5	Br1	K7	85.88(5)
K7	O85	K5	104.3(2)	K1[9]	Br1	K2[3]	82.04(19)
C32	N31	C40	112.7(6)	K1[9]	Br1	K5	169.03(8)
C32	N31	C46[1]	115.8(6)	K1[9]	Br1	K7	88.97(6)
C32	N31	K2	121.1(8)	K7	Br1	K2[3]	89.9(2)
C32	N31	K2A	115.0(10)	K7[2]	O104	K8	108.5(2)
C40	N31	C46[1]	111.4(6)	K3	O101	K1	86.2(3)
C40	N31	K2	85.0(5)	K9	O106	K7[1]	89.8(3)
C40	N31	K2A	86.7(8)	K1[9]	Br1A	K5	165.1(5)
C46[1]	N31	K2	106.9(7)	K1[9]	Br1A	K7	99.8(3)
C46[1]	N31	K2A	111.8(9)	K1[9]	Br1A	K2A[3]	98.2(7)
C11	N10	C19	112.4(7)	K7	Br1A	K5	85.8(2)
C11	N10	C25	116.4(7)	K7	Br1A	K2A[3]	109.3(7)
C11	N10	K9[5]	115.2(5)	K2A[3]	Br1A	K5	92.9(6)
C19	N10	C25	112.1(6)	S27[1]	K2A	C39	123.1(12)
C19	N10	K9[5]	84.5(4)	S27[1]	K2A	K1[1]	45.0(5)
C25	N10	K9[5]	112.0(5)	O38	K2A	S27[1]	121.3(13)
S90	O91	K9	130.2(4)	O38	K2A	O24	88.8(10)
S69	O70	K6[4]	129.4(3)	O38	K2A	N31	56.3(7)
C58	C53	N52	118.3(7)	O38	K2A	O30[1]	98.8(13)
C54	C53	N52	123.5(8)	O38	K2A	C40	60.2(7)
C54	C53	C58	118.1(8)	O38	K2A	O28[1]	145.9(14)
C79	C74	N73	118.4(7)	O38	K2A	C39	21.6(4)
C75	C74	N73	123.5(7)	O38	K2A	K1[1]	138.6(10)

C75	C74	C79	118.0(8)	O38	K2A	Br1A^{3}	136.5(12)
C74	N73	K6	112.5(5)	O24	K2A	S27^{1}	149.6(16)
C74	N73	C82	113.7(6)	O24	K2A	N31	92.1(10)
C74	N73	C88	115.7(6)	O24	K2A	C40	65.1(7)
C82	N73	K6	86.9(4)	O24	K2A	O28^{1}	125.1(15)
C82	N73	C88	111.2(6)	O24	K2A	C39	86.0(10)
C88	N73	K6	113.6(5)	O24	K2A	K1^{1}	110.5(12)
K3	O29	K1	84.7(2)	O24	K2A	Br1A^{3}	71.9(10)
S27	O29	K3	167.5(5)	N31	K2A	S27^{1}	101.6(9)
S27	O29	K1	93.5(4)	N31	K2A	C40	27.0(3)
S69	O71	K9^{4}	157.8(4)	N31	K2A	O28^{1}	113.3(12)
S69	O71	K7	92.6(3)	N31	K2A	C39	77.8(9)
K9^{4}	O71	K7	84.92(18)	N31	K2A	K1^{1}	85.8(9)
S90	O92	K2^{6}	146.9(7)	N31	K2A	Br1A^{3}	85.1(10)
S90	O92	K2A^{6}	152.5(10)	O92^{7}	K2A	S27^{1}	86.9(9)
C16	C11	N10	119.1(8)	O92^{7}	K2A	O38	101.2(15)
C12	C11	N10	123.8(8)	O92^{7}	K2A	O24	90.8(10)
C12	C11	C16	117.1(8)	O92^{7}	K2A	N31	157.2(19)
S84	O87	K8	146.2(4)	O92^{7}	K2A	O30^{1}	93.2(11)
S84	O87	K8^{2}	102.7(3)	O92^{7}	K2A	C40	148.3(14)
S84	O87	K5	99.7(3)	O92^{7}	K2A	O28^{1}	82.9(10)
K8^{2}	O87	K8	76.29(16)	O92^{7}	K2A	C39	79.9(11)
K8^{2}	O87	K5	127.5(2)	O92^{7}	K2A	K1^{1}	114.2(11)
K8	O87	K5	107.6(2)	O92^{7}	K2A	Br1A^{3}	117.2(14)
O80	C79	C74	115.7(7)	O30^{1}	K2A	S27^{1}	22.7(3)
O80	C79	C78	125.0(7)	O30^{1}	K2A	O24	170.6(19)
C78	C79	C74	119.3(8)	O30^{1}	K2A	N31	87.5(10)
C53	N52	K3	114.8(5)	O30^{1}	K2A	C40	113.8(11)
C53	N52	C61	112.9(6)	O30^{1}	K2A	O28^{1}	47.2(6)
C53	N52	C67	116.2(6)	O30^{1}	K2A	C39	103.0(13)
C61	N52	K3	86.2(4)	O30^{1}	K2A	K1^{1}	60.1(8)
C61	N52	C67	110.5(6)	O30^{1}	K2A	Br1A^{3}	98.7(12)
C67	N52	K3	112.4(5)	C40	K2A	S27^{1}	124.4(11)
S69	O72	K7	108.4(3)	C40	K2A	C39	78.3(9)
S017	O65	K4^{3}	133.8(4)	C40	K2A	K1^{1}	94.2(9)
S017	O65	K4	145.5(5)	C40	K2A	Br1A^{3}	76.2(9)
K4	O65	K4^{3}	73.2(2)	O28^{1}	K2A	S27^{1}	24.6(3)
C35	C36	C37	121.0(8)	O28^{1}	K2A	C40	127.3(13)
S27	O30	K2^{4}	103.2(7)	O28^{1}	K2A	C39	144.5(13)
S27	O30	K2A^{4}	108.5(10)	O28^{1}	K2A	K1^{1}	33.5(5)

