

Crystallographic data

Crystal structure [DSA-H₄] · 1.5 MeOH

Table 1

Operator	Dr. Volker Huch	
Diffractometer	Bruker X8 Apex	
Identification code	sh2725a	
Empirical formula	C _{21.50} H ₂₁ N ₃ O _{9.50} S ₂	
Formula weight	537.53 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 16.181(5) Å	α = 90°
	b = 16.416(5) Å	β = 91.782(18)°
	c = 21.898(7) Å	γ = 90°
Volume	5814(3) Å ³	
Z	8	
Density (calculated)	1.228 mg/m ³	
Absorption coefficient	0.233 mm ⁻¹	
F(000)	2232	
Crystal size	0.2 x 0.3 x 0.4 mm ³	
Theta range for data collection	1.77 to 26.00°	
Index ranges	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -26 ≤ l ≤ 26	
Reflections collected	48374	
Independent reflections	5699 [R(int) = 0.0480]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5699 / 7 / 348	

Goodness-of-fit on F^2	1.075
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0674$, $wR_2 = 0.2021$
R indices (all data)	$R_1 = 0.0764$, $wR_2 = 0.2104$
Largest diff. peak and hole	1.360 and -0.609 e.Å ⁻³

Table 2

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² $\times 10^3$) for the crystal structure [DSA-H₄] · 1.5 MeOH. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

atom	x	y	z	U(eq)
C(11)	-3143(2)	943(2)	5462(1)	25(1)
O(11)	-3382(1)	1735(1)	5489(1)	27(1)
C(12)	-2302(2)	760(2)	5549(1)	24(1)
C(13)	-2041(2)	-54(2)	5520(2)	34(1)
C(14)	-2604(2)	-667(2)	5401(2)	41(1)
C(15)	-3437(2)	-482(2)	5312(2)	41(1)
C(16)	-3709(2)	312(2)	5343(2)	33(1)
C(21)	-1687(2)	1397(2)	5675(1)	22(1)
N(22)	-1866(1)	2194(1)	5764(1)	21(1)
C(23)	-1170(2)	2609(2)	5893(1)	23(1)
N(24)	-568(1)	2044(1)	5861(1)	21(1)
N(25)	-885(1)	1280(1)	5730(1)	23(1)
C(31)	-1139(2)	3471(2)	6035(1)	26(1)
C(32)	-1879(2)	3919(2)	6055(1)	29(1)
O(32)	-2605(1)	3530(1)	5935(1)	32(1)
C(33)	-1859(2)	4746(2)	6194(2)	41(1)
C(34)	-1117(2)	5136(2)	6306(2)	49(1)
C(35)	-372(2)	4702(2)	6289(2)	49(1)
C(36)	-386(2)	3883(2)	6153(2)	35(1)

C(41)	311(2)	2088(2)	6004(1)	23(1)
C(42)	877(2)	2230(2)	5550(1)	22(1)
S(1)	577(1)	2403(1)	4767(1)	24(1)
O(1)	-10(1)	3077(1)	4785(1)	31(1)
O(2)	1329(1)	2612(1)	4466(1)	34(1)
O(3)	206(2)	1643(1)	4557(1)	38(1)
C(43)	1719(2)	2210(2)	5714(1)	26(1)
C(44)	1986(2)	2052(2)	6310(1)	31(1)
C(45)	1412(2)	1902(2)	6755(1)	36(1)
C(46)	563(2)	1924(2)	6603(1)	31(1)
S(2A)	1803(1)	1746(1)	7514(1)	45(1)
O(4A)	1177(3)	1324(4)	7818(2)	80(2)
O(5A)	1951(6)	2490(4)	7799(3)	133(3)
O(6A)	2516(3)	1229(6)	7433(5)	103(2)
S(2B)	1626(3)	1486(4)	7522(3)	45(1)
O(4B)	1068(8)	866(9)	7679(6)	80(2)
O(5B)	1469(13)	2180(8)	7863(7)	133(3)
O(6B)	2468(6)	1193(12)	7532(15)	103(2)
O(1M)	-3994(2)	4231(2)	5974(2)	62(1)
C(1M)	-758(3)	-37(2)	4137(3)	73(2)
O(2M)	1234(6)	-828(7)	7638(5)	116(3)
C(2M)	856(8)	-907(8)	8193(6)	93(3)

Table 3Bond lengths [Å] and bond angles [°] for [DSA-H₄] · 1.5 MeOH.

atom	bond length	atom	bond angle
C(11)-O(11)	1.358(3)	O(11)-C(11)-C(16)	122.0(2)
C(11)-C(16)	1.401(4)	O(11)-C(11)-C(12)	118.4(2)
C(11)-C(12)	1.402(4)	C(16)-C(11)-C(12)	119.6(3)
C(12)-C(13)	1.402(4)	C(13)-C(12)-C(11)	119.3(3)
C(12)-C(21)	1.463(4)	C(13)-C(12)-C(21)	119.0(2)
C(13)-C(14)	1.377(4)	C(11)-C(12)-C(21)	121.6(2)
C(14)-C(15)	1.389(5)	C(14)-C(13)-C(12)	120.5(3)
C(15)-C(16)	1.379(5)	C(13)-C(14)-C(15)	119.9(3)
C(21)-N(25)	1.313(3)	C(16)-C(15)-C(14)	120.7(3)
C(21)-N(22)	1.356(4)	C(15)-C(16)-C(11)	119.9(3)
N(22)-C(23)	1.337(4)	N(25)-C(21)-N(22)	110.0(2)
C(23)-N(24)	1.349(3)	N(25)-C(21)-C(12)	125.2(2)
C(23)-C(31)	1.451(4)	N(22)-C(21)-C(12)	124.8(2)
N(24)-N(25)	1.381(3)	C(23)-N(22)-C(21)	109.9(2)
N(24)-C(41)	1.447(3)	N(22)-C(23)-N(24)	104.1(2)
C(31)-C(32)	1.407(4)	N(22)-C(23)-C(31)	124.5(2)
C(31)-C(36)	1.409(4)	N(24)-C(23)-C(31)	131.4(2)
C(32)-O(32)	1.357(3)	C(23)-N(24)-N(25)	111.7(2)
C(32)-C(33)	1.390(4)	C(23)-N(24)-C(41)	131.4(2)
C(33)-C(34)	1.376(5)	N(25)-N(24)-C(41)	116.5(2)
C(34)-C(35)	1.402(5)	C(21)-N(25)-N(24)	104.3(2)
C(35)-C(36)	1.378(5)	C(32)-C(31)-C(36)	118.4(3)
C(41)-C(46)	1.390(4)	C(32)-C(31)-C(23)	119.5(2)
C(41)-C(42)	1.393(4)	C(36)-C(31)-C(23)	122.1(3)
C(42)-C(43)	1.399(4)	O(32)-C(32)-C(33)	121.1(3)

C(42)-S(1)	1.790(3)	O(32)-C(32)-C(31)	118.7(3)
S(1)-O(2)	1.442(2)	C(33)-C(32)-C(31)	120.2(3)
S(1)-O(3)	1.454(2)	C(34)-C(33)-C(32)	120.5(3)
S(1)-O(1)	1.459(2)	C(33)-C(34)-C(35)	120.3(3)
C(43)-C(44)	1.387(4)	C(36)-C(35)-C(34)	119.5(3)
C(44)-C(45)	1.389(4)	C(35)-C(36)-C(31)	121.1(3)
C(45)-C(46)	1.404(4)	C(46)-C(41)-C(42)	121.8(2)
C(45)-S(2A)	1.778(4)	C(46)-C(41)-N(24)	116.9(2)
C(45)-S(2B)	1.837(7)	C(42)-C(41)-N(24)	121.2(2)
S(2A)-O(5A)	1.389(6)	C(41)-C(42)-C(43)	118.0(2)
S(2A)-O(4A)	1.410(5)	C(41)-C(42)-S(1)	123.1(2)
S(2A)-O(6A)	1.448(4)	C(43)-C(42)-S(1)	118.9(2)
S(2B)-O(5B)	1.391(7)	O(2)-S(1)-O(3)	113.91(14)
S(2B)-O(4B)	1.408(6)	O(2)-S(1)-O(1)	113.05(13)
S(2B)-O(6B)	1.445(5)	O(3)-S(1)-O(1)	113.42(14)
O(1M)-C(1M)#1	1.402(5)	O(2)-S(1)-C(42)	105.56(13)
C(1M)-O(1M)#1	1.402(5)	O(3)-S(1)-C(42)	105.21(13)
O(2M)-C(2M)	1.384(15)	O(1)-S(1)-C(42)	104.54(12)
		C(44)-C(43)-C(42)	121.3(3)
		C(43)-C(44)-C(45)	119.8(3)
		C(44)-C(45)-C(46)	120.1(3)
		C(44)-C(45)-S(2A)	117.0(2)
		C(46)-C(45)-S(2A)	122.8(2)
		C(44)-C(45)-S(2B)	126.6(3)
		C(46)-C(45)-S(2B)	112.4(3)
		S(2A)-C(45)-S(2B)	16.29(15)
		C(41)-C(46)-C(45)	119.0(3)
		O(5A)-S(2A)-O(4A)	109.6(5)

O(5A)-S(2A)-O(6A)	116.3(5)
O(4A)-S(2A)-O(6A)	110.9(4)
O(5A)-S(2A)-C(45)	110.2(4)
O(4A)-S(2A)-C(45)	105.8(2)
O(6A)-S(2A)-C(45)	103.4(5)
O(5B)-S(2B)-O(4B)	109.4(7)
O(5B)-S(2B)-O(6B)	116.9(8)
O(4B)-S(2B)-O(6B)	111.6(7)
O(5B)-S(2B)-C(45)	98.8(8)
O(4B)-S(2B)-C(45)	112.7(6)
O(6B)-S(2B)-C(45)	106.7(13)

Symmetry transformations used to generate equivalent atoms:

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

Crystal structure $\text{Cs}_4[\text{DSA-H}_2]_2 \cdot (\text{H}_2\text{O})_{13/6} \cdot \text{MeOH}$

Table 1

Operator	Dr. Volker Huch	
Diffractometer	Bruker X8 Apex	
Identification code	sh3040	
Empirical formula	$\text{C}_{20.50} \text{H}_{17.17} \text{Cs}_2 \text{N}_3 \text{O}_{9.58} \text{S}_2$	
Formula weight	788.80 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	$a = 10.8806(6) \text{ Å}$	$\alpha = 91.971(3)^\circ$
	$b = 16.1975(9) \text{ Å}$	$\beta = 106.856(3)^\circ$
	$c = 16.3259(9) \text{ Å}$	$\gamma = 96.096(3)^\circ$
Volume	$2731.6(3) \text{ Å}^3$	
Z	4	
Density (calculated)	1.918 mg/m^3	
Absorption coefficient	2.876 mm^{-1}	
F(000)	1519	
Crystal size	$0.22 \times 0.11 \times 0.04 \text{ mm}^3$	
Theta range for data collection	1.97 to 30.00°	
Index ranges	$-15 \leq h \leq 15, -22 \leq k \leq 22, -22 \leq l \leq 22$	
Reflections collected	60393	
Independent reflections	15842 [R(int) = 0.0959]	
Completeness to theta = 30.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8936 and 0.5703	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15842 / 0 / 633	
Goodness-of-fit on F^2	0.883	

Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0543$, $wR_2 = 0.1045$
R indices (all data)	$R_1 = 0.1103$, $wR_2 = 0.1183$
Largest diff. peak and hole	2.191 and -1.801 e. $\text{\AA}^{-3}$

Table 2

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the crystal structure $\text{Cs}_4[\text{DSA-H}_2]_2 \cdot (\text{H}_2\text{O})_{13/6} \cdot \text{MeOH}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

atom	x	y	z	$U(\text{eq})$
Cs(1)	8399(1)	5555(1)	3742(1)	22(1)
Cs(2)	7929(1)	2995(1)	2362(1)	32(1)
Cs(3)	10346(1)	1773(1)	4909(1)	35(1)
Cs(4)	15596(1)	6535(1)	855(1)	39(1)
C(11)	10631(6)	2228(4)	-1174(4)	34(2)
O(11)	11096(5)	1880(3)	-418(3)	54(1)
C(12)	10018(7)	1697(5)	-1912(4)	45(2)
C(13)	9531(7)	2032(4)	-2684(4)	41(2)
C(14)	9597(6)	2876(5)	-2769(4)	38(2)
C(15)	10212(6)	3420(4)	-2041(3)	31(2)
C(16)	10724(6)	3095(4)	-1244(4)	27(1)
C(21)	11282(5)	3678(4)	-491(3)	24(1)
N(22)	11316(4)	4515(3)	-516(3)	23(1)
C(23)	11860(5)	4811(4)	305(3)	23(1)
N(24)	12154(4)	4166(3)	795(3)	21(1)
N(25)	11790(4)	3426(3)	294(3)	25(1)
C(31)	11705(6)	6259(4)	-92(4)	27(1)
O(31)	11218(4)	6006(3)	-944(2)	34(1)
C(32)	11901(6)	7115(4)	124(4)	33(2)
C(33)	12375(6)	7416(4)	961(4)	32(2)
C(34)	12710(6)	6884(4)	1597(4)	34(2)

