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TWO IONIC SACCHARINATES:
(1a) SODIUM SACCHARINATE 2/3 HYDRATE, $C_7H_4NO_3SNa \cdot 2/3H_2O$
(1b) MAGNESIUM DISACCHARINATE HEPTAHYDRATE, $(C_7H_4NO_3S)_2Mg \cdot 7H_2O$

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Preliminary information. Up to now very little is known about the crystal structure of metal saccharinates. As part of the investigation of these compounds several saccharinates have been studied (Jovanovski & Kamenar, 1981). This paper reports the crystal structures of sodium and magnesium saccharinates.

Sodium saccharinate hydrate was prepared from warm aqueous solution of saccharin and Na_2CO_3 (Defournel, 1901), Mg saccharinate heptahydrate analogously from saccharin and $MgCO_3$.

Crystal data. Needle-like triclinic crystals of both saccharinates were obtained by recrystallization from ethanol. From single crystal diffractometry, MoKα, λ = 0.7107 Å, for (1a): a = 15.237(8), b = 11.640(5), c = 7.346(3) Å, α = 96.31(3), β = 87.64(3), γ = 107.55(3)°, V = 1234.7 Å^3, Z = 6, D_{obs} = 1.70, D_{calc} = 1.760 g cm^{-3}, $F(000)$ = 664, μ(MoKα) = 4.22 cm^{-1}, space group $P\bar{1}$, crystal size 0.60 x 0.13 x 0.12 mm^3.
(1b): a = 14.305(13), b = 11.288(10), c = 7.017(7) Å, α = 97.02(2), β = 78.11(3), γ = 100.13(3)°, V = 1087.1 Å^3, Z = 2, D_{obs} = 1.50, D_{calc} = 1.460 g cm^3, $F(000)$ = 536, μ(MoKα) = 3.19 cm^{-1}, space group $P\bar{1}$, crystal size 0.31 x 0.35 x 0.49 mm^3.

Intensity data, structure determination and refinement. Intensity data for both crystals were collected on a Philips PW 1100 four circle diffractometer using graphite monochromatized MoKα radiation. The structures were solved using MULTAN program (Declerq et. al. 1973). The hydrogen atoms were located in difference Fourier maps. The structures were refined by block-diagonal least-squares procedure with anisotropic thermal parameters for all atoms except hydrogens for which isotropic parameter B = 2.5 was assigned.

(1*a*) Out of total 6641 independent reflections measured by the $\omega - 2\theta$ scan technique (scan width 1.20°, scan speed 0.04° s^{-1}) in the range $4<2\theta<60^{\circ}$, 5365 with $I>3\sigma(I)$ were used in structure refinement. The final *R* factor was 0.039.

(1*b*) Out of 5166 reflections ($\theta - 2\theta$ scan technique, scan width 1.60°, scan speed 0.08° s^{-1}, range $4<2\theta<60^{\circ}$) 4769 with $I>3\sigma(I)$ were used for structure solution and refinement. The final *R* was 0.038.

Table 1. Atomic coordinates ($x10^4$, for hydrogens $x10^3$) with their e.s.d.'s for (1*a*)

	x/a	*y/b*	*z/c*		*x/a*	*y/b*	*z/c*
Na(1)	3076(1)	1463(1)	3711(2)	S(3)	3519(0)	4506(1)	6017(1)
S(1)	1906(0)	446(1)	7109(1)	N(3)	4180(1)	5840(2)	5755(3)
N(1)	2238(1)	845(2)	9178(3)	O(31)	3885(1)	3968(2)	7373(3)
O(11)	1760(1)	1427(2)	6245(3)	O(32)	3319(1)	3764(2)	4269(2)
O(12)	2512(1)	-131(2)	6058(3)	O(33)	4076(1)	7775(2)	6035(3)
O(13)	1782(1)	241(2)	12011(3)	C(31)	2541(2)	4914(2)	6853(3)
C(11)	860(2)	-658(2)	7551(3)	C(32)	1689(2)	4214(2)	7391(4)
C(12)	161(2)	-1314(3)	6379(4)	C(33)	1058(2)	4826(3)	8008(4)
C(13)	-595(2)	-2111(3)	7152(4)	C(34)	1283(2)	6078(3)	8054(4)
C(14)	-626(2)	-2240(3)	9017(4)	C(35)	2141(2)	6764(2)	7486(4)
C(15)	88(2)	-1565(3)	10168(4)	C(36)	2774(2)	6165(2)	6884(3)
C(16)	839(2)	-756(2)	9412(3)	C(37)	3734(2)	6682(2)	6194(3)
C(17)	1661(2)	150(2)	10350(3)	H(11)	337	172	24
Ow(1)	3871(1)	2190(2)	1073(3)	H(12)	422	185	54
Ow(2)	4268(1)	1763(2)	5800(3)	H(21)	482	201	532
Na(2)	5962(1)	222(1)	3275(2)	H(22)	422	230	653
S(2)	6182(0)	1235(1)	8640(1)	H(122)	19	-129	498
N(2)	5568(1)	2110(2)	9303(3)	H(133)	-111	-270	636
O(21)	6397(1)	668(2)	10150(3)	H(144)	-117	-279	953
O(22)	5764(1)	384(2)	7087(3)	H(155)	-7	-155	1161
O(23)	5689(1)	4122(2)	9436(3)	H(222)	816	149	698