S21	O22	K8[7]	126.2(4)	O28[1]	K2A	Br1A[3]	63.5(9)
S21	O22	K8[3]	92.3(4)	C39	K2A	K1[1]	157.2(10)
K8[7]	O22	K8[3]	70.66(18)	Br1A[3]	K2A	S27[1]	82.3(9)
S48	O50	K3	115.1(4)	Br1A[3]	K2A	C39	151.6(11)
N31	C32	C37	117.8(7)	Br1A[3]	K2A	K1[1]	38.6(5)
C33	C32	N31	123.5(7)				

[1]+X,1+Y,+Z; [2]1-X,1-Y,1-Z; [3]2-X,1-Y,1-Z; [4]+X,-1+Y,+Z; [5]1+X,-1+Y,+Z; [6]-1+X,+Y,+Z; [7]1+X,+Y,+Z; [8]-1+X,1+Y,+Z; [9]2-X,-Y,1-Z

Table 14 Hydrogen Bonds for 2.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C57	H57	O30[1]	0.95	2.51	3.186(11)	128.1
C62	H62A	O85	0.99	2.21	3.101(10)	149.6
C83	H83B	O22[2]	0.99	2.36	3.200(11)	141.7
O102	H10A	O49[3]	0.87	2.24	3.089(12)	163.1
O102	H10B	O66[4]	0.87	2.24	2.967(10)	141.3
O100	H10E	O101[3]	0.88	2.00	2.821(15)	153.4
O103	H10G	O106[5]	0.93	2.14	2.972(16)	148.3
O103	H10H	O93	0.93	1.89	2.782(11)	158.4
O107	H10J	O102	0.97	2.19	2.857(17)	125.2
O107	H10J	O105[4]	0.97	2.25	2.904(16)	123.8
O108	H10K	O107	1.01	2.45	3.15(2)	125.4
O108	H10L	O28	1.01	1.79	2.722(13)	151.5