C(35)	12558(6)	6044(4)	1397(4)	27(1)
C(36)	12059(5)	5703(4)	557(4)	26(1)
C(41)	12717(5)	4126(3)	1708(3)	17(1)
C(42)	11855(5)	4067(4)	2196(3)	22(1)
C(43)	12319(5)	4032(3)	3070(3)	20(1)
C(44)	13637(5)	4054(4)	3452(3)	21(1)
C(45)	14480(5)	4113(4)	2959(3)	22(1)
C(46)	14043(5)	4152(3)	2080(3)	19(1)
S(1)	15170(1)	4223(1)	1476(1)	22(1)
O(1)	15185(4)	3375(3)	1160(2)	30(1)
O(2)	16389(4)	4575(3)	2081(2)	31(1)
O(3)	14664(4)	4741(3)	787(3)	34(1)
S(2)	11200(2)	3977(1)	3680(1)	29(1)
O(4)	10702(4)	3117(3)	3623(3)	38(1)
O(5)	10218(4)	4476(3)	3248(3)	44(1)
O(6)	11941(5)	4337(4)	4524(3)	61(2)
C(51)	6709(6)	-293(4)	7982(4)	29(1)
O(51)	7385(4)	471(3)	8177(3)	42(1)
C(52)	7097(7)	-921(4)	8534(4)	41(2)
C(53)	6440(6)	-1723(4)	8352(4)	40(2)
C(54)	5401(6)	-1904(4)	7635(4)	34(2)
C(55)	5007(6)	-1290(4)	7088(4)	30(1)
C(56)	5644(5)	-479(4)	7249(4)	23(1)
C(61)	5210(5)	147(4)	6646(4)	24(1)
N(62)	4171(4)	-5(3)	5924(3)	26(1)
C(63)	4107(5)	710(4)	5547(4)	21(1)
N(64)	5069(4)	1283(3)	6035(3)	24(1)
N(65)	5804(5)	921(3)	6731(3)	24(1)
C(71)	2140(6)	162(4)	4406(4)	32(2)
O(71)	2021(4)	-551(3)	4808(3)	37(1)
C(72)	1208(7)	230(4)	3615(4)	42(2)
C(73)	1254(7)	922(4)	3169(4)	39(2)

C(74)	2233(6)	1571(4)	3494(4)	35(2)
C(75)	3156(6)	1519(4)	4265(4)	27(1)
C(76)	3134(5)	818(4)	4735(4)	22(1)
C(81)	5488(5)	2120(3)	5904(3)	19(1)
C(82)	5046(5)	2815(4)	6230(3)	23(1)
C(83)	5513(6)	3600(4)	6074(4)	25(1)
C(84)	6349(5)	3720(4)	5593(4)	26(1)
C(85)	6749(5)	3038(3)	5253(3)	19(1)
C(86)	6351(5)	2245(4)	5419(3)	21(1)
S(3)	7842(1)	3168(1)	4620(1)	21(1)
O(7)	7703(4)	2365(2)	4153(2)	24(1)
O(8)	7419(4)	3817(3)	4060(3)	30(1)
O(9)	9115(4)	3379(3)	5228(2)	28(1)
S(4)	3877(2)	2705(1)	6808(1)	35(1)
O(10)	3955(5)	3527(3)	7218(3)	49(1)
O(13)	4240(5)	2110(3)	7419(4)	64(2)
O(12)	2690(5)	2523(5)	6139(3)	83(2)

Table 3

Bond length in [Å]

atom	bond length	atom	bond length
Cs(1)-O(6)#1	2.961(4)	Cs(3)-O(71)#5	3.230(5)
Cs(1)-O(8)	3.019(4)	Cs(3)-C(74)#6	3.535(6)
Cs(1)-O(5)	3.030(4)	Cs(3)-C(73)#6	3.548(6)
Cs(1)-O(9)#1	3.050(4)	Cs(3)-C(75)#6	3.567(6)
Cs(1)-O(10)#2	3.142(5)	Cs(3)-C(72)#6	3.586(6)
Cs(1)-O(2)#3	3.191(4)	Cs(3)-C(76)#6	3.624(5)
Cs(1)-O(12)#2	3.465(7)	Cs(3)-C(71)#6	3.627(6)
Cs(1)-C(14)#4	3.853(7)	Cs(3)-S(3)	3.6596(14)
Cs(1)-C(15)#4	3.869(6)	Cs(4)-O(3)	2.961(5)
Cs(1)-S(4)#2	3.9056(18)	Cs(4)-O(10)#1	3.047(4)
Cs(1)-S(2)#1	4.1383(15)	Cs(4)-O(1)#7	3.163(4)
Cs(1)-Cs(3)#1	4.6699(6)	Cs(4)-O(3)#7	3.255(4)
Cs(2)-O(4)	3.102(4)	Cs(4)-O(13)#1	3.463(5)
Cs(2)-O(31)#4	3.167(4)	Cs(4)-C(21)#7	3.662(6)
Cs(2)-O(2)#3	3.180(4)	Cs(4)-C(35)	3.678(6)
Cs(2)-O(7)	3.197(4)	Cs(4)-C(34)	3.766(6)
Cs(2)-O(1)#3	3.198(4)	Cs(4)-S(1)#7	3.7819(14)
Cs(2)-O(5)	3.233(5)	Cs(4)-C(36)	3.825(6)
Cs(2)-O(8)	3.250(4)	Cs(4)-S(4)#1	3.8285(16)
Cs(2)-S(3)	3.7156(14)	Cs(4)-N(25)#7	3.831(5)
Cs(2)-S(2)	3.7342(17)	C(11)-O(11)	1.357(8)
Cs(2)-S(1)#3	3.7425(14)	C(11)-C(12)	1.405(9)
Cs(2)-C(54)#5	3.860(6)	C(11)-C(16)	1.408(9)
Cs(2)-Cs(3)	4.8423(6)	C(12)-C(13)	1.374(9)
Cs(3)-O(12)#6	2.868(5)	C(13)-C(14)	1.376(9)
Cs(3)-O(7)	3.053(4)	C(14)-C(15)	1.406(8)
Cs(3)-O(9)	3.144(4)	C(14)-Cs(1)#4	3.853(7)
Cs(3)-O(4)	3.147(4)	C(15)-C(16)	1.404(8)

C(15)-Cs(1)#4	3.869(6)	S(1)-Cs(4)#7	3.7819(14)
C(16)-C(21)	1.461(8)	O(1)-Cs(4)#7	3.163(4)
C(16)-Cs(4)#7	3.845(6)	O(1)-Cs(2)#6	3.198(4)
C(21)-N(25)	1.337(7)	O(2)-Cs(2)#6	3.180(4)
C(21)-N(22)	1.355(7)	O(2)-Cs(1)#6	3.191(4)
C(21)-Cs(4)#7	3.662(5)	O(3)-Cs(4)#7	3.255(4)
N(22)-C(23)	1.346(7)	S(2)-O(4)	1.429(5)
C(23)-N(24)	1.347(7)	S(2)-O(5)	1.442(4)
C(23)-C(36)	1.465(8)	S(2)-O(6)	1.446(5)
N(24)-N(25)	1.381(6)	S(2)-Cs(1)#1	4.1383(15)
N(24)-C(41)	1.444(6)	O(6)-Cs(1)#1	2.961(4)
N(25)-Cs(4)#7	3.831(5)	C(51)-O(51)	1.348(7)
C(31)-O(31)	1.368(7)	C(51)-C(52)	1.399(9)
C(31)-C(32)	1.396(8)	C(51)-C(56)	1.401(8)
C(31)-C(36)	1.409(8)	C(52)-C(53)	1.393(9)
O(31)-Cs(2)#4	3.167(4)	C(53)-C(54)	1.369(9)
C(32)-C(33)	1.367(8)	C(54)-C(55)	1.377(8)
C(33)-C(34)	1.363(9)	C(54)-Cs(2)#5	3.860(6)
C(34)-C(35)	1.370(8)	C(55)-C(56)	1.397(8)
C(35)-C(36)	1.389(8)	C(56)-C(61)	1.456(8)
C(41)-C(46)	1.389(7)	C(61)-N(65)	1.332(7)
C(41)-C(42)	1.394(7)	C(61)-N(62)	1.370(7)
C(42)-C(43)	1.373(7)	N(62)-C(63)	1.330(7)
C(43)-C(44)	1.384(7)	C(63)-N(64)	1.360(7)
C(43)-S(2)	1.781(5)	C(63)-C(76)	1.467(8)
C(44)-C(45)	1.382(7)	N(64)-N(65)	1.377(6)
C(45)-C(46)	1.381(7)	N(64)-C(81)	1.426(7)
C(46)-S(1)	1.780(5)	C(71)-O(71)	1.360(8)
S(1)-O(3)	1.441(4)	C(71)-C(76)	1.403(8)
S(1)-O(2)	1.449(4)	C(71)-C(72)	1.407(8)
S(1)-O(1)	1.453(4)	C(71)-Cs(3)#3	3.627(6)
S(1)-Cs(2)#6	3.7425(14)	O(71)-Cs(3)#5	3.230(5)

C(72)-C(73)	1.361(9)	C(85)-S(3)	1.790(5)
C(72)-Cs(3)#3	3.586(6)	S(3)-O(8)	1.440(4)
C(73)-C(74)	1.385(9)	S(3)-O(9)	1.449(4)
C(73)-Cs(3)#3	3.548(6)	S(3)-O(7)	1.457(4)
C(74)-C(75)	1.375(8)	O(9)-Cs(1)#1	3.050(4)
C(74)-Cs(3)#3	3.535(6)	S(4)-O(13)	1.414(5)
C(75)-C(76)	1.394(8)	S(4)-O(12)	1.424(5)
C(75)-Cs(3)#3	3.567(6)	S(4)-O(10)	1.452(5)
C(76)-Cs(3)#3	3.624(5)	S(4)-Cs(4)#1	3.8285(16)
C(81)-C(86)	1.397(7)	S(4)-Cs(1)#2	3.9056(18)
C(81)-C(82)	1.416(7)	O(10)-Cs(4)#1	3.047(4)
C(82)-C(83)	1.379(8)	O(10)-Cs(1)#2	3.142(5)
C(82)-S(4)	1.788(5)	O(13)-Cs(4)#1	3.463(5)
C(83)-C(84)	1.368(8)	O(12)-Cs(3)#3	2.868(5)
C(84)-C(85)	1.385(7)	O(12)-Cs(1)#2	3.465(7)
C(85)-C(86)	1.372(8)		

Table 4

Bond angles in [°].

atom	angle	atom	angle
O(6)#1-Cs(1)-O(8)	73.88(14)	O(6)#1-Cs(1)-C(15)#4	148.53(15)
O(6)#1-Cs(1)-O(5)	123.57(14)	O(8)-Cs(1)-C(15)#4	136.52(12)
O(8)-Cs(1)-O(5)	76.16(12)	O(5)-Cs(1)-C(15)#4	69.62(13)
O(6)#1-Cs(1)-O(9)#1	78.09(12)	O(9)#1-Cs(1)-C(15)#4	75.04(12)
O(8)-Cs(1)-O(9)#1	127.66(11)	O(10)#2-Cs(1)-C(15)#4	80.43(12)
O(5)-Cs(1)-O(9)#1	84.19(12)	O(2)#3-Cs(1)-C(15)#4	82.28(12)
O(6)#1-Cs(1)-O(10)#2	98.18(13)	O(12)#2-Cs(1)-C(15)#4	82.29(13)
O(8)-Cs(1)-O(10)#2	109.37(12)	C(14)#4-Cs(1)-C(15)#4	20.98(13)
O(5)-Cs(1)-O(10)#2	136.85(12)	O(6)#1-Cs(1)-S(4)#2	86.56(11)
O(9)#1-Cs(1)-O(10)#2	117.77(12)	O(8)-Cs(1)-S(4)#2	121.86(8)
O(6)#1-Cs(1)-O(2)#3	125.56(12)	O(5)-Cs(1)-S(4)#2	149.48(9)
O(8)-Cs(1)-O(2)#3	66.69(11)	O(9)#1-Cs(1)-S(4)#2	99.14(8)
O(5)-Cs(1)-O(2)#3	81.71(12)	O(10)#2-Cs(1)-S(4)#2	20.31(9)
O(9)#1-Cs(1)-O(2)#3	156.36(10)	O(2)#3-Cs(1)-S(4)#2	83.95(8)
O(10)#2-Cs(1)-O(2)#3	63.65(12)	O(12)#2-Cs(1)-S(4)#2	21.21(9)
O(6)#1-Cs(1)-O(12)#2	76.65(15)	C(14)#4-Cs(1)-S(4)#2	79.03(11)
O(8)-Cs(1)-O(12)#2	133.48(12)	C(15)#4-Cs(1)-S(4)#2	81.87(9)
O(5)-Cs(1)-O(12)#2	150.12(13)	O(6)#1-Cs(1)-S(2)#1	13.76(10)
O(9)#1-Cs(1)-O(12)#2	78.77(11)	O(8)-Cs(1)-S(2)#1	83.41(8)
O(10)#2-Cs(1)-O(12)#2	41.46(12)	O(5)-Cs(1)-S(2)#1	118.43(9)
O(2)#3-Cs(1)-O(12)#2	104.99(11)	O(9)#1-Cs(1)-S(2)#1	64.34(7)
O(6)#1-Cs(1)-C(14)#4	127.80(15)	O(10)#2-Cs(1)-S(2)#1	104.70(8)
O(8)-Cs(1)-C(14)#4	153.21(13)	O(2)#3-Cs(1)-S(2)#1	139.30(8)
O(5)-Cs(1)-C(14)#4	78.03(14)	O(12)#2-Cs(1)-S(2)#1	75.55(9)
O(9)#1-Cs(1)-C(14)#4	55.71(12)	C(14)#4-Cs(1)-S(2)#1	115.57(10)
O(10)#2-Cs(1)-C(14)#4	84.97(14)	C(15)#4-Cs(1)-S(2)#1	136.55(10)
O(2)#3-Cs(1)-C(14)#4	102.59(12)	S(4)#2-Cs(1)-S(2)#1	89.65(3)
O(12)#2-Cs(1)-C(14)#4	72.10(14)	O(6)#1-Cs(1)-Cs(3)#1	67.37(12)