Table 1. (cont.)

	x/a	y/b	z/c		x/a	y/b	z/c
C(21)	7162(2)	2360(2)	7934(3)	H(233)	926	332	623
C(22)	7989(2)	2273(2)	7188(4)	H(244)	888	522	682
C(23)	8636(2)	3350(3)	6788(4)	H(255)	749	528	806
C(24)	8456(2)	4454(3)	7147(4)	H(322)	155	335	739
C(25)	7616(2)	4516(2)	7891(4)	H(333)	47	436	841
C(26)	6964(2)	3449(2)	8265(3)	H(344)	80	651	844
C(27)	6015(2)	3269(2)	9046(3)	H(355)	235	768	751
Na(3)	5452(1)	5737(1)	8196(2)				

Table 2. Atomic coordinates (x10^4, for hydrogens x10^3) with their e.s.d.'s for (1b)

	x/a	y/b	z/c		x/a	y/b	z/c
Mg	4453(1)	2360(1)	237(1)	C(26)	1973(2)	-1607(2)	5734(3)
Ow(1)	4413(1)	825(2)	1716(3)	C(27)	3001(2)	-999(2)	5339(4)
Ow(2)	2973(1)	2002(2)	654(3)	O(23)	3698(1)	-1560(2)	5012(3)
Ow(3)	4348(2)	3367(2)	2853(3)	O(22)	1900(1)	1189(2)	4140(3)
Ow(4)	4414(1)	3780(2)	-1290(3)	O(21)	1900(1)	1402(2)	7629(3)
Ow(5)	4584(1)	1216(2)	-2374(3)	H(11)	403	73	268
Ow(6)	5739(1)	3783(2)	5067(3)	H(12)	488	51	160
Ow(7)	2815(2)	4237(2)	5267(3)	H(21)	257	183	166
N(1)	6842(1)	4405(2)	-379(3)	H(22)	260	191	-13
S(1)	7985(0)	4933(1)	-763(1)	H(31)	482	362	353
C(11)	8413(2)	3560(2)	-825(4)	H(32)	382	356	362
C(12)	9347(2)	3306(3)	-1109(4)	H(41)	415	442	-100
C(13)	9445(2)	2103(3)	-1088(4)	H(42)	484	397	-229
C(14)	8643(2)	1208(3)	-797(4)	H(51)	415	88	-298
C(15)	7710(2)	1480(2)	-538(4)	H(52)	511	120	-328
C(16)	7609(2)	2676(2)	-552(3)	H(61)	620	440	472
C(17)	6700(2)	3203(2)	-323(3)	H(62)	602	315	493
O(13)	5901(1)	2543(2)	-101(3)	H(71)	247	429	444
O(12)	8302(1)	5404(2)	-2660(3)	H(72)	251	407	644
O(11)	8244(2)	5763(2)	849(3)	H(122)	987	395	-113
N(2)	3100(1)	217(2)	5369(3)	H(133)	1005	184	-123
S(2)	2052(0)	659(1)	5802(1)	H(144)	869	36	-66
C(21)	1343(2)	-774(2)	6023(3)	H(155)	713	92	-38
C(22)	350(2)	-1098(3)	6405(4)	H(222)	-9	-48	658
C(23)	0(2)	-2323(3)	6486(4)	H(233)	-66	-249	686
C(24)	618(2)	-3168(3)	6207(4)	H(244)	31	-400	615
C(25)	1615(2)	-2826(2)	5817(4)	H(255)	206	-341	571