[1]2-X,1/2+Y,1/2-Z; [2]-1+X,+Y,+Z; [3]2-X,-Y,1-Z; [4]2-X,1-Y,1-Z; [5]1-X,2-Y,1-Z

Table 15 Torsion Angles for 2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
K3	S48	O49	K6[1]	69(3)	O23	S21	O24	K2	-171.3(9)
K3	S48	C47	C46	136.5(5)	O23	S21	O24	K5[2]	5.7(4)
K3	S48	O51	K1	-64.9(9)	O23	S21	O24	K2A	-167.0(13)
K3	O59	C58	C53	24.6(10)	O23	S21	O22	K8[2]	3.1(4)
K3	O59	C58	C57	-155.3(6)	O23	S21	O22	K8[4]	-64.5(6)
K3	N52	C61	C62	-173.3(7)	O23	S21	C20	C19	-62.9(7)
K3	N52	C67	C68	-71.5(7)	C14	C13	C12	C11	-3.7(13)
K6	S017	O66	K5	169.2(4)	C19	N10	C11	C16	71.1(9)
K6	S017	O65	K4	135.5(5)	C19	N10	C11	C12	-108.0(9)
K6	S017	O65	K4[2]	2.0(9)	C19	N10	C25	C26	-164.7(7)
K6	S017	C62	C61	142.9(5)	C18	O17	C16	C11	179.6(7)
K6	O80	C79	C74	-27.9(9)	C18	O17	C16	C15	0.4(12)
K6	O80	C79	C78	150.3(7)	C61	N52	C67	C68	-165.9(7)

K6	N73	C82	C83	-174.9(6)	C62	S017	O66	K6	-105.5(4)
K6	N73	C88	C89	67.1(7)	C62	S017	O66	K5	63.7(4)
S48	C47	C46	N31[1]	-175.2(5)	C62	S017	O65	K4	-40.3(8)
O17	C16	C15	C14	176.9(8)	C62	S017	O65	K4[2]	-173.8(5)
O86	S84	O85	K5	-133.8(3)	C62	S017	O64	K6	107.5(4)
O86	S84	O85	K7	-27.5(4)	O43	S42	O45	K3	-50.4(7)
O86	S84	O87	K8	-83.0(7)	O43	S42	O45	K4	130.3(5)
O86	S84	O87	K8[3]	1.3(4)	O43	S42	O44	K4[2]	150.1(6)
O86	S84	O87	K5	133.4(3)	O43	S42	O44	K4	-134.5(4)
O86	S84	C83	C82	-178.0(6)	O43	S42	O44	K5[2]	13.1(5)
O66	S017	O65	K4[2]	-55.7(7)	O43	S42	C41	C40	-51.1(8)
O66	S017	O65	K4	77.8(8)	C67	N52	C61	K3	112.5(6)
O66	S017	C62	C61	-162.0(6)	C67	N52	C61	C62	-60.7(9)
O66	S017	O64	K6	-7.8(4)	C83	S84	O86	K8[3]	-116.1(3)
O80	C79	C78	C77	-176.0(8)	C83	S84	O86	K9[1]	58.1(6)
O24	S21	O22	K8[4]	63.9(6)	C83	S84	O86	K7	144.8(3)
O24	S21	O22	K8[2]	131.5(3)	C83	S84	O85	K5	108.3(3)
O24	S21	O23	K8[2]	-131.6(3)	C83	S84	O85	K7	-145.4(3)
O24	S21	O23	K5[2]	-6.1(4)	C83	S84	O87	K8	33.2(7)
O24	S21	C20	C19	177.5(6)	C83	S84	O87	K8[3]	117.4(3)
O45	S42	O44	K4	-6.0(4)	C83	S84	O87	K5	-110.4(3)
O45	S42	O44	K4[2]	-81.4(6)	C12	C11	C16	O17	-177.5(7)
O45	S42	O44	K5[2]	141.6(4)	C12	C11	C16	C15	1.7(12)
O45	S42	O43	K5[2]	-133.8(4)	C12	C13	C14	C15	3.1(13)
O45	S42	C41	C40	-179.2(6)	C20	S21	O24	K2	-58.4(10)
O85	S84	O86	K8[3]	125.3(3)	C20	S21	O24	K5[2]	118.7(4)
O85	S84	O86	K9[1]	-60.5(6)	C20	S21	O24	K2A	-54.1(13)
O85	S84	O86	K7	26.2(4)	C20	S21	O22	K8[2]	-110.6(4)
O85	S84	O87	K8[3]	-125.7(3)	C20	S21	O22	K8[4]	-178.2(4)
O85	S84	O87	K8	150.1(6)	C20	S21	O23	K8[2]	113.9(4)
O85	S84	O87	K5	6.5(4)	C20	S21	O23	K5[2]	-120.7(4)
O85	S84	C83	C82	-56.9(7)	C35	C36	C37	O38	-178.2(8)
N31	C32	C33	C34	-178.9(8)	C35	C36	C37	C32	2.1(13)
N31	C32	C37	O38	-3.0(10)	C47	S48	O50	K3	-107.5(4)
N31	C32	C37	C36	176.7(7)	C47	S48	O49	K6[1]	-96(2)
N31	C40	C41	S42	-169.9(6)	C47	S48	O51	K3	110.0(3)
N10	C11	C16	O17	3.3(11)	C47	S48	O51	K1	45.2(10)
N10	C11	C16	C15	-177.5(7)	O28	S27	O29	K3	-100(2)
N10	C11	C12	C13	-179.6(8)	O28	S27	O29	K1	-18.2(5)
N10	C19	C20	S21	161.1(6)	O28	S27	O30	K2[1]	-1.4(6)