O(8)-Cs(1)-Cs(3)#1	141.20(8)	O(31)#4-Cs(2)-S(3)	143.16(8)
O(5)-Cs(1)-Cs(3)#1	124.35(9)	O(2)#3-Cs(2)-S(3)	86.52(7)
O(9)#1-Cs(1)-Cs(3)#1	41.83(7)	O(7)-Cs(2)-S(3)	22.78(7)
O(10)#2-Cs(1)-Cs(3)#1	78.88(9)	O(1)#3-Cs(2)-S(3)	107.67(7)
O(2)#3-Cs(1)-Cs(3)#1	141.13(8)	O(5)-Cs(2)-S(3)	76.62(9)
O(12)#2-Cs(1)-Cs(3)#1	37.74(8)	O(8)-Cs(2)-S(3)	22.61(7)
C(14)#4-Cs(1)-Cs(3)#1	62.20(10)	O(4)-Cs(2)-S(2)	21.71(8)
C(15)#4-Cs(1)-Cs(3)#1	81.64(9)	O(31)#4-Cs(2)-S(2)	80.54(8)
S(4)#2-Cs(1)-Cs(3)#1	58.86(3)	O(2)#3-Cs(2)-S(2)	100.74(8)
S(2)#1-Cs(1)-Cs(3)#1	58.09(3)	O(7)-Cs(2)-S(2)	83.89(7)
O(4)-Cs(2)-O(31)#4	94.73(11)	O(1)#3-Cs(2)-S(2)	143.91(8)
O(4)-Cs(2)-O(2)#3	120.84(11)	O(5)-Cs(2)-S(2)	22.43(8)
O(31)#4-Cs(2)-O(2)#3	73.17(10)	O(8)-Cs(2)-S(2)	76.02(7)
O(4)-Cs(2)-O(7)	72.10(10)	S(3)-Cs(2)-S(2)	73.32(3)
O(31)#4-Cs(2)-O(7)	163.45(10)	O(4)-Cs(2)-S(1)#3	143.15(9)
O(2)#3-Cs(2)-O(7)	104.50(10)	O(31)#4-Cs(2)-S(1)#3	76.75(8)
O(4)-Cs(2)-O(1)#3	165.28(11)	O(2)#3-Cs(2)-S(1)#3	22.32(7)
O(31)#4-Cs(2)-O(1)#3	79.15(10)	O(7)-Cs(2)-S(1)#3	107.54(7)
O(2)#3-Cs(2)-O(1)#3	44.64(10)	O(1)#3-Cs(2)-S(1)#3	22.45(7)
O(7)-Cs(2)-O(1)#3	111.11(10)	O(5)-Cs(2)-S(1)#3	100.65(8)
O(4)-Cs(2)-O(5)	44.01(11)	O(8)-Cs(2)-S(1)#3	76.21(7)
O(31)#4-Cs(2)-O(5)	69.57(11)	S(3)-Cs(2)-S(1)#3	95.99(3)
O(2)#3-Cs(2)-O(5)	78.81(10)	S(2)-Cs(2)-S(1)#3	122.85(4)
O(7)-Cs(2)-O(5)	93.88(11)	O(4)-Cs(2)-C(54)#5	134.17(12)
O(1)#3-Cs(2)-O(5)	121.48(11)	O(31)#4-Cs(2)-C(54)#5	130.96(12)
O(4)-Cs(2)-O(8)	80.44(10)	O(2)#3-Cs(2)-C(54)#5	82.01(12)
O(31)#4-Cs(2)-O(8)	125.54(10)	O(7)-Cs(2)-C(54)#5	63.42(12)
O(2)#3-Cs(2)-O(8)	64.19(10)	O(1)#3-Cs(2)-C(54)#5	54.21(12)
O(7)-Cs(2)-O(8)	43.88(10)	O(5)-Cs(2)-C(54)#5	145.31(12)
O(1)#3-Cs(2)-O(8)	92.16(9)	O(8)-Cs(2)-C(54)#5	75.41(12)
O(5)-Cs(2)-O(8)	70.27(10)	S(3)-Cs(2)-C(54)#5	73.59(10)
O(4)-Cs(2)-S(3)	69.40(8)	S(2)-Cs(2)-C(54)#5	146.55(10)

S(1)#3-Cs(2)-C(54)#5	65.67(10)	C(74)#6-Cs(3)-C(73)#6	22.56(15)
O(4)-Cs(2)-Cs(3)	39.55(8)	O(12)#6-Cs(3)-C(75)#6	67.13(14)
O(31)#4-Cs(2)-Cs(3)	132.65(8)	O(7)-Cs(3)-C(75)#6	138.01(11)
O(2)#3-Cs(2)-Cs(3)	132.88(7)	O(9)-Cs(3)-C(75)#6	131.17(13)
O(7)-Cs(2)-Cs(3)	38.15(7)	O(4)-Cs(3)-C(75)#6	70.03(12)
O(1)#3-Cs(2)-Cs(3)	148.19(7)	O(71)#5-Cs(3)-C(75)#6	135.93(13)
O(5)-Cs(2)-Cs(3)	77.77(8)	C(74)#6-Cs(3)-C(75)#6	22.33(13)
O(8)-Cs(2)-Cs(3)	69.57(7)	C(73)#6-Cs(3)-C(75)#6	39.33(15)
S(3)-Cs(2)-Cs(3)	48.46(2)	O(12)#6-Cs(3)-C(72)#6	107.29(16)
S(2)-Cs(2)-Cs(3)	58.51(3)	O(7)-Cs(3)-C(72)#6	116.05(12)
S(1)#3-Cs(2)-Cs(3)	144.18(2)	O(9)-Cs(3)-C(72)#6	154.75(13)
C(54)#5-Cs(2)-Cs(3)	95.08(9)	O(4)-Cs(3)-C(72)#6	89.87(14)
O(12)#6-Cs(3)-O(7)	132.92(15)	O(71)#5-Cs(3)-C(72)#6	93.67(15)
O(12)#6-Cs(3)-O(9)	87.09(15)	C(74)#6-Cs(3)-C(72)#6	38.96(17)
O(7)-Cs(3)-O(9)	45.87(10)	C(73)#6-Cs(3)-C(72)#6	21.98(15)
O(12)#6-Cs(3)-O(4)	89.71(16)	C(75)#6-Cs(3)-C(72)#6	45.28(16)
O(7)-Cs(3)-O(4)	73.44(10)	O(12)#6-Cs(3)-C(76)#6	68.10(15)
O(9)-Cs(3)-O(4)	69.09(10)	O(7)-Cs(3)-C(76)#6	152.84(11)
O(12)#6-Cs(3)-O(71)#5	129.57(14)	O(9)-Cs(3)-C(76)#6	149.37(12)
O(7)-Cs(3)-O(71)#5	66.33(10)	O(4)-Cs(3)-C(76)#6	92.25(12)
O(9)-Cs(3)-O(71)#5	92.63(10)	O(71)#5-Cs(3)-C(76)#6	116.82(12)
O(4)-Cs(3)-O(71)#5	136.71(11)	C(74)#6-Cs(3)-C(76)#6	39.37(14)
O(12)#6-Cs(3)-C(74)#6	86.29(15)	C(73)#6-Cs(3)-C(76)#6	45.88(14)
O(7)-Cs(3)-C(74)#6	116.46(12)	C(75)#6-Cs(3)-C(76)#6	22.34(13)
O(9)-Cs(3)-C(74)#6	125.24(13)	C(72)#6-Cs(3)-C(76)#6	39.28(14)
O(4)-Cs(3)-C(74)#6	56.58(13)	O(12)#6-Cs(3)-C(71)#6	88.37(16)
O(71)#5-Cs(3)-C(74)#6	131.20(14)	O(7)-Cs(3)-C(71)#6	137.53(12)
O(12)#6-Cs(3)-C(73)#6	106.43(15)	O(9)-Cs(3)-C(71)#6	170.11(13)
O(7)-Cs(3)-C(73)#6	106.97(12)	O(4)-Cs(3)-C(71)#6	102.11(13)
O(9)-Cs(3)-C(73)#6	134.60(13)	O(71)#5-Cs(3)-C(71)#6	97.03(13)
O(4)-Cs(3)-C(73)#6	67.89(14)	C(74)#6-Cs(3)-C(71)#6	45.59(16)
O(71)#5-Cs(3)-C(73)#6	108.97(15)	C(73)#6-Cs(3)-C(71)#6	39.26(15)

C(75)#6-Cs(3)-C(71)#6	39.03(15)	O(3)#7-Cs(4)-C(35)	104.76(12)
C(72)#6-Cs(3)-C(71)#6	22.49(13)	O(13)#1-Cs(4)-C(35)	73.54(12)
C(76)#6-Cs(3)-C(71)#6	22.32(13)	C(21)#7-Cs(4)-C(35)	161.31(13)
O(12)#6-Cs(3)-S(3)	110.11(13)	O(3)-Cs(4)-C(34)	85.49(12)
O(7)-Cs(3)-S(3)	22.85(7)	O(10)#1-Cs(4)-C(34)	65.33(13)
O(9)-Cs(3)-S(3)	23.03(7)	O(1)#7-Cs(4)-C(34)	108.46(12)
O(4)-Cs(3)-S(3)	69.73(7)	O(3)#7-Cs(4)-C(34)	121.49(12)
O(71)#5-Cs(3)-S(3)	78.72(8)	O(13)#1-Cs(4)-C(34)	56.64(13)
C(74)#6-Cs(3)-S(3)	123.82(11)	C(21)#7-Cs(4)-C(34)	170.59(12)
C(73)#6-Cs(3)-S(3)	122.70(11)	C(35)-Cs(4)-C(34)	21.17(13)
C(75)#6-Cs(3)-S(3)	139.67(10)	O(3)-Cs(4)-S(1)#7	74.93(8)
C(72)#6-Cs(3)-S(3)	136.83(11)	O(10)#1-Cs(4)-S(1)#7	159.33(10)
C(76)#6-Cs(3)-S(3)	161.98(10)	O(1)#7-Cs(4)-S(1)#7	21.90(8)
C(71)#6-Cs(3)-S(3)	159.26(10)	O(3)#7-Cs(4)-S(1)#7	22.04(7)
O(3)-Cs(4)-O(10)#1	84.66(12)	O(13)#1-Cs(4)-S(1)#7	157.08(9)
O(3)-Cs(4)-O(1)#7	94.69(11)	C(21)#7-Cs(4)-S(1)#7	74.09(9)
O(10)#1-Cs(4)-O(1)#7	173.78(11)	C(35)-Cs(4)-S(1)#7	105.15(9)
O(3)-Cs(4)-O(3)#7	57.32(12)	C(34)-Cs(4)-S(1)#7	115.31(10)
O(10)#1-Cs(4)-O(3)#7	138.34(11)	O(3)-Cs(4)-C(36)	56.70(12)
O(1)#7-Cs(4)-O(3)#7	43.82(10)	O(10)#1-Cs(4)-C(36)	87.66(13)
O(3)-Cs(4)-O(13)#1	122.15(11)	O(1)#7-Cs(4)-C(36)	86.83(11)
O(10)#1-Cs(4)-O(13)#1	42.09(12)	O(3)#7-Cs(4)-C(36)	84.93(11)
O(1)#7-Cs(4)-O(13)#1	135.47(11)	O(13)#1-Cs(4)-C(36)	93.26(12)
O(3)#7-Cs(4)-O(13)#1	178.06(12)	C(21)#7-Cs(4)-C(36)	150.49(13)
O(3)-Cs(4)-C(21)#7	97.91(12)	C(35)-Cs(4)-C(36)	21.23(12)
O(10)#1-Cs(4)-C(21)#7	106.12(12)	C(34)-Cs(4)-C(36)	37.09(12)
O(1)#7-Cs(4)-C(21)#7	80.10(11)	S(1)#7-Cs(4)-C(36)	83.93(9)
O(3)#7-Cs(4)-C(21)#7	67.32(11)	O(3)-Cs(4)-S(4)#1	104.02(8)
O(13)#1-Cs(4)-C(21)#7	114.59(12)	O(10)#1-Cs(4)-S(4)#1	20.64(9)
O(3)-Cs(4)-C(35)	64.44(12)	O(1)#7-Cs(4)-S(4)#1	157.03(8)
O(10)#1-Cs(4)-C(35)	67.82(13)	O(3)#7-Cs(4)-S(4)#1	158.95(8)
O(1)#7-Cs(4)-C(35)	106.31(12)	O(13)#1-Cs(4)-S(4)#1	21.62(9)