Comments. Tables 1 and 2 give atomic coordinates while Tables 3 and 4 interatomic distances and angles. Both structures consist of cations (Na^+ and Mg^{2+}, respectively), saccharinate anions and water molecules (Figure 1 and 2). In (1a) two

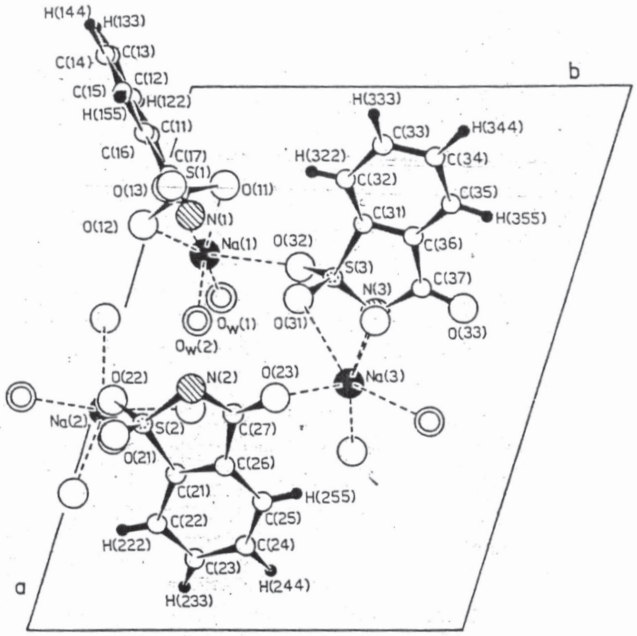

Figure 1

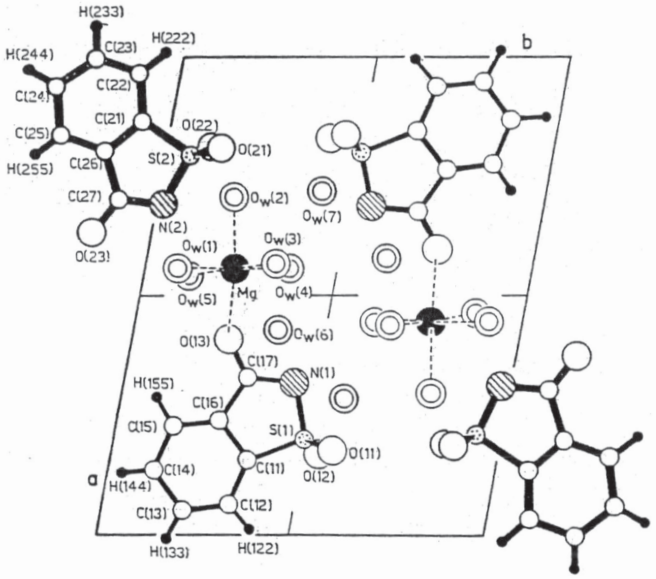

Figure 2

crystallographically independent Na^+ ions have C.N. six, being surrounded by oxygen atoms from water molecules, CO and SO_2 groups from saccharinates, while the third crystallographically independent Na^+ ion has also C.N. six but realized by five oxygen atoms from the same groups and by one saccharinate nitrogen atom. Coordination polyhedra are irregular. Within coordination polyhedra the sodium-to-oxygen distances vary from 2.304 to 2.796 Å, while the sodium-to-nitrogen distance amounts to 2.731 Å. In (1*b*) Mg^{2+} is octahedrally surrounded by five oxygen atoms from water molecules and one oxygen atom from the CO group of a neighbouring saccharinate ion. Magnesium-to-oxygen distances range from 2.012 to 2.113 Å, the angles in the octahedron from 86.2 to 96.9°. In both structures the oxygen and nitrogen atoms from saccharinate ions participate in hydrogen bonding with water molecules. Saccharinate ions are planar within the experimental errors. Bond lengths and angles in these ions are within expected values and not very different from those found in saccharin itself (Bart, 1968 and Okaya 1969).