N10	C25	C26	S27	176.9(6)	O28	S27	O30	K2A[1]	-5.3(9)
O91	S90	O92	K2[5]	-80.3(10)	O28	S27	C26	C25	-72.5(7)
O91	S90	O92	K2A[5]	-74(2)	C89	S90	O91	K9	-95.5(5)
O91	S90	C89	C88	-179.8(6)	C89	S90	O92	K2[5]	162.6(9)
O70	S69	O71	K9[1]	55.9(11)	C89	S90	O92	K2A[5]	169(2)
O70	S69	O71	K7	138.8(3)	C60	O59	C58	C53	-179.8(7)
O70	S69	O72	K7	-141.7(3)	C60	O59	C58	C57	0.3(12)
O70	S69	C68	C67	179.1(6)	C41	S42	O45	K3	73.6(6)
C53	N52	C61	K3	-115.4(6)	C41	S42	O45	K4	-105.7(4)
C53	N52	C61	C62	71.4(9)	C41	S42	O44	K4[2]	33.1(7)
C53	N52	C67	C68	63.7(9)	C41	S42	O44	K4	108.5(4)
C74	N73	C82	K6	113.2(6)	C41	S42	O44	K5[2]	-103.9(4)
C74	N73	C82	C83	-61.6(9)	C41	S42	O43	K5[2]	103.1(4)
C74	N73	C88	C89	-65.2(9)	C81	O80	C79	C74	-176.8(7)
C74	C79	C78	C77	2.2(13)	C81	O80	C79	C78	1.4(12)
C74	C75	C76	C77	4.2(12)	C46[7]	N31	C32	C33	-25.6(11)
N73	C74	C79	O80	-4.8(10)	C46[7]	N31	C32	C37	157.2(7)
N73	C74	C79	C78	176.9(7)	C46[7]	N31	C40	C41	69.3(9)
N73	C74	C75	C76	-179.9(7)	C46[7]	N31	C40	K2	-106.2(8)
N73	C82	C83	S84	-159.9(6)	C46[7]	N31	C40	K2A	-112.1(10)
N73	C88	C89	S90	175.8(5)	C39	O38	C37	C36	-2.1(11)
O29	S27	O30	K2[1]	-127.9(6)	C39	O38	C37	C32	177.7(7)
O29	S27	O30	K2A[1]	-131.7(9)	C25	N10	C11	C16	-157.6(7)
O29	S27	O28	K2[1]	127.8(6)	C25	N10	C11	C12	23.2(11)
O29	S27	O28	K1	19.6(5)	C25	N10	C19	C20	-73.4(9)
O29	S27	O28	K2A[1]	131.0(8)	C25	N10	C19	K9[6]	111.6(6)
O29	S27	C26	C25	50.0(8)	C26	S27	O29	K3	142(2)
O71	S69	O70	K6[1]	-151.4(4)	C26	S27	O29	K1	-136.3(3)
O71	S69	O72	K7	-13.6(4)	C26	S27	O30	K2[1]	112.7(6)
O71	S69	C68	C67	56.9(7)	C26	S27	O30	K2A[1]	108.9(9)
O92	S90	O91	K9	146.9(4)	C26	S27	O28	K2[1]	-113.0(5)
O92	S90	C89	C88	-57.9(7)	C26	S27	O28	K1	138.8(3)
C11	N10	C19	C20	59.9(9)	C26	S27	O28	K2A[1]	-109.8(8)
C11	N10	C19	K9[6]	-115.1(6)	O64	S017	O66	K6	8.6(5)
C11	N10	C25	C26	63.9(9)	O64	S017	O66	K5	177.7(4)
C11	C16	C15	C14	-2.3(13)	O64	S017	O65	K4	-155.4(7)
O87	S84	O86	K8[3]	-1.2(4)	O64	S017	O65	K4[2]	71.1(7)
O87	S84	O86	K9[1]	173.0(4)	O64	S017	C62	C61	79.8(7)
O87	S84	O86	K7	-100.3(3)	C68	S69	O70	K6[1]	90.9(5)
O87	S84	O85	K5	-6.5(4)	C68	S69	O71	K9[1]	173.7(10)