C(21)#7-Cs(4)-S(4)#1	109.83(9)	C(21)-C(16)-Cs(4)#7	71.8(3)
C(35)-Cs(4)-S(4)#1	71.11(9)	N(25)-C(21)-N(22)	113.8(5)
C(34)-Cs(4)-S(4)#1	60.78(10)	N(25)-C(21)-C(16)	122.5(5)
S(1)#7-Cs(4)-S(4)#1	176.08(3)	N(22)-C(21)-C(16)	123.8(5)
C(36)-Cs(4)-S(4)#1	92.34(9)	N(25)-C(21)-Cs(4)#7	86.9(3)
O(3)-Cs(4)-N(25)#7	103.37(11)	N(22)-C(21)-Cs(4)#7	98.5(3)
O(10)#1-Cs(4)-N(25)#7	125.82(11)	C(16)-C(21)-Cs(4)#7	85.9(3)
O(1)#7-Cs(4)-N(25)#7	60.35(10)	C(23)-N(22)-C(21)	104.6(5)
O(3)#7-Cs(4)-N(25)#7	57.77(10)	N(22)-C(23)-N(24)	108.8(5)
O(13)#1-Cs(4)-N(25)#7	123.88(11)	N(22)-C(23)-C(36)	121.9(5)
C(21)#7-Cs(4)-N(25)#7	20.40(10)	N(24)-C(23)-C(36)	129.2(5)
C(35)-Cs(4)-N(25)#7	162.39(11)	C(23)-N(24)-N(25)	110.1(4)
C(34)-Cs(4)-N(25)#7	165.84(13)	C(23)-N(24)-C(41)	132.0(5)
S(1)#7-Cs(4)-N(25)#7	57.99(7)	N(25)-N(24)-C(41)	117.9(4)
C(36)-Cs(4)-N(25)#7	141.48(11)	C(21)-N(25)-N(24)	102.7(5)
S(4)#1-Cs(4)-N(25)#7	125.84(7)	C(21)-N(25)-Cs(4)#7	72.7(3)
O(11)-C(11)-C(12)	118.3(6)	N(24)-N(25)-Cs(4)#7	101.8(3)
O(11)-C(11)-C(16)	122.6(6)	O(31)-C(31)-C(32)	117.2(5)
C(12)-C(11)-C(16)	119.1(6)	O(31)-C(31)-C(36)	123.1(5)
C(13)-C(12)-C(11)	119.5(7)	C(32)-C(31)-C(36)	119.6(6)
C(12)-C(13)-C(14)	122.7(6)	C(31)-O(31)-Cs(2)#4	121.4(4)
C(13)-C(14)-C(15)	118.8(6)	C(33)-C(32)-C(31)	120.7(6)
C(13)-C(14)-Cs(1)#4	134.6(5)	C(34)-C(33)-C(32)	120.2(6)
C(15)-C(14)-Cs(1)#4	80.2(4)	C(33)-C(34)-C(35)	120.0(6)
C(16)-C(15)-C(14)	119.8(6)	C(33)-C(34)-Cs(4)	88.4(4)
C(16)-C(15)-Cs(1)#4	136.0(4)	C(35)-C(34)-Cs(4)	75.8(4)
C(14)-C(15)-Cs(1)#4	78.9(4)	C(34)-C(35)-C(36)	122.1(6)
C(15)-C(16)-C(11)	120.1(6)	C(34)-C(35)-Cs(4)	83.0(4)
C(15)-C(16)-C(21)	118.2(6)	C(36)-C(35)-Cs(4)	85.3(3)
C(11)-C(16)-C(21)	121.6(5)	C(35)-C(36)-C(31)	117.3(6)
C(15)-C(16)-Cs(4)#7	103.9(4)	C(35)-C(36)-C(23)	124.7(6)
C(11)-C(16)-Cs(4)#7	97.0(4)	C(31)-C(36)-C(23)	118.1(5)

C(35)-C(36)-Cs(4)	73.4(3)	O(1)-S(1)-Cs(4)	141.33(17)
C(31)-C(36)-Cs(4)	88.2(4)	C(46)-S(1)-Cs(4)	107.70(18)
C(23)-C(36)-Cs(4)	109.0(3)	Cs(2)#6-S(1)-Cs(4)	123.83(4)
C(46)-C(41)-C(42)	121.9(5)	Cs(4)#7-S(1)-Cs(4)	90.08(3)
C(46)-C(41)-N(24)	121.9(5)	S(1)-O(1)-Cs(4)#7	103.8(2)
C(42)-C(41)-N(24)	116.2(5)	S(1)-O(1)-Cs(2)#6	100.4(2)
C(43)-C(42)-C(41)	119.6(5)	Cs(4)#7-O(1)-Cs(2)#6	125.93(12)
C(42)-C(43)-C(44)	119.4(5)	S(1)-O(2)-Cs(2)#6	101.2(2)
C(42)-C(43)-S(2)	118.7(4)	S(1)-O(2)-Cs(1)#6	160.2(2)
C(44)-C(43)-S(2)	121.9(4)	Cs(2)#6-O(2)-Cs(1)#6	91.31(10)
C(45)-C(44)-C(43)	120.3(5)	S(1)-O(3)-Cs(4)	122.5(2)
C(46)-C(45)-C(44)	121.6(5)	S(1)-O(3)-Cs(4)#7	100.0(2)
C(45)-C(46)-C(41)	117.2(5)	Cs(4)-O(3)-Cs(4)#7	122.68(12)
C(45)-C(46)-S(1)	119.8(4)	O(4)-S(2)-O(5)	111.8(3)
C(41)-C(46)-S(1)	123.0(4)	O(4)-S(2)-O(6)	116.4(3)
O(3)-S(1)-O(2)	114.4(3)	O(5)-S(2)-O(6)	112.5(3)
O(3)-S(1)-O(1)	111.8(3)	O(4)-S(2)-C(43)	105.4(2)
O(2)-S(1)-O(1)	113.2(2)	O(5)-S(2)-C(43)	104.7(3)
O(3)-S(1)-C(46)	105.9(2)	O(6)-S(2)-C(43)	104.9(3)
O(2)-S(1)-C(46)	105.1(2)	O(4)-S(2)-Cs(2)	53.39(18)
O(1)-S(1)-C(46)	105.6(2)	O(5)-S(2)-Cs(2)	58.8(2)
O(3)-S(1)-Cs(2)#6	141.89(16)	O(6)-S(2)-Cs(2)	143.9(2)
O(2)-S(1)-Cs(2)#6	56.47(17)	C(43)-S(2)-Cs(2)	111.24(19)
O(1)-S(1)-Cs(2)#6	57.19(17)	O(4)-S(2)-Cs(1)#1	96.79(19)
C(46)-S(1)-Cs(2)#6	112.22(18)	O(5)-S(2)-Cs(1)#1	104.33(19)
O(3)-S(1)-Cs(4)#7	57.95(18)	O(6)-S(2)-Cs(1)#1	29.2(2)
O(2)-S(1)-Cs(4)#7	129.98(16)	C(43)-S(2)-Cs(1)#1	133.19(19)
O(1)-S(1)-Cs(4)#7	54.31(16)	Cs(2)-S(2)-Cs(1)#1	115.10(4)
C(46)-S(1)-Cs(4)#7	124.88(18)	S(2)-O(4)-Cs(2)	104.9(2)
Cs(2)#6-S(1)-Cs(4)#7	97.69(3)	S(2)-O(4)-Cs(3)	136.8(3)
O(3)-S(1)-Cs(4)	39.46(19)	Cs(2)-O(4)-Cs(3)	101.58(12)
O(2)-S(1)-Cs(4)	76.32(18)	S(2)-O(5)-Cs(1)	137.0(3)

S(2)-O(5)-Cs(2)	98.7(2)	C(71)-O(71)-Cs(3)#5	135.8(3)
Cs(1)-O(5)-Cs(2)	93.31(11)	C(73)-C(72)-C(71)	121.2(7)
S(2)-O(6)-Cs(1)#1	137.1(3)	C(73)-C(72)-Cs(3)#3	77.4(4)
O(51)-C(51)-C(52)	118.4(6)	C(71)-C(72)-Cs(3)#3	80.4(3)
O(51)-C(51)-C(56)	122.4(6)	C(72)-C(73)-C(74)	119.7(6)
C(52)-C(51)-C(56)	119.2(6)	C(72)-C(73)-Cs(3)#3	80.6(4)
C(53)-C(52)-C(51)	120.4(6)	C(74)-C(73)-Cs(3)#3	78.2(4)
C(54)-C(53)-C(52)	120.3(6)	C(75)-C(74)-C(73)	120.3(6)
C(53)-C(54)-C(55)	119.8(6)	C(75)-C(74)-Cs(3)#3	80.2(3)
C(53)-C(54)-Cs(2)#5	124.3(4)	C(73)-C(74)-Cs(3)#3	79.3(4)
C(55)-C(54)-Cs(2)#5	99.7(4)	C(74)-C(75)-C(76)	121.2(6)
C(54)-C(55)-C(56)	121.5(6)	C(74)-C(75)-Cs(3)#3	77.5(3)
C(55)-C(56)-C(51)	118.8(6)	C(76)-C(75)-Cs(3)#3	81.1(3)
C(55)-C(56)-C(61)	119.6(5)	C(75)-C(76)-C(71)	118.5(5)
C(51)-C(56)-C(61)	121.6(6)	C(75)-C(76)-C(63)	124.1(6)
N(65)-C(61)-N(62)	113.2(5)	C(71)-C(76)-C(63)	117.4(5)
N(65)-C(61)-C(56)	123.2(5)	C(75)-C(76)-Cs(3)#3	76.5(3)
N(62)-C(61)-C(56)	123.6(6)	C(71)-C(76)-Cs(3)#3	79.0(3)
C(63)-N(62)-C(61)	105.0(5)	C(63)-C(76)-Cs(3)#3	116.0(3)
N(62)-C(63)-N(64)	108.8(5)	C(86)-C(81)-C(82)	119.5(5)
N(62)-C(63)-C(76)	123.1(5)	C(86)-C(81)-N(64)	117.8(5)
N(64)-C(63)-C(76)	128.2(5)	C(82)-C(81)-N(64)	122.7(5)
C(63)-N(64)-N(65)	109.8(5)	C(83)-C(82)-C(81)	118.4(5)
C(63)-N(64)-C(81)	132.0(5)	C(83)-C(82)-S(4)	119.3(4)
N(65)-N(64)-C(81)	117.9(5)	C(81)-C(82)-S(4)	122.3(5)
C(61)-N(65)-N(64)	103.2(5)	C(84)-C(83)-C(82)	121.9(5)
O(71)-C(71)-C(76)	123.6(5)	C(83)-C(84)-C(85)	119.5(6)
O(71)-C(71)-C(72)	117.3(6)	C(86)-C(85)-C(84)	120.7(5)
C(76)-C(71)-C(72)	119.2(6)	C(86)-C(85)-S(3)	118.3(4)
O(71)-C(71)-Cs(3)#3	114.5(4)	C(84)-C(85)-S(3)	120.9(5)
C(76)-C(71)-Cs(3)#3	78.7(3)	C(85)-C(86)-C(81)	119.9(5)
C(72)-C(71)-Cs(3)#3	77.1(3)	O(8)-S(3)-O(9)	114.1(3)