Table 3. Interatomic distances and angles with their e.s.d.'s for (1*a*)

Distances (Å)

Na(1) - Ow(1)	2.344(2)	S(1) - N(1)	1.596(2)
Na(1) - Ow(2)	2.345(2)	S(1) - O(11)	1.443(2)
Na(1) - O(32)	2.580(2)	S(1) - O(12)	1.450(2)
Na(1) - O(11)	2.674(2)	S(1) - C(11)	1.764(2)
Na(1) - $O(12)_{i}$	2.602(2)	N(1) - C(17)	1.354(3)
Na(1) - $O(13)_{ii}$	2.365(2)	C(17) - O(13)	1.230(3)
Na(2) - $Ow(2)_{i}$	2.400(2)	C(16) - C(17)	1.506(3)
Na(2) - O(21)	2.431(2)	C(11) - C(16)	1.382(4)
Na(2) - O(22)	2.796(2)	C(11) - C(12)	1.378(3)
Na(2) - $O(22)_{ii}$	2.527(2)	C(12) - C(13)	1.388(4)
Na(2) - $O(33)_{iii}$	2.349(2)	C(13) - C(14)	1.392(5)
Na(2) - $O(12)_{ii}$	2.430(2)	C(14) - C(15)	1.389(4)
Na(3) - $Ow(1)_{iii}$	2.331(2)	C(15) - C(16)	1.385(3)
Na(3) - N(3)	2.731(3)	C(12) - H(122)	1.03
Na(3) - O(31)	2.681(2)	C(13) - H(133)	1.03
Na(3) - $O(32)_{iii}$	2.534(2)	C(14) - H(144)	0.97
Na(3) - $O(23)_{iv}$	2.304(2)	C(15) - H(155)	1.06
Na(3) - $O(23)_{iv}$	2.437(2)		

Table 3. (cont.)

S(2) - N(2)	1.606(2)	S(3) - O(32)	1.455(2)
S(2) - O(21)	1.446(2)	S(3) - C(31)	1.764(3)
S(2) - O(22)	1.456(2)	N(3) - C(37)	1.357(4)
S(2) - C(21)	1.767(2)	C(37) - O(33)	1.237(3)
N(2) - C(27)	1.346(3)	C(36) - C(37)	1.494(3)
C(27) - O(23)	1.241(4)	C(31) - C(36)	1.389(3)
C(26) - C(27)	1.496(3)	C(31) - C(32)	1.377(3)
C(21) - C(26)	1.384(4)	C(32) - C(33)	1.395(4)
C(21) - C(22)	1.381(4)	C(33) - C(34)	1.390(4)
C(22) - C(23)	1.393(3)	C(34) - C(35)	1.386(4)
C(23) - C(24)	1.389(4)	C(35) - C(36)	1.384(4)
C(24) - C(25)	1.390(4)	C(32) - H(322)	0.96
C(25) - C(26)	1.383(3)	C(33) - H(333)	0.95
C(22) - H(222)	1.01	C(34) - H(344)	1.02
C(23) - H(233)	0.99	C(35) - H(355)	1.01
C(24) - H(244)	0.98	Ow(1) - H(11)	0.99
C(25) - H(255)	0.97	Ow(1) - H(12)	0.82
S(3) - N(3)	1.603(2)	Ow(2) - H(21)	0.87
S(3) - O(31)	1.445(2)	Ow(2) - H(22)	0.79

Hydrogen bonds

$Ow(1)\cdots N(1)^{i}$	2.833(3)	$Ow(2)\cdots O(33)^{iii}$	2.746(4)
$Ow(1)\cdots N(2)^{i}$	2.869(3)	Ow(2)···O(31)	2.908(3)

Angles (°)