O87	S84	O85	K7	99.8(3)	C68	S69	O71	K7	-103.4(3)
O87	S84	C83	C82	61.9(7)	C68	S69	O72	K7	101.8(3)
C79	O80	C81	K6	154.1(8)	O51	S48	O50	K3	6.3(5)
C79	C74	N73	K6	27.7(8)	O51	S48	O49	K6[1]	148(2)
C79	C74	N73	C82	-69.1(9)	O51	S48	C47	C46	65.1(7)
C79	C74	N73	C88	160.5(7)	K8[3]	S84	O86	K9[1]	174.2(5)
C79	C74	C75	C76	-2.5(11)	K8[3]	S84	O86	K7	-99.1(2)
C79	C78	C77	C76	-0.5(13)	K8[3]	S84	O85	K5	-64.8(3)
N52	C53	C58	O59	4.8(11)	K8[3]	S84	O85	K7	41.5(4)
N52	C53	C58	C57	-175.3(7)	K8[3]	S84	O87	K8	-84.3(6)
N52	C53	C54	C55	178.1(7)	K8[3]	S84	O87	K5	132.1(3)
N52	C61	C62	S017	-164.3(6)	K8[3]	S84	C83	C82	117.0(5)
N52	C67	C68	S69	-176.2(6)	K8[2]	S21	O24	K2	136.3(8)
O72	S69	O70	K6[1]	-25.1(5)	K8[2]	S21	O24	K5[2]	-46.7(4)
O72	S69	O71	K9[1]	-71.5(11)	K8[2]	S21	O24	K2A	140.6(12)
O72	S69	O71	K7	11.4(3)	K8[2]	S21	O22	K8[4]	-67.6(4)
O72	S69	C68	C67	-60.7(7)	K8[2]	S21	O23	K5[2]	125.5(4)
O65	S017	O66	K6	135.9(4)	K8[2]	S21	C20	C19	-13.9(8)
O65	S017	O66	K5	-54.9(5)	K9[6]	O17	C16	C11	22.8(10)
O65	S017	C62	C61	-40.1(8)	K9[6]	O17	C16	C15	-156.4(6)
O65	S017	O64	K6	-135.6(3)	K9[6]	N10	C11	C16	-23.5(9)
O30	S27	O29	K3	24(3)	K9[6]	N10	C11	C12	157.4(7)
O30	S27	O29	K1	105.2(4)	K9[6]	N10	C19	C20	175.0(7)
O30	S27	O28	K2[1]	1.4(6)	K9[6]	N10	C25	C26	-71.6(7)
O30	S27	O28	K1	-106.8(4)	K4	S42	O45	K3	179.3(6)
O30	S27	O28	K2A[1]	4.6(8)	K4	S42	O44	K4[2]	-75.4(5)
O30	S27	C26	C25	172.5(6)	K4	S42	O44	K5[2]	147.6(5)
O22	S21	O24	K2	61.6(10)	K4	S42	O43	K5[2]	-66.3(5)
O22	S21	O24	K5[2]	-121.4(4)	K4	S42	C41	C40	121.1(6)
O22	S21	O24	K2A	65.9(13)	K2[1]	S27	O29	K3	-37(3)
O22	S21	O23	K8[2]	-3.8(5)	K2[1]	S27	O29	K1	44.9(8)
O22	S21	O23	K5[2]	121.7(4)	K2[1]	S27	O28	K1	-108.2(5)
O22	S21	C20	C19	55.8(8)	K2[1]	S27	C26	C25	-131.0(8)
O50	S48	O49	K6[1]	23(3)	K2	O38	C37	C36	159.0(7)
O50	S48	C47	C46	-177.7(6)	K2	O38	C37	C32	-21.2(10)
O50	S48	O51	K3	-4.7(4)	K2	N31	C32	C33	-157.6(7)
O50	S48	O51	K1	-69.6(9)	K2	N31	C32	C37	25.2(9)
C32	N31	C40	C41	-62.8(9)	K2	N31	C40	C41	175.5(9)
C32	N31	C40	K2	121.7(8)	K5	S84	O86	K8[3]	62.9(4)
C32	N31	C40	K2A	115.8(10)	K5	S84	O86	K9[1]	-122.9(4)