O(8)-S(3)-O(7)	112.6(2)	O(13)-S(4)-O(12)	118.6(4)
O(9)-S(3)-O(7)	112.6(2)	O(13)-S(4)-O(10)	111.6(3)
O(8)-S(3)-C(85)	106.2(2)	O(12)-S(4)-O(10)	110.1(3)
O(9)-S(3)-C(85)	105.6(2)	O(13)-S(4)-C(82)	108.1(3)
O(7)-S(3)-C(85)	105.0(2)	O(12)-S(4)-C(82)	102.6(3)
O(8)-S(3)-Cs(3)	135.80(17)	O(10)-S(4)-C(82)	104.6(3)
O(9)-S(3)-Cs(3)	58.08(16)	O(13)-S(4)-Cs(4)#1	64.5(2)
O(7)-S(3)-Cs(3)	54.47(16)	O(12)-S(4)-Cs(4)#1	128.4(2)
C(85)-S(3)-Cs(3)	117.94(18)	O(10)-S(4)-Cs(4)#1	47.70(18)
O(8)-S(3)-Cs(2)	60.20(16)	C(82)-S(4)-Cs(4)#1	126.40(19)
O(9)-S(3)-Cs(2)	112.75(16)	O(13)-S(4)-Cs(1)#2	140.67(18)
O(7)-S(3)-Cs(2)	58.18(16)	O(12)-S(4)-Cs(1)#2	61.7(3)
C(85)-S(3)-Cs(2)	141.62(18)	O(10)-S(4)-Cs(1)#2	48.7(2)
Cs(3)-S(3)-Cs(2)	82.07(3)	C(82)-S(4)-Cs(1)#2	110.0(2)
S(3)-O(7)-Cs(3)	102.68(19)	Cs(4)#1-S(4)-Cs(1)#2	84.87(3)
S(3)-O(7)-Cs(2)	99.04(19)	S(4)-O(10)-Cs(4)#1	111.7(2)
Cs(3)-O(7)-Cs(2)	101.55(10)	S(4)-O(10)-Cs(1)#2	111.0(3)
S(3)-O(8)-Cs(1)	139.0(2)	Cs(4)#1-O(10)-Cs(1)#2	114.98(12)
S(3)-O(8)-Cs(2)	97.19(19)	S(4)-O(13)-Cs(4)#1	93.9(2)
Cs(1)-O(8)-Cs(2)	93.17(10)	S(4)-O(12)-Cs(3)#3	166.8(5)
S(3)-O(9)-Cs(1)#1	158.8(2)	S(4)-O(12)-Cs(1)#2	97.1(3)
S(3)-O(9)-Cs(3)	98.89(19)	Cs(3)#3-O(12)-Cs(1)#2	94.55(16)
Cs(1)#1-O(9)-Cs(3)	97.85(10)		

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+2,-y+1,-z #5 -x+1,-y,-z+1 #6 x+1,y,z

#7 -x+3,-y+1,-z

Crystal structure Cs₅[Fe(DSA)₂] · 10.74 H₂O

Table1

Operator	Dr. Volker Huch	
Diffractometer	Bruker X8 Area	
Identification code	sh2862a	
Empirical formula	C ₄₀ H _{43.48} Cs ₅ Fe N ₆ O _{26.74} S ₄	
Formula weight	1884.77 g/mol	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.0813(6) Å	α = 90°
	b = 11.2287(4) Å	β = 98.059(2)°
	c = 26.4674(8) Å	γ = 90°
Volume	6203.4(3) Å ³	
Z	4	
Density (calculated)	2.018 mg/m ³	
Absorption coefficient	3.352 mm ⁻¹	
F(000)	3618	
Crystal size	0.59 x 0.23 x 0.19 mm ³	
Theta range for data collection	1.55 to 26.00°	
Index ranges	-26 ≤ h ≤ 26, -13 ≤ k ≤ 13, -32 ≤ l ≤ 32	
Reflections collected	44730	
Independent reflections	6104 [R(int) = 0.0322]	
Completeness to theta = 26.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5684 and 0.2445	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6104 / 0 / 420	

Goodness-of-fit on F^2	1.256
Final R indices [$I > 2 \sigma(I)$]	$R_1 = 0.0682$, $wR_2 = 0.1524$
R indices (all data)	$R_1 = 0.0778$, $wR_2 = 0.1588$
Largest diff. peak and hole	1.896 and -1.060 e.Å ⁻³

Table 2

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the crystal structure $\text{Cs}_5[\text{Fe}(\text{HSS})_2] \cdot 10.74 \text{ H}_2\text{O}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

atom	x	y	z	U(eq)
Fe(1)	5000	4541(2)	7500	24(1)
C(11)	4221(4)	2421(9)	7685(3)	27(2)
C(12)	3838(4)	2400(8)	7194(3)	27(2)
C(13)	3502(5)	1367(10)	7037(4)	40(2)
C(14)	3511(6)	386(9)	7347(4)	43(3)
C(15)	3853(6)	417(10)	7828(4)	45(3)
C(16)	4206(5)	1384(10)	7992(4)	36(2)
O(11)	4557(3)	3345(6)	7864(2)	31(1)
C(21)	3778(4)	3454(8)	6876(3)	24(2)
N(22)	4158(3)	4445(7)	6968(3)	24(2)
C(23)	3947(4)	5213(8)	6609(3)	22(2)
N(24)	3452(4)	4694(7)	6309(3)	26(2)
N(25)	3333(4)	3591(7)	6483(3)	28(2)
C(31)	4193(4)	6429(8)	6578(3)	24(2)
C(32)	4817(4)	6653(8)	6822(3)	23(2)
C(33)	5032(5)	7851(9)	6846(4)	32(2)
C(34)	4628(5)	8776(10)	6627(4)	38(2)
C(35)	4030(5)	8513(10)	6376(4)	35(2)
C(36)	3809(5)	7350(9)	6363(3)	29(2)
O(32)	5219(3)	5821(6)	7026(2)	28(1)

C(41)	3046(4)	5098(8)	5856(3)	23(2)
C(42)	2415(4)	5334(8)	5899(3)	27(2)
C(43)	1999(4)	5695(8)	5469(3)	26(2)
C(44)	2228(5)	5914(9)	5014(3)	32(2)
C(45)	2868(4)	5652(9)	4980(3)	32(2)
C(46)	3273(4)	5189(9)	5385(3)	27(2)
S(1)	1167(1)	5815(3)	5499(1)	38(1)
O(1)	861(3)	5280(8)	5030(3)	48(2)
O(2)	1040(4)	5121(10)	5932(3)	58(2)
O(3)	1029(5)	7061(9)	5539(4)	73(3)
S(2)	4042(1)	4669(2)	5277(1)	30(1)
O(4)	4482(3)	5631(7)	5394(3)	50(2)
O(5)	4191(3)	3647(7)	5607(3)	38(2)
O(6)	3937(4)	4337(9)	4741(3)	54(2)
Cs(1)	5611(1)	4202(1)	6109(1)	41(1)
Cs(2)	5159(1)	7908(1)	5450(1)	40(1)
Cs(3)	7384(1)	7113(2)	5592(1)	50(1)
Cs(4)	7209(4)	6972(10)	5900(3)	88(3)
O(1W)	6443(5)	7857(11)	6258(4)	61(3)
O(2W)	3469(4)	6436(12)	7872(4)	84(4)
O(3A)	2488(11)	7180(20)	7009(10)	73(7)
O(3B)	2600(14)	6500(30)	7062(11)	60(8)
O(4A)	8714(17)	6260(20)	5674(11)	70(8)
O(4B)	8437(11)	6662(19)	5345(10)	95(7)
O(5A)	7018(11)	5280(20)	6396(8)	76(6)
O(5B)	7131(10)	4450(20)	6530(11)	83(8)
O(6W)	7241(10)	3040(20)	6285(8)	79(6)

Table 3

Bond lengths in [Å]

atom	bond length	atom	bond length
Fe(1)-O(11)#1	1.963(6)	C(31)-C(36)	1.386(13)
Fe(1)-O(11)	1.963(7)	C(31)-C(32)	1.404(12)
Fe(1)-O(32)	2.003(7)	C(32)-O(32)	1.324(11)
Fe(1)-O(32)#1	2.003(6)	C(32)-C(33)	1.418(13)
Fe(1)-N(22)	2.109(7)	C(32)-Cs(1)	3.850(9)
Fe(1)-N(22)#1	2.109(7)	C(33)-C(34)	1.414(15)
Fe(1)-Cs(1)	4.0851(6)	C(33)-Cs(2)	3.744(9)
Fe(1)-Cs(1)#1	4.0851(6)	C(34)-C(35)	1.374(14)
C(11)-O(11)	1.306(11)	C(34)-Cs(2)	3.591(10)
C(11)-C(16)	1.424(14)	C(35)-C(36)	1.385(14)
C(11)-C(12)	1.431(13)	C(35)-Cs(2)	3.712(10)
C(11)-Cs(1)#1	3.741(9)	O(32)-Cs(1)	3.233(6)
C(12)-C(13)	1.392(14)	C(41)-C(42)	1.377(12)
C(12)-C(21)	1.448(12)	C(41)-C(46)	1.400(12)
C(13)-C(14)	1.373(14)	C(41)-Cs(3)#2	3.660(9)
C(13)-Cs(4)#2	3.828(13)	C(42)-C(43)	1.394(12)
C(14)-C(15)	1.372(15)	C(42)-Cs(3)#2	3.706(10)
C(15)-C(16)	1.353(16)	C(42)-Cs(4)#2	3.801(14)
O(11)-Cs(1)#1	2.952(6)	C(43)-C(44)	1.382(13)
C(21)-N(25)	1.308(11)	C(43)-S(1)	1.773(9)
C(21)-N(22)	1.372(12)	C(44)-C(45)	1.396(13)
N(22)-C(23)	1.314(11)	C(44)-Cs(3)#3	3.893(11)
C(23)-N(24)	1.352(11)	C(45)-C(46)	1.374(12)
C(23)-C(31)	1.467(12)	C(45)-Cs(3)#3	3.463(11)
N(24)-N(25)	1.356(11)	C(45)-Cs(4)#3	3.746(15)
N(24)-C(41)	1.446(10)	C(46)-S(2)	1.785(9)
N(25)-Cs(4)#2	3.206(11)	C(46)-Cs(3)#3	3.780(10)
N(25)-Cs(3)#2	3.316(7)	S(1)-O(3)	1.436(10)

S(1)-O(2)	1.441(9)	Cs(2)-O(1W)	3.207(11)
S(1)-O(1)	1.447(8)	Cs(2)-O(6)#3	3.241(9)
S(1)-Cs(2)#4	3.769(3)	Cs(2)-O(2)#7	3.254(10)
S(1)-Cs(2)#2	3.886(3)	Cs(2)-O(1)#7	3.313(9)
O(1)-Cs(2)#4	3.100(8)	Cs(2)-O(3)#4	3.359(11)
O(1)-Cs(2)#2	3.313(9)	Cs(2)-O(5)#3	3.717(7)
O(2)-Cs(2)#2	3.254(10)	Cs(2)-S(1)#4	3.769(3)
O(3)-Cs(1)#5	3.034(9)	Cs(3)-O(4A)	2.94(3)
O(3)-Cs(2)#4	3.359(11)	Cs(3)-O(1W)	2.953(10)
S(2)-O(4)	1.429(8)	Cs(3)-O(5A)	3.13(3)
S(2)-O(5)	1.450(8)	Cs(3)-O(6)#3	3.239(9)
S(2)-O(6)	1.452(8)	Cs(3)-N(25)#7	3.316(8)
S(2)-Cs(1)	3.744(2)	Cs(3)-Cs(3)#8	3.353(5)
S(2)-Cs(2)#3	3.975(3)	Cs(3)-C(45)#3	3.463(11)
S(2)-Cs(1)#3	4.043(2)	Cs(3)-C(41)#7	3.660(9)
S(2)-Cs(3)#3	4.048(3)	Cs(3)-C(42)#7	3.706(10)
O(4)-Cs(2)	2.922(8)	Cs(3)-C(46)#3	3.780(10)
O(4)-Cs(1)	3.248(8)	Cs(3)-C(44)#3	3.893(11)
O(5)-Cs(1)	3.161(7)	Cs(3)-S(2)#3	4.049(3)
O(5)-Cs(2)#3	3.717(7)	Cs(4)-O(1W)	2.217(16)
O(6)-Cs(1)#3	3.044(8)	Cs(4)-O(6)#3	3.118(11)
O(6)-Cs(4)#3	3.118(11)	Cs(4)-O(4B)	3.17(3)
O(6)-Cs(3)#3	3.239(8)	Cs(4)-N(25)#7	3.206(11)
O(6)-Cs(2)#3	3.241(9)	Cs(4)-O(5B)	3.30(3)
Cs(1)-O(11)#1	2.952(6)	Cs(4)-O(4B)#8	3.72(3)
Cs(1)-O(3)#6	3.034(9)	Cs(4)-C(45)#3	3.746(15)
Cs(1)-O(6)#3	3.044(8)	Cs(4)-O(2W)#1	3.778(14)
Cs(1)-O(5A)	3.20(2)	Cs(4)-C(42)#7	3.801(14)
Cs(1)-O(5B)	3.253(19)	Cs(4)-C(13)#7	3.828(13)
Cs(1)-O(6W)	3.64(2)	O(2W)-Cs(4)#1	3.778(14)
Cs(1)-C(11)#1	3.741(9)	O(4B)-Cs(4)#8	3.72(3)
Cs(2)-O(1)#4	3.100(8)	O(5B)-O(6W)	1.74(3)