S(1)-N(1)-C(17)	111.4(2)	C(14)-C(13)-H(133)	117
C(11)-S(1)-N(1)	97.9(1)	C(13)-C(14)-H(144	119
O(11)-S(1)-O(12)	112.9(1)	C(15)-C(14)-H(144)	119
O(11)-S(1)-C(11)	111.9(1)	C(14)-C(15)-H(155)	125
O(11)-S(1)-N(1)	112.3(1)	C(16)-C(15)-H(155)	117
O(12)-S(1)-N(1)	111.6(1)	S(2)-N(2)-C(27)	111.3(2)
O(12)-S(1)-C(11)	109.3(1)	C(21)-S(2)-N(2)	97.5(1)
N(1)-C(17)-C(16)	113.0(2)	O(21)-S(2)-O(22)	113.9(1)
N(1)-C(17)-O(13)	124.2(2)	O(21)-S(2)-C(21)	111.1(1)
O(13)-C(17)-C(16)	122.8(2)	O(21)-S(2)-N(2)	111.4(1)
C(11)-C(16)-C(17)	111.2(2)	O(22)-S(2)-N(2)	111.1(1)
C(11)-C(16)-C(15)	119.4(2)	O(22)-S(2)-C(21)	110.6(1)
C(15)-C(16)-C(17)	129.3(2)	N(2)-C(27)-C(26)	113.7(2)
S(1)-C(11)-C(16)	106.2(2)	N(2)-C(27)-O(23)	124.0(2)
S(1)-C(11)-C(12)	130.2(2)	O(23)-C(27)-C(26)	122.3(2)
C(12)-C(11)-C(16)	123.6(2)	C(21)-C(26)-C(27)	111.1(2)
C(11)-C(12)-C(13)	116.7(3)	C(21)-C(26)-C(25)	120.1(2)
C(12)-C(13)-C(14)	120.9(2)	C(25)-C(26)-C(27)	128.8(2)
C(13)-C(14)-C(15)	121.3(2)	S(2)-C(21)-C(26)	106.4(2)
C(14)-C(15)-C(16)	118.2(3)	S(2)-C(21)-C(22)	130.8(2)
C(11)-C(12)-H(122)	124	C(22)-C(21)-C(26)	122.8(2)
C(13)-C(12)-H(122)	119	C(21)-C(22)-C(23)	116.7(3)
C(12)-C(13)-H(133)	122	C(22)-C(23)-C(24)	121.2(3)

Table 3. (cont.)

C(23)-C(24)-C(25)	120.9(2)	Ow(1)-Na(1)-Ow(2)	102.7(1)
C(24)-C(25)-C(26)	118.3(3)	Ow(1)-Na(1)-O(32)	76.9(1)
C(21)-C(22)-H(222)	124	Ow(1)-Na(1)-O(12)^{i}	153.5(1)
C(23)-C(22)-H(222)	119	Ow(1)-Na(1)-O(13)^{i}	92.5(1)
C(22)-C(23)-H(233)	119	Ow(2)-Na(1)-O(32)	87.0(1)
C(24)-C(23)-H(233)	120	Ow(2)-Na(1)-O(11)^{i}	95.7(1)
C(23)-C(24)-H(244)	123	Ow(2)-Na(1)-O(13)^{i}	152.9(1)
C(25)-C(24)-H(244)	116	O(32)-Na(1)-O(11)	81.8(1)
C(24)-C(25)-H(255)	120	O(32)-Na(1)-O(12)	127.6(1)
C(26)-C(25)-H(255)	122	O(11)-Na(1)-O(12)^{i}	54.4(1)
S(3)-N(3)-C(37)	111.0(2)	O(11)-Na(1)-O(13)^{i}	80.5(1)
C(31)-S(3)-N(3)	97.8(1)	O(12)-Na(1)-O(13)^{i}	84.2(1)
O(31)-S(3)-O(32)	114.0(1)	Ow(2)^{ii}-Na(2)-O(21)^{i}	121.5(1)
O(31)-S(3)-C(31)	111.5(1)	Ow(2)^{ii}-Na(2)-O(22)^{iii}	72.4(1)
O(31)-S(3)-N(3)	110.8(1)	Ow(2)^{ii}-Na(2)-O(33)^{ii}	149.8(1)
O(32)-S(3)-N(3)	111.2(1)	Ow(2)^{ii}-Na(2)-O(12)	74.5(1)
O(32)-S(3)-C(31)	110.4(1)	O(21)^{i}-Na(2)-O(22)^{ii}	163.9(1)
N(3)-C(37)-C(36)	113.5(2)	O(21)^{i}-Na(2)-O(12)^{ii}	98.1(1)
N(3)-C(37)-O(33)	124.0(2)	O(22)^{ii}-Na(2)-O(33)^{iii}	92.4(1)
O(33)-C(37)-C(36)	122.5(2)	O(22)^{ii}-Na(2)-O(12)^{ii}	90.6(1)
C(31)-C(36)-C(37)	111.3(2)	O(22)^{iii}-Na(2)-O(33)^{iii}	78.1(1)
C(31)-C(36)-C(35)	120.1(2)	O(22)^{ii}-Na(2)-O(12)^{ii}	87.5(1)
C(35)-C(36)-C(37)	128.6(2)	O(33)^{iii}-Na(2)-O(12)^{ii}	160.9(1)
S(3)-C(31)-C(36)	106.3(2)	Ow(1)^{iii}-Na(3)-N(3)	108.8(1)
S(3)-C(31)-C(32)	130.8(2)	Ow(1)^{iii}-Na(3)-O(31)	98.6(1)
C(32)-C(31)-C(36)	122.9(3)	Ow(1)^{iii}-Na(3)-O(23)^{iv}	145.9(1)
C(31)-C(32)-C(33)	116.6(2)	Ow(1)^{iii}-Na(3)-O(23)	129.8(1)
C(32)-C(33)-C(34)	121.2(2)	N(3)-Na(3)-O(31)^{iii}	86.8(1)
C(33)-C(34)-C(35)	121.3(3)	N(3)-Na(3)-O(32)^{iv}	55.3(1)
C(34)-C(35)-C(36)	118.0(2)	N(3)-Na(3)-O(23)^{iii}	89.2(1)
C(31)-C(32)-H(322)	122	O(31)-Na(3)-O(32)^{iii}	86.3(1)
C(33)-C(32)-H(322)	122	O(31)-Na(3)-O(23)	118.4(1)
C(32)-C(33)-H(333)	118	O(32)^{iii}-Na(3)-O(23)^{iv}	77.7(1)
C(34)-C(33)-H(333)	121	O(32)^{iii}-Na(3)-O(23)	104.4(1)
C(33)-C(34)-H(344)	120	O(23)-Na(3)-O(23)^{iv}	163.3(1)
C(35)-C(34)-H(344)	118	C(36)-C(35)-H(355)	90.5(1)
C(34)-C(35)-H(355)	125		118