C32	C33	C34	C35	2.7(13)	K5	S84	O86	K7	-36.2(4)
C33	C32	C37	O38	179.6(7)	K5	S84	O85	K7	106.3(3)
C33	C32	C37	C36	-0.6(12)	K5	S84	O87	$K8^{3}$	-132.1(3)
C33	C34	C35	C36	-1.3(13)	K5	S84	O87	K8	143.6(7)
C37	O38	C39	K2A	160.6(11)	K5	S84	C83	C82	2.7(7)
C37	C36	C35	C34	-1.1(14)	$K5^{2}$	S42	O45	K3	-135.1(3)
C37	C32	C33	C34	-1.8(12)	$K5^{2}$	S42	O45	K4	45.5(5)
C57	C56	C55	C54	1.8(13)	$K5^{2}$	S42	O44	$K4^{2}$	137.0(8)
O93	S90	O91	K9	20.4(6)	$K5^{2}$	S42	O44	K4	-147.6(5)
O93	S90	O92	$K2^{5}$	47.4(10)	$K5^{2}$	S42	C41	C40	20.7(7)
O93	S90	O92	$K2A^{5}$	54(2)	$K5^{2}$	S21	O24	K2	-177.0(10)
O93	S90	C89	C88	60.0(7)	$K5^{2}$	S21	O24	K2A	-172.8(13)
O49	S48	O50	K3	132.5(4)	$K5^{2}$	S21	O22	$K8^{2}$	63.5(3)
O49	S48	C47	C46	-55.5(7)	$K5^{2}$	S21	O22	$K8^{4}$	-4.1(7)
O49	S48	O51	K3	-131.3(3)	$K5^{2}$	S21	O23	$K8^{2}$	-125.5(4)
O49	S48	O51	K1	163.8(8)	$K5^{2}$	S21	C20	C19	-118.7(6)
C82	N73	C88	C89	163.2(7)	K5	S017	O66	K6	-169.2(4)
C56	C57	C58	O59	177.0(8)	K5	S017	O65	$K4^{2}$	-92.1(5)
C56	C57	C58	C53	-3.0(13)	K5	S017	O65	K4	41.4(7)
C56	C55	C54	C53	-2.9(13)	K5	S017	C62	C61	-121.5(6)
C58	C53	N52	K3	-26.6(9)	K5	S017	O64	K6	-3.5(9)
C58	C53	N52	C61	70.1(9)	K1	S27	O29	K3	-82(2)
C58	C53	N52	C67	-160.7(7)	K1	S27	O30	$K2^{1}$	-60.3(5)
C58	C53	C54	C55	1.2(12)	K1	S27	O30	$K2A^{1}$	-64.1(9)
C58	C57	C56	C55	1.2(13)	K1	S27	O28	$K2^{1}$	108.2(5)
C75	C74	N73	K6	-154.9(6)	K1	S27	O28	$K2A^{1}$	111.4(8)
C75	C74	N73	C82	108.4(8)	K1	S27	C26	C25	-17.3(9)
C75	C74	N73	C88	-22.1(10)	K7	S69	O70	$K6^{1}$	-75.5(6)
C75	C74	C79	O80	177.7(7)	K7	S69	O71	$K9^{1}$	-82.9(10)
C75	C74	C79	C78	-0.6(12)	K7	S69	C68	C67	-9.6(6)
C75	C76	C77	C78	-2.7(12)	K7	S84	O86	$K8^{3}$	99.1(2)
C88	N73	C82	K6	-114.1(6)	K7	S84	O86	$K9^{1}$	-86.7(4)
C88	N73	C82	C83	71.0(9)	K7	S84	O85	K5	-106.3(3)
O44	S42	O45	K3	-174.9(5)	K7	S84	O87	K8	-149.0(5)
O44	S42	O45	K4	5.8(4)	K7	S84	O87	$K8^{3}$	-64.7(2)
O44	S42	O43	$K5^{2}$	-9.7(4)	K7	S84	O87	K5	67.4(2)
O44	S42	C41	C40	65.7(7)	K7	S84	C83	C82	-114.4(6)
C16	C11	C12	C13	1.2(13)	$K2A^{1}$	S27	O29	K3	-30(3)
C16	C15	C14	C13	-0.1(13)	$K2A^{1}$	S27	O29	K1	51.1(11)
C40	N31	C32	C33	104.3(9)	$K2A^{1}$	S27	O28	K1	-111.4(8)