Table 4

Bond angles in [°]

atom	angles	atom	angles
O(11)#1-Fe(1)-O(11)	93.7(4)	O(11)-C(11)-C(16)	119.8(8)
O(11)#1-Fe(1)-O(32)	91.0(3)	O(11)-C(11)-C(12)	123.4(8)
O(11)-Fe(1)-O(32)	164.7(2)	C(16)-C(11)-C(12)	116.8(9)
O(11)#1-Fe(1)-O(32)#1	164.7(2)	O(11)-C(11)-Cs(1)#1	44.4(4)
O(11)-Fe(1)-O(32)#1	91.0(3)	C(16)-C(11)-Cs(1)#1	87.5(6)
O(32)-Fe(1)-O(32)#1	88.3(4)	C(12)-C(11)-Cs(1)#1	139.2(6)
O(11)#1-Fe(1)-N(22)	93.0(3)	C(13)-C(12)-C(11)	118.9(9)
O(11)-Fe(1)-N(22)	83.0(3)	C(13)-C(12)-C(21)	120.5(8)
O(32)-Fe(1)-N(22)	82.2(3)	C(11)-C(12)-C(21)	120.5(8)
O(32)#1-Fe(1)-N(22)	102.0(3)	C(14)-C(13)-C(12)	121.8(10)
O(11)#1-Fe(1)-N(22)#1	83.0(3)	C(14)-C(13)-Cs(4)#2	124.1(8)
O(11)-Fe(1)-N(22)#1	93.0(3)	C(12)-C(13)-Cs(4)#2	111.3(7)
O(32)-Fe(1)-N(22)#1	102.0(3)	C(15)-C(14)-C(13)	119.7(10)
O(32)#1-Fe(1)-N(22)#1	82.2(3)	C(16)-C(15)-C(14)	120.9(10)
N(22)-Fe(1)-N(22)#1	174.1(4)	C(15)-C(16)-C(11)	121.8(10)
O(11)#1-Fe(1)-Cs(1)	42.5(2)	C(11)-O(11)-Fe(1)	129.5(6)
O(11)-Fe(1)-Cs(1)	127.6(2)	C(11)-O(11)-Cs(1)#1	117.6(5)
O(32)-Fe(1)-Cs(1)	51.22(19)	Fe(1)-O(11)-Cs(1)#1	110.8(3)
O(32)#1-Fe(1)-Cs(1)	139.5(2)	N(25)-C(21)-N(22)	112.4(8)
N(22)-Fe(1)-Cs(1)	74.66(19)	N(25)-C(21)-C(12)	123.6(8)
N(22)#1-Fe(1)-Cs(1)	104.78(19)	N(22)-C(21)-C(12)	123.9(7)
O(11)#1-Fe(1)-Cs(1)#1	127.6(2)	C(23)-N(22)-C(21)	105.9(7)
O(11)-Fe(1)-Cs(1)#1	42.5(2)	C(23)-N(22)-Fe(1)	128.1(6)
O(32)-Fe(1)-Cs(1)#1	139.5(2)	C(21)-N(22)-Fe(1)	125.2(6)
O(32)#1-Fe(1)-Cs(1)#1	51.22(19)	N(22)-C(23)-N(24)	107.2(8)
N(22)-Fe(1)-Cs(1)#1	104.78(19)	N(22)-C(23)-C(31)	124.4(8)
N(22)#1-Fe(1)-Cs(1)#1	74.66(19)	N(24)-C(23)-C(31)	128.2(8)
Cs(1)-Fe(1)-Cs(1)#1	169.32(6)	C(23)-N(24)-N(25)	111.1(7)

C(23)-N(24)-C(41)	132.1(8)	C(46)-C(41)-N(24)	121.6(8)
N(25)-N(24)-C(41)	116.8(7)	C(42)-C(41)-Cs(3)#2	81.1(5)
C(21)-N(25)-N(24)	103.3(7)	C(46)-C(41)-Cs(3)#2	93.8(6)
C(21)-N(25)-Cs(4)#2	135.7(6)	N(24)-C(41)-Cs(3)#2	92.1(5)
N(24)-N(25)-Cs(4)#2	120.9(5)	C(41)-C(42)-C(43)	119.5(8)
C(21)-N(25)-Cs(3)#2	143.2(6)	C(41)-C(42)-Cs(3)#2	77.3(5)
N(24)-N(25)-Cs(3)#2	109.8(5)	C(43)-C(42)-Cs(3)#2	96.6(6)
Cs(4)#2-N(25)-Cs(3)#2	16.73(17)	C(41)-C(42)-Cs(4)#2	85.4(6)
C(36)-C(31)-C(32)	120.7(8)	C(43)-C(42)-Cs(4)#2	103.3(6)
C(36)-C(31)-C(23)	121.8(8)	Cs(3)#2-C(42)-Cs(4)#2	14.54(15)
C(32)-C(31)-C(23)	117.2(8)	C(44)-C(43)-C(42)	120.4(8)
O(32)-C(32)-C(31)	124.4(8)	C(44)-C(43)-S(1)	119.6(7)
O(32)-C(32)-C(33)	117.9(8)	C(42)-C(43)-S(1)	119.9(7)
C(31)-C(32)-C(33)	117.6(8)	C(43)-C(44)-C(45)	118.5(8)
O(32)-C(32)-Cs(1)	53.1(4)	C(43)-C(44)-Cs(3)#3	108.8(6)
C(31)-C(32)-Cs(1)	95.2(5)	C(45)-C(44)-Cs(3)#3	61.9(6)
C(33)-C(32)-Cs(1)	122.8(6)	C(46)-C(45)-C(44)	122.0(8)
C(34)-C(33)-C(32)	120.5(9)	C(46)-C(45)-Cs(3)#3	92.4(6)
C(34)-C(33)-Cs(2)	72.9(6)	C(44)-C(45)-Cs(3)#3	97.2(6)
C(32)-C(33)-Cs(2)	92.2(5)	C(46)-C(45)-Cs(4)#3	99.0(7)
C(35)-C(34)-C(33)	120.0(10)	C(44)-C(45)-Cs(4)#3	104.3(6)
C(35)-C(34)-Cs(2)	84.1(6)	Cs(3)#3-C(45)-Cs(4)#3	14.55(14)
C(33)-C(34)-Cs(2)	85.0(6)	C(45)-C(46)-C(41)	118.0(8)
C(34)-C(35)-C(36)	119.8(10)	C(45)-C(46)-S(2)	118.5(7)
C(34)-C(35)-Cs(2)	74.2(6)	C(41)-C(46)-S(2)	123.5(7)
C(36)-C(35)-Cs(2)	93.2(6)	C(45)-C(46)-Cs(3)#3	66.2(6)
C(35)-C(36)-C(31)	121.2(9)	C(41)-C(46)-Cs(3)#3	114.9(6)
C(32)-O(32)-Fe(1)	124.9(5)	S(2)-C(46)-Cs(3)#3	85.4(3)
C(32)-O(32)-Cs(1)	107.8(5)	O(3)-S(1)-O(2)	114.0(6)
Fe(1)-O(32)-Cs(1)	99.9(2)	O(3)-S(1)-O(1)	113.5(6)
C(42)-C(41)-C(46)	120.9(8)	O(2)-S(1)-O(1)	110.4(6)
C(42)-C(41)-N(24)	117.3(8)	O(3)-S(1)-C(43)	106.8(6)

O(2)-S(1)-C(43)	106.8(5)	Cs(1)-S(2)-Cs(2)#3	77.51(5)
O(1)-S(1)-C(43)	104.7(4)	O(4)-S(2)-Cs(1)#3	76.5(4)
O(3)-S(1)-Cs(2)#4	62.6(4)	O(5)-S(2)-Cs(1)#3	138.1(3)
O(2)-S(1)-Cs(2)#4	122.2(3)	O(6)-S(2)-Cs(1)#3	38.5(4)
O(1)-S(1)-Cs(2)#4	52.2(3)	C(46)-S(2)-Cs(1)#3	109.1(3)
C(43)-S(1)-Cs(2)#4	130.2(3)	Cs(1)-S(2)-Cs(1)#3	108.70(5)
O(3)-S(1)-Cs(2)#2	134.9(5)	Cs(2)#3-S(2)-Cs(1)#3	69.33(4)
O(2)-S(1)-Cs(2)#2	53.9(4)	O(4)-S(2)-Cs(3)#3	154.8(4)
O(1)-S(1)-Cs(2)#2	56.4(4)	O(5)-S(2)-Cs(3)#3	91.8(3)
C(43)-S(1)-Cs(2)#2	118.3(3)	O(6)-S(2)-Cs(3)#3	47.1(3)
Cs(2)#4-S(1)-Cs(2)#2	86.94(6)	C(46)-S(2)-Cs(3)#3	68.5(3)
S(1)-O(1)-Cs(2)#4	106.1(4)	Cs(1)-S(2)-Cs(3)#3	142.11(8)
S(1)-O(1)-Cs(2)#2	102.2(4)	Cs(2)#3-S(2)-Cs(3)#3	72.36(5)
Cs(2)#4-O(1)-Cs(2)#2	110.4(2)	Cs(1)#3-S(2)-Cs(3)#3	81.62(6)
S(1)-O(2)-Cs(2)#2	105.1(4)	S(2)-O(4)-Cs(2)	165.9(5)
S(1)-O(3)-Cs(1)#5	152.3(6)	S(2)-O(4)-Cs(1)	98.8(4)
S(1)-O(3)-Cs(2)#4	95.1(5)	Cs(2)-O(4)-Cs(1)	95.2(2)
Cs(1)#5-O(3)-Cs(2)#4	98.2(3)	S(2)-O(5)-Cs(1)	102.1(3)
O(4)-S(2)-O(5)	112.8(5)	S(2)-O(5)-Cs(2)#3	89.4(3)
O(4)-S(2)-O(6)	114.4(5)	Cs(1)-O(5)-Cs(2)#3	88.97(16)
O(5)-S(2)-O(6)	112.1(5)	S(2)-O(6)-Cs(1)#3	124.2(5)
O(4)-S(2)-C(46)	107.1(5)	S(2)-O(6)-Cs(4)#3	130.8(4)
O(5)-S(2)-C(46)	106.7(4)	Cs(1)#3-O(6)-Cs(4)#3	98.7(3)
O(6)-S(2)-C(46)	102.9(4)	S(2)-O(6)-Cs(3)#3	113.7(4)
O(4)-S(2)-Cs(1)	59.0(3)	Cs(1)#3-O(6)-Cs(3)#3	114.6(2)
O(5)-S(2)-Cs(1)	55.6(3)	Cs(4)#3-O(6)-Cs(3)#3	17.14(17)
O(6)-S(2)-Cs(1)	122.7(3)	S(2)-O(6)-Cs(2)#3	109.8(4)
C(46)-S(2)-Cs(1)	134.3(3)	Cs(1)#3-O(6)-Cs(2)#3	93.00(19)
O(4)-S(2)-Cs(2)#3	110.5(3)	Cs(4)#3-O(6)-Cs(2)#3	88.6(3)
O(5)-S(2)-Cs(2)#3	69.2(3)	Cs(3)#3-O(6)-Cs(2)#3	93.9(3)
O(6)-S(2)-Cs(2)#3	50.1(4)	O(11)#1-Cs(1)-O(3)#6	106.3(3)
C(46)-S(2)-Cs(2)#3	140.5(3)	O(11)#1-Cs(1)-O(6)#3	161.3(2)

O(3)#6-Cs(1)-O(6)#3	85.2(3)	O(4)-Cs(1)-O(6W)	148.4(4)
O(11)#1-Cs(1)-O(5)	95.40(18)	O(5B)-Cs(1)-O(6W)	28.4(5)
O(3)#6-Cs(1)-O(5)	87.6(2)	O(11)#1-Cs(1)-C(11)#1	18.01(19)
O(6)#3-Cs(1)-O(5)	99.9(2)	O(3)#6-Cs(1)-C(11)#1	90.1(3)
O(11)#1-Cs(1)-O(5A)	97.6(5)	O(6)#3-Cs(1)-C(11)#1	156.5(2)
O(3)#6-Cs(1)-O(5A)	95.4(5)	O(5)-Cs(1)-C(11)#1	102.93(19)
O(6)#3-Cs(1)-O(5A)	66.1(5)	O(5A)-Cs(1)-C(11)#1	91.5(5)
O(5)-Cs(1)-O(5A)	165.2(5)	O(32)-Cs(1)-C(11)#1	70.32(18)
O(11)#1-Cs(1)-O(32)	54.21(17)	O(4)-Cs(1)-C(11)#1	137.28(19)
O(3)#6-Cs(1)-O(32)	160.4(2)	O(5B)-Cs(1)-C(11)#1	77.4(6)
O(6)#3-Cs(1)-O(32)	113.1(2)	O(6W)-Cs(1)-C(11)#1	74.0(4)
O(5)-Cs(1)-O(32)	95.72(17)	O(11)#1-Cs(1)-S(2)	112.19(13)
O(5A)-Cs(1)-O(32)	86.3(4)	O(3)#6-Cs(1)-S(2)	96.5(2)
O(11)#1-Cs(1)-O(4)	121.67(19)	O(6)#3-Cs(1)-S(2)	80.32(15)
O(3)#6-Cs(1)-O(4)	110.0(2)	O(5)-Cs(1)-S(2)	22.26(14)
O(6)#3-Cs(1)-O(4)	65.4(2)	O(5A)-Cs(1)-S(2)	143.2(5)
O(5)-Cs(1)-O(4)	43.92(19)	O(32)-Cs(1)-S(2)	93.75(11)
O(5A)-Cs(1)-O(4)	122.0(5)	O(4)-Cs(1)-S(2)	22.16(14)
O(32)-Cs(1)-O(4)	85.19(18)	O(5B)-Cs(1)-S(2)	159.4(5)
O(11)#1-Cs(1)-O(5B)	87.2(6)	O(6W)-Cs(1)-S(2)	149.8(3)
O(3)#6-Cs(1)-O(5B)	84.0(5)	C(11)#1-Cs(1)-S(2)	123.15(14)
O(6)#3-Cs(1)-O(5B)	79.2(6)	O(11)#1-Cs(1)-C(32)	70.44(18)
O(5)-Cs(1)-O(5B)	171.7(5)	O(3)#6-Cs(1)-C(32)	170.6(2)
O(5A)-Cs(1)-O(5B)	18.2(5)	O(6)#3-Cs(1)-C(32)	100.4(2)
O(32)-Cs(1)-O(5B)	92.2(5)	O(5)-Cs(1)-C(32)	84.03(18)
O(4)-Cs(1)-O(5B)	139.8(5)	O(5A)-Cs(1)-C(32)	93.7(5)
O(11)#1-Cs(1)-O(6W)	89.9(4)	O(32)-Cs(1)-C(32)	19.12(16)
O(3)#6-Cs(1)-O(6W)	56.3(4)	O(4)-Cs(1)-C(32)	66.4(2)
O(6)#3-Cs(1)-O(6W)	84.3(4)	O(5B)-Cs(1)-C(32)	104.3(5)
O(5)-Cs(1)-O(6W)	143.4(4)	O(6W)-Cs(1)-C(32)	131.3(4)
O(5A)-Cs(1)-O(6W)	43.8(6)	C(11)#1-Cs(1)-C(32)	87.68(19)
O(32)-Cs(1)-O(6W)	116.2(4)	S(2)-Cs(1)-C(32)	77.27(13)

O(4)-Cs(2)-O(1)#4	104.4(2)	O(2)#7-Cs(2)-C(35)	89.1(2)
O(4)-Cs(2)-O(1W)	112.2(3)	O(1)#7-Cs(2)-C(35)	115.6(2)
O(1)#4-Cs(2)-O(1W)	139.2(3)	O(3)#4-Cs(2)-C(35)	92.0(2)
O(4)-Cs(2)-O(6)#3	66.8(2)	C(34)-Cs(2)-C(35)	21.6(2)
O(1)#4-Cs(2)-O(6)#3	146.73(19)	O(4)-Cs(2)-O(5)#3	77.3(2)
O(1W)-Cs(2)-O(6)#3	68.3(2)	O(1)#4-Cs(2)-O(5)#3	107.96(18)
O(4)-Cs(2)-O(2)#7	159.4(2)	O(1W)-Cs(2)-O(5)#3	97.4(2)
O(1)#4-Cs(2)-O(2)#7	89.1(2)	O(6)#3-Cs(2)-O(5)#3	39.76(17)
O(1W)-Cs(2)-O(2)#7	50.9(3)	O(2)#7-Cs(2)-O(5)#3	113.80(17)
O(6)#3-Cs(2)-O(2)#7	109.8(2)	O(1)#7-Cs(2)-O(5)#3	84.04(17)
O(4)-Cs(2)-O(1)#7	157.6(2)	O(3)#4-Cs(2)-O(5)#3	74.45(19)
O(1)#4-Cs(2)-O(1)#7	69.6(2)	C(34)-Cs(2)-O(5)#3	166.6(2)
O(1W)-Cs(2)-O(1)#7	82.1(2)	C(35)-Cs(2)-O(5)#3	157.06(19)
O(6)#3-Cs(2)-O(1)#7	105.8(2)	O(4)-Cs(2)-C(33)	86.1(2)
O(2)#7-Cs(2)-O(1)#7	42.31(19)	O(1)#4-Cs(2)-C(33)	105.9(2)
O(4)-Cs(2)-O(3)#4	70.4(3)	O(1W)-Cs(2)-C(33)	60.7(2)
O(1)#4-Cs(2)-O(3)#4	43.6(2)	O(6)#3-Cs(2)-C(33)	105.4(2)
O(1W)-Cs(2)-O(3)#4	170.9(2)	O(2)#7-Cs(2)-C(33)	75.0(2)
O(6)#3-Cs(2)-O(3)#4	106.1(2)	O(1)#7-Cs(2)-C(33)	116.24(19)
O(2)#7-Cs(2)-O(3)#4	128.3(2)	O(3)#4-Cs(2)-C(33)	128.4(2)
O(1)#7-Cs(2)-O(3)#4	92.8(2)	C(34)-Cs(2)-C(33)	22.1(2)
O(4)-Cs(2)-C(34)	94.1(2)	C(35)-Cs(2)-C(33)	37.8(2)
O(1)#4-Cs(2)-C(34)	83.9(2)	O(5)#3-Cs(2)-C(33)	145.0(2)
O(1W)-Cs(2)-C(34)	76.2(2)	O(4)-Cs(2)-S(1)#4	89.32(17)
O(6)#3-Cs(2)-C(34)	127.4(2)	O(1)#4-Cs(2)-S(1)#4	21.65(15)
O(2)#7-Cs(2)-C(34)	71.5(2)	O(1W)-Cs(2)-S(1)#4	158.3(2)
O(1)#7-Cs(2)-C(34)	106.3(2)	O(6)#3-Cs(2)-S(1)#4	126.13(14)
O(3)#4-Cs(2)-C(34)	112.6(2)	O(2)#7-Cs(2)-S(1)#4	107.44(16)
O(4)-Cs(2)-C(35)	80.7(2)	O(1)#7-Cs(2)-S(1)#4	78.17(13)
O(1)#4-Cs(2)-C(35)	71.2(2)	O(3)#4-Cs(2)-S(1)#4	22.30(17)
O(1W)-Cs(2)-C(35)	97.0(2)	C(34)-Cs(2)-S(1)#4	100.52(18)
O(6)#3-Cs(2)-C(35)	133.7(2)	C(35)-Cs(2)-S(1)#4	83.43(16)

O(5)#3-Cs(2)-S(1)#4	89.69(12)	O(5A)-Cs(3)-C(42)#7	119.4(5)
C(33)-Cs(2)-S(1)#4	121.01(17)	O(6)#3-Cs(3)-C(42)#7	122.6(2)
O(4A)-Cs(3)-O(1W)	139.6(6)	N(25)#7-Cs(3)-C(42)#7	50.6(2)
O(4A)-Cs(3)-O(5A)	93.4(7)	Cs(3)#8-Cs(3)-C(42)#7	87.22(17)
O(1W)-Cs(3)-O(5A)	62.0(5)	C(45)#3-Cs(3)-C(42)#7	165.4(2)
O(4A)-Cs(3)-O(6)#3	129.1(5)	C(41)#7-Cs(3)-C(42)#7	21.53(19)
O(1W)-Cs(3)-O(6)#3	71.4(3)	O(4A)-Cs(3)-C(46)#3	94.7(5)
O(5A)-Cs(3)-O(6)#3	64.6(4)	O(1W)-Cs(3)-C(46)#3	112.9(3)
O(4A)-Cs(3)-N(25)#7	68.7(5)	O(5A)-Cs(3)-C(46)#3	85.1(4)
O(1W)-Cs(3)-N(25)#7	79.8(3)	O(6)#3-Cs(3)-C(46)#3	41.54(19)
O(5A)-Cs(3)-N(25)#7	91.6(4)	N(25)#7-Cs(3)-C(46)#3	162.9(2)
O(6)#3-Cs(3)-N(25)#7	148.8(2)	Cs(3)#8-Cs(3)-C(46)#3	67.99(14)
O(4A)-Cs(3)-Cs(3)#8	83.7(5)	C(45)#3-Cs(3)-C(46)#3	21.3(2)
O(1W)-Cs(3)-Cs(3)#8	133.1(2)	C(41)#7-Cs(3)-C(46)#3	148.2(2)
O(5A)-Cs(3)-Cs(3)#8	152.5(4)	C(42)#7-Cs(3)-C(46)#3	144.2(2)
O(6)#3-Cs(3)-Cs(3)#8	96.23(15)	O(4A)-Cs(3)-C(44)#3	59.5(5)
N(25)#7-Cs(3)-Cs(3)#8	112.47(16)	O(1W)-Cs(3)-C(44)#3	133.7(3)
O(4A)-Cs(3)-C(45)#3	80.0(5)	O(5A)-Cs(3)-C(44)#3	78.0(5)
O(1W)-Cs(3)-C(45)#3	116.1(3)	O(6)#3-Cs(3)-C(44)#3	70.8(2)
O(5A)-Cs(3)-C(45)#3	70.8(4)	N(25)#7-Cs(3)-C(44)#3	126.1(2)
O(6)#3-Cs(3)-C(45)#3	50.0(2)	Cs(3)#8-Cs(3)-C(44)#3	76.99(15)
N(25)#7-Cs(3)-C(45)#3	143.2(2)	C(45)#3-Cs(3)-C(44)#3	20.8(2)
Cs(3)#8-Cs(3)-C(45)#3	81.78(16)	C(41)#7-Cs(3)-C(44)#3	141.4(2)
O(4A)-Cs(3)-C(41)#7	87.1(5)	C(42)#7-Cs(3)-C(44)#3	160.8(2)
O(1W)-Cs(3)-C(41)#7	84.1(3)	C(46)#3-Cs(3)-C(44)#3	36.78(19)
O(5A)-Cs(3)-C(41)#7	126.5(4)	O(4A)-Cs(3)-S(2)#3	120.3(5)
O(6)#3-Cs(3)-C(41)#7	143.4(2)	O(1W)-Cs(3)-S(2)#3	88.4(2)
N(25)#7-Cs(3)-C(41)#7	39.64(19)	O(5A)-Cs(3)-S(2)#3	80.0(3)
Cs(3)#8-Cs(3)-C(41)#7	80.76(16)	O(6)#3-Cs(3)-S(2)#3	19.17(13)
C(45)#3-Cs(3)-C(41)#7	159.3(2)	N(25)#7-Cs(3)-S(2)#3	167.75(15)
O(4A)-Cs(3)-C(42)#7	108.3(5)	Cs(3)#8-Cs(3)-S(2)#3	77.97(7)
O(1W)-Cs(3)-C(42)#7	65.5(3)	C(45)#3-Cs(3)-S(2)#3	41.60(16)

C(41)#7-Cs(3)-S(2)#3	142.55(15)	O(1W)-Cs(4)-C(42)#7	69.2(4)
C(42)#7-Cs(3)-S(2)#3	126.55(15)	O(6)#3-Cs(4)-C(42)#7	123.2(4)
C(46)#3-Cs(3)-S(2)#3	26.07(14)	O(4B)-Cs(4)-C(42)#7	90.4(4)
C(44)#3-Cs(3)-S(2)#3	61.11(14)	N(25)#7-Cs(4)-C(42)#7	50.2(2)
O(1W)-Cs(4)-O(6)#3	83.7(4)	O(5B)-Cs(4)-C(42)#7	150.1(5)
O(1W)-Cs(4)-O(4B)	159.6(6)	O(4B)#8-Cs(4)-C(42)#7	67.5(3)
O(6)#3-Cs(4)-O(4B)	108.5(5)	C(45)#3-Cs(4)-C(42)#7	140.9(3)
O(1W)-Cs(4)-N(25)#7	94.2(5)	O(2W)#1-Cs(4)-C(42)#7	102.5(4)
O(6)#3-Cs(4)-N(25)#7	173.3(4)	O(1W)-Cs(4)-C(13)#7	103.0(4)
O(4B)-Cs(4)-N(25)#7	71.8(4)	O(6)#3-Cs(4)-C(13)#7	139.1(4)
O(1W)-Cs(4)-O(5B)	94.5(6)	O(4B)-Cs(4)-C(13)#7	78.8(6)
O(6)#3-Cs(4)-O(5B)	77.3(4)	N(25)#7-Cs(4)-C(13)#7	47.6(2)
O(4B)-Cs(4)-O(5B)	103.9(7)	O(5B)-Cs(4)-C(13)#7	62.1(4)
N(25)#7-Cs(4)-O(5B)	109.2(4)	O(4B)#8-Cs(4)-C(13)#7	154.5(4)
O(1W)-Cs(4)-O(4B)#8	89.8(5)	C(45)#3-Cs(4)-C(13)#7	108.3(4)
O(6)#3-Cs(4)-O(4B)#8	63.4(3)	O(2W)#1-Cs(4)-C(13)#7	67.0(3)
O(4B)-Cs(4)-O(4B)#8	81.7(7)	C(42)#7-Cs(4)-C(13)#7	96.2(3)
N(25)#7-Cs(4)-O(4B)#8	110.3(4)	O(1W)-Cs(4)-Cs(2)	43.2(3)
O(5B)-Cs(4)-O(4B)#8	139.8(5)	O(6)#3-Cs(4)-Cs(2)	46.8(2)
O(1W)-Cs(4)-C(45)#3	130.4(4)	O(4B)-Cs(4)-Cs(2)	136.7(5)
O(6)#3-Cs(4)-C(45)#3	47.8(3)	N(25)#7-Cs(4)-Cs(2)	128.3(4)
O(4B)-Cs(4)-C(45)#3	66.0(4)	O(5B)-Cs(4)-Cs(2)	102.9(4)
N(25)#7-Cs(4)-C(45)#3	135.2(4)	O(4B)#8-Cs(4)-Cs(2)	56.2(4)
O(5B)-Cs(4)-C(45)#3	68.8(5)	C(45)#3-Cs(4)-Cs(2)	93.6(2)
O(4B)#8-Cs(4)-C(45)#3	78.1(4)	O(2W)#1-Cs(4)-Cs(2)	78.3(2)
O(1W)-Cs(4)-O(2W)#1	47.0(4)	C(42)#7-Cs(4)-Cs(2)	82.6(2)
O(6)#3-Cs(4)-O(2W)#1	92.1(3)	C(13)#7-Cs(4)-Cs(2)	144.3(3)
O(4B)-Cs(4)-O(2W)#1	144.4(6)	O(1W)-Cs(4)-Cs(1)	70.6(4)
N(25)#7-Cs(4)-O(2W)#1	91.1(3)	O(6)#3-Cs(4)-Cs(1)	40.08(18)
O(5B)-Cs(4)-O(2W)#1	51.5(5)	O(4B)-Cs(4)-Cs(1)	129.1(5)
O(4B)#8-Cs(4)-O(2W)#1	133.9(5)	N(25)#7-Cs(4)-Cs(1)	144.8(3)
C(45)#3-Cs(4)-O(2W)#1	114.9(3)	O(5B)-Cs(4)-Cs(1)	44.1(3)

O(4B)#8-Cs(4)-Cs(1)	101.5(3)	Cs(3)-O(1W)-Cs(2)	100.4(3)
C(45)#3-Cs(4)-Cs(1)	65.2(2)	Cs(4)-O(4B)-Cs(4)#8	98.3(7)
O(2W)#1-Cs(4)-Cs(1)	55.0(2)	Cs(3)-O(5A)-Cs(1)	113.4(7)
C(42)#7-Cs(4)-Cs(1)	138.2(3)	O(6W)-O(5B)-Cs(1)	88.4(10)
C(13)#7-Cs(4)-Cs(1)	103.6(2)	O(6W)-O(5B)-Cs(4)	125.0(16)
Cs(2)-Cs(4)-Cs(1)	59.97(11)	Cs(1)-O(5B)-Cs(4)	90.9(6)
Cs(4)-O(1W)-Cs(3)	13.7(2)	O(5B)-O(6W)-Cs(1)	63.2(9)
Cs(4)-O(1W)-Cs(2)	108.6(4)		

Symmetry transformations used to generate equivalent atoms:

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

#4 $-x+1/2, -y+3/2, -z+1$ #5 $x-1/2, y+1/2, z$ #6 $x+1/2, y-1/2, z$

#7 $x+1/2, y+1/2, z$ #8 $-x+3/2, -y+3/2, -z+1$

Crystal structure $\text{Na}_3[\text{Cu}(\text{DSA})(\text{HCO}_3)] \cdot 2.5 \text{H}_2\text{O} \cdot 1.5 \text{MeOH}$

Table 1

Operator	Dr. Volker Huch	
Diffractometer	Stoe IPDS	
Identification code	sh2986	
Empirical formula	$\text{C}_{22.50} \text{H}_{22} \text{Cu N}_3 \text{Na}_3 \text{O}_{15} \text{S}_2$	
Formula weight	771.06 g/mol	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	$a = 10.343(4) \text{ Å}$	$\alpha = 71.75(7)^\circ$
	$b = 10.962(8) \text{ Å}$	$\beta = 74.37(5)^\circ$
	$c = 14.304(7) \text{ Å}$	$\gamma = 76.27(7)^\circ$
Volume	$1462.4(14) \text{ Å}^3$	
Z	2	
Density (calculated)	1.751 mg/m^3	
Absorption coefficient	1.014 mm^{-1}	
F(000)	784	
Crystal size	$0.39 \times 0.22 \times 0.09 \text{ mm}^3$	
Theta range for data collection	2.30 to 27.00°	
Index ranges	$-13 \leq h \leq 13, -14 \leq k \leq 14, -18 \leq l \leq 18$	
Reflections collected	16103	
Independent reflections	5929 [$R(\text{int}) = 0.0881$]	
Completeness to $\theta = 27.00^\circ$	93.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5929 / 0 / 431	
Goodness-of-fit on F^2	0.945	
Final R indices [$ I > 2\sigma(I)$]	$R_1 = 0.0575, wR_2 = 0.1449$	

R indices (all data)

 $R_1 = 0.0870$, $wR_2 = 0.1589$

Largest diff. peak and hole

1.254 and -0.811 e. $\text{\AA}^{-3}$ **Table 2**

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the crystal structure $\text{Na}_3[\text{Cu}(\text{DSA})(\text{HCO}_3)] \cdot 2.5 \text{ H}_2\text{O} \cdot 1.5 \text{ MeOH}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

atom	x	y	z	U(eq)
Cu(1)	2455(1)	1640(1)	863(1)	30(1)
C(31)	3239(4)	-1290(4)	427(3)	24(1)
C(32)	2586(4)	-1198(4)	1408(3)	24(1)
O(32)	2191(3)	-81(3)	1660(2)	29(1)
C(33)	2299(5)	-2353(5)	2161(3)	30(1)
C(34)	2673(5)	-3549(5)	1958(4)	35(1)
C(35)	3345(5)	-3637(5)	995(4)	36(1)
C(36)	3620(5)	-2526(4)	239(4)	30(1)
C(21)	3660(4)	1865(4)	-1291(3)	21(1)
N(22)	3340(3)	1096(3)	-342(3)	22(1)
C(23)	3500(4)	-136(4)	-432(3)	22(1)
N(24)	3883(4)	-182(3)	-1386(3)	26(1)
N(25)	3969(3)	1103(3)	-1925(3)	23(1)
C(11)	3074(4)	3949(4)	-812(3)	28(1)
O(11)	2573(4)	3424(3)	153(2)	37(1)
C(12)	3650(4)	3273(4)	-1568(3)	24(1)
C(13)	4201(5)	3963(5)	-2562(4)	32(1)
C(14)	4137(6)	5297(5)	-2844(4)	41(1)
C(15)	3522(6)	5978(5)	-2125(4)	41(1)
C(16)	3015(5)	5340(5)	-1147(4)	37(1)
C(41)	4400(4)	1354(4)	-3008(3)	21(1)
C(42)	5791(4)	1038(4)	-3387(3)	22(1)

C(43)	6264(4)	1176(4)	-4414(3)	20(1)
S(1)	8041(1)	701(1)	-4858(1)	21(1)
O(1)	8213(3)	-681(3)	-4721(3)	41(1)
O(2)	8396(3)	1469(3)	-5909(2)	36(1)
O(3)	8708(3)	1002(3)	-4199(2)	32(1)
C(44)	5362(4)	1596(4)	-5078(3)	22(1)
C(45)	3978(4)	1920(4)	-4694(3)	25(1)
C(46)	3480(4)	1804(4)	-3666(3)	22(1)
S(2)	1663(1)	2201(1)	-3219(1)	27(1)
O(4)	1140(3)	2981(3)	-4130(3)	35(1)
O(5)	1190(3)	969(4)	-2762(3)	42(1)
O(6)	1479(3)	2975(4)	-2530(3)	43(1)
C(1C)	1939(5)	2770(4)	2562(3)	30(1)
O(1C)	1160(3)	3412(3)	3124(3)	37(1)
O(2C)	1491(3)	2188(4)	2094(3)	39(1)
O(3C)	3465(5)	2661(6)	2407(4)	84(2)
Na(1)	168(2)	2518(2)	4775(1)	27(1)
Na(2)	140(2)	448(2)	2859(1)	36(1)
Na(3)	-880(3)	4714(4)	2573(3)	33(1)
Na(4)	-943(6)	3460(8)	2592(5)	88(2)
O(1LM)	-1486(4)	4423(4)	4449(3)	56(1)
C(1LM)	-2777(6)	4477(6)	5107(5)	52(2)
O(1W)	-1170(7)	1634(7)	1618(6)	126(3)
O(2W)	277(5)	5036(6)	947(4)	90(2)
O(2LM)	-120(12)	2440(11)	-586(9)	83(3)
O(3W)	164(16)	2089(15)	141(13)	118(5)
C(2LM)	60(20)	1070(20)	-193(17)	109(6)

Table 3

Bond length in [Å].

atom	bond length	atom	bond length
Cu(1)-O(32)	1.914(3)	C(15)-Na(4)#1	2.804(8)
Cu(1)-O(11)	1.916(4)	C(41)-C(42)	1.395(6)
Cu(1)-N(22)	1.923(4)	C(41)-C(46)	1.416(5)
Cu(1)-O(2C)	1.972(4)	C(42)-C(43)	1.389(6)
Cu(1)-Na(2)	3.326(3)	C(43)-C(44)	1.409(5)
C(31)-C(32)	1.406(6)	C(43)-S(1)	1.783(4)
C(31)-C(36)	1.408(6)	S(1)-O(1)	1.438(4)
C(31)-C(23)	1.481(6)	S(1)-O(3)	1.458(3)
C(32)-O(32)	1.326(5)	S(1)-O(2)	1.469(4)
C(32)-C(33)	1.416(6)	S(1)-Na(1)#2	3.143(3)
O(32)-Na(2)	2.420(4)	O(1)-Na(1)#3	2.301(4)
C(33)-C(34)	1.374(7)	O(2)-Na(2)#2	2.485(4)
C(34)-C(35)	1.388(7)	O(2)-Na(4)#2	2.611(8)
C(35)-C(36)	1.381(7)	O(2)-Na(1)#2	2.882(4)
C(21)-N(25)	1.347(6)	O(3)-Na(1)#2	2.380(4)
C(21)-N(22)	1.355(5)	O(3)-Na(2)#3	2.459(4)
C(21)-C(12)	1.467(6)	C(44)-C(45)	1.391(6)
N(22)-C(23)	1.364(6)	C(45)-C(46)	1.396(6)
C(23)-N(24)	1.328(6)	C(46)-S(2)	1.808(4)
N(24)-N(25)	1.389(5)	S(2)-O(6)	1.440(4)
N(25)-C(41)	1.446(5)	S(2)-O(5)	1.441(4)
C(11)-O(11)	1.327(5)	S(2)-O(4)	1.477(4)
C(11)-C(12)	1.421(7)	O(4)-Na(1)#4	2.306(4)
C(11)-C(16)	1.439(7)	O(5)-Na(2)#5	2.362(4)
C(12)-C(13)	1.419(6)	O(6)-Na(3)#1	2.447(6)
C(13)-C(14)	1.380(7)	C(1C)-O(1C)	1.236(6)
C(14)-C(15)	1.386(8)	C(1C)-O(2C)	1.283(6)
C(15)-C(16)	1.374(7)	C(1C)-O(3C)	1.514(7)

C(1C)-Na(4)	2.888(7)	Na(2)-O(1W)	2.386(7)
O(1C)-Na(1)	2.304(4)	Na(2)-O(3)#3	2.459(4)
O(1C)-Na(3)	2.423(5)	Na(