(i=x,y,z-1; ii=1-x,-y,1-z; iii=1-x,1-y,1-z; iv=1-x,1-y,2-z)

Table 4. Interatomic distances and angles with their e.s.d.'s for (1b)

Distances (Å)

Mg - O(13)	2.012(2)	Mg - Ow(4)	2.049(2)
Mg - Ow(1)	2.113(2)	Mg - Ow(5)	2.104(2)
Mg - Ow(2)	2.051(2)	S(1) - N(1)	1.618(2)
Mg - Ow(3)	2.030(2)	S(1) - O(11)	1.445(2)

Table 4. (cont.)

S(1) - O(12)	1.449(2)	C(21) - C(22)	1.381(3)
S(1) - C(11)	1.756(3)	C(22) - C(23)	1.390(4)
N(1) - C(17)	1.340(3)	C(23) - C(24)	1.382(4)
C(17) - O(13)	1.242(3)	C(24) - C(25)	1.388(4)
C(16) - C(17)	1.495(4)	C(25) - C(26)	1.385(3)
C(11) - C(16)	1.381(3)	C(22) - H(222)	1.00
C(11) - C(12)	1.385(4)	C(23) - H(233)	0.92
C(12) - C(13)	1.391(5)	C(24) - H(244)	0.97
C(13) - C(14)	1.387(4)	C(25) - H(255)	0.98
C(14) - C(15)	1.392(5)	Ow(1) - H(11)	0.78
C(15) - C(16)	1.384(4)	Ow(1) - H(12)	0.80
C(12) - H(122)	0.95	Ow(2) - H(21)	0.83
C(13) - H(133)	0.95	Ow(2) - H(22)	0.83
C(14) - H(144)	0.99	Ow(3) - H(31)	0.89
C(15) - H(155)	0.95	Ow(3) - H(32)	0.87
S(2) - N(2)	1.620(2)	Ow(4) - H(41)	0.85
S(2) - O(21)	1.442(2)	Ow(4) - H(42)	0.85
S(2) - O(22)	1.445(2)	Ow(5) - H(51)	0.83
S(2) - C(21)	1.757(2)	Ow(5) - H(52)	0.88
N(2) - C(27)	1.353(3)	Ow(6) - H(61)	0.89
C(27) - O(23)	1.240(3)	Ow(6) - H(62)	0.87
C(26) - C(27)	1.495(3)	Ow(7) - H(71)	0.85
C(21) - C(26)	1.384(4)	Ow(7) - H(72)	0.87