C40	N31	C32	C37	-72.9(9)	K2A[1]	S27	C26	C25	-135.7(9)
C54	C53	N52	K3	156.6(6)	K2A	O38	C37	C36	155.6(12)
C54	C53	N52	C61	-106.8(9)	K2A	O38	C37	C32	-24.6(13)
C54	C53	N52	C67	22.4(11)	K2A	N31	C32	C33	-158.5(10)
C54	C53	C58	O59	-178.2(7)	K2A	N31	C32	C37	24.3(11)
C54	C53	C58	C57	1.8(12)	K2A	N31	C40	C41	-178.6(11)

[1]+X,-1+Y,+Z; [2]2-X,1-Y,1-Z; [3]1-X,1-Y,1-Z; [4]1+X,+Y,+Z; [5]-1+X,+Y,+Z; [6]1+X,-1+Y,+Z; [7]+X,1+Y,+Z

Table 16 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2.

Atom	*x*	*y*	*z*	U(eq)
H36	11180	5456	2352	35
H33	9325	6185	3109	29
H13	11432	3327	2360	34
H57	8650	3542	2339	32
H82A	6270	5846	4097	25
H82B	6512	5312	3708	25
H56	7371	3654	2024	34
H75	4296	6158	3077	28
H76	3917	5716	2374	31
H34	8974	5648	2406	32
H88A	5389	7080	4032	26
H88B	4695	6576	3702	26
H55	6449	3197	2394	31
H78	6100	5334	2307	32
H40A	11269	5990	4132	23
H40B	11501	5421	3747	23
H54	6831	2706	3099	28
H15	13641	3600	2302	30
H14	12355	3802	1994	39
H19A	14013	3506	3706	26
H19B	13729	2970	4081	26
H18A	14719	2673	2572	43
H18B	15314	2890	3005	43
H18C	14805	3800	2765	43
H61A	8956	3674	3697	28
H61B	8858	3058	4102	28
H62A	7715	3836	4106	28
H62B	7626	4252	3639	28

H67A	7229	2324	3736	28
H67B	7927	1806	4059	28
H83A	5481	4246	3587	26
H83B	5020	4947	3845	26
H12	11795	2806	3048	29
H20A	12519	3962	3831	33
H20B	13011	4640	3581	33
H35	9906	5261	2042	36
H77	4833	5233	1996	32
H47A	9679	-2064	3213	25
H47B	10410	-1502	3490	25
H89A	4794	7923	3214	24
H89B	5445	8443	3566	24
H60A	10339	2927	3037	43
H60B	9815	3835	2807	43
H60C	9734	2716	2607	43
H41A	10374	4467	3613	30
H41B	10030	5132	3937	30
H81A	7207	6235	2582	37
H81B	7287	5086	2750	37
H81C	7818	5961	3002	37
H46A	10398	-2701	4044	23
H46B	9710	-3290	3741	23
H39A	12365	5180	2859	39
H39B	12849	6149	3064	39
H39C	12245	6260	2627	39
H25A	12166	2276	3670	31
H25B	12851	1712	3985	31
H26A	12900	487	3456	29
H26B	12188	1035	3157	29
H68A	7959	458	3583	21
H68B	7300	991	3241	21
H10A	10998	2380	5585	70
H10B	11431	2942	5346	70
H10C	6798	7526	4564	94
H10D	6596	8502	4381	94
H10E	10909	-262	5466	88
H10F	11338	664	5479	88
H10G	5670	8643	5087	102
H10H	5418	8536	4622	102

H10I	12430	1900	4731	134
H10J	11961	2093	5064	134
H10K	13068	832	4967	203
H10L	12704	121	4582	203

Table 17 Atomic Occupancy for 2.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
K2	0.75(11)	Br1	0.883(3)	Br1A	0.117(3)
K2A	0.25(11)				