Hydrogen bonds

Ow(1)···N(2)	2.926(3)	Ow(4)···N(1)^{iii}	2.939(3)
Ow(1)···Ow(5)^{ii}	3.046(3)	Ow(5)···O(23)^{ii}	2.754(2)
Ow(2)···O(22)$_{i}$	2.772(3)	Ow(5)···N(2)^{i}	2.898(3)
Ow(2)···O(21)^{i}	2.818(2)	Ow(6)···O(23)^{iv}	2.757(2)
Ow(3)···Ow(6)	2.714(3)	Ow(6)···Ow(7)^{v}	2.763(3)
Ow(3)···Ow(7)$_{i}$	2.732(3)	Ow(7)···O(12)^{iii}	2.770(3)
Ow(4)···Ow(6)^{i}	2.852(3)	Ow(7)···O(11)^{v}	2.832(3)

Angles (°)

S(1)-N(1)-C(17)	110.6(2)	C(12)-C(11)-C(16)	122.6(3)
C(11)-S(1)-N(1)	97.6(1)	C(11)-C(12)-C(13)	116.6(2)
O(11)-S(1)-O(12)	114.4(1)	C(12)-C(13)-C(14)	121.1(3)
O(11)-S(1)-C(11)	111.2(1)	C(13)-C(14)-C(15)	121.2(3)
O(11)-S(1)-N(1)	111.6(1)	C(14)-C(15)-C(16)	117.7(2)
O(12)-S(1)-N(1)	111.4(1)	C(11)-C(12)-H(122)	119
O(12)-S(1)-C(11)	109.4(1)	C(13)-C(12)-H(122)	124
N(1)-C(17)-C(16)	114.2(2)	C(12)-C(13)-H(133)	123
N(1)-C(17)-O(13)	125.4(2)	C(14)-C(13)-H(133)	115
O(13)-C(17)-C(16)	120.5(2)	C(13)-C(14)-H(144)	123
C(11)-C(16)-C(17)	111.0(2)	C(15)-C(14)-H(144)	116
C(11)-C(16)-C(15)	120.6(2)	C(14)-C(15)-H(155)	126
C(15)-C(16)-C(17)	128.4(2)	C(16)-C(15)-H(155)	116
S(1)-C(11)-C(16)	106.6(2)	S(2)-N(2)-C(27)	110.8(2)
S(1)-C(11)-C(12)	130.8(2)	C(21)-S(2)-N(2)	97.3(1)

Table 4. (cont.)

O(21)-S(2)-C(21)	110.5(1)	C(23)-C(22)-H(222)	122
O(21)-S(2)-O(22)	114.7(1)	C(22)-C(23)-H(233)	114
O(21)-S(2)-N(2)	111.5(1)	C(24)-C(23)-H(233)	124
O(22)-S(2)-N(2)	111.1(1)	C(23)-C(24)-H(244)	115
O(22)-S(2)-C(21)	110.4(1)	C(25)-C(24)-H(244)	123
N(2)-C(27)-C(26)	113.8(2)	C(24)-C(25)-H(255)	122
N(2)-C(27)-O(23)	123.3(2)	C(26)-C(25)-H(255)	120
O(23)-C(27)-C(26)	122.9(2)	O(13)-Mg-Ow(1)	86.2(1)
C(21)-C(26)-C(27)	111.0(2)	O(13)-Mg-Ow(3)	92.0(1)
C(21)-C(26)-C(25)	120.0(2)	O(13)-Mg-Ow(4)	96.9(1)
C(25)-C(26)-C(27)	129.0(2)	O(13)-Mg-Ow(5)	86.8(1)
S(2)-C(21)-C(26)	107.1(2)	Ow(1)-Mg-Ow(2)	88.2(1)
S(2)-C(21)-C(22)	130.1(2)	Ow(1)-Mg-Ow(3)	88.7(1)
C(22)-C(21)-C(26)	122.8(2)	Ow(1)-Mg-Ow(5)	87.3(1)
C(21)-C(22)-C(23)	116.6(3)	Ow(2)-Mg-Ow(3)	89.3(1)
C(22)-C(23)-C(24)	121.4(2)	Ow(2)-Mg-Ow(4)	88.6(1)
C(23)-C(24)-C(25)	121.2(2)	Ow(2)-Mg-Ow(5)	91.5(1)
C(24)-C(25)-C(26)	117.9(3)	Ow(3)-Mg-Ow(4)	93.9(1)
C(21)-C(22)-H(222)	121	Ow(4)-Mg-Ow(5)	90.2(1)

(i=x,y,z-1; ii=1-x,-y,-z; iii=1-x,1-y,-z; iv=1-x,-y,1-z; v=1-x,1-y,1-z)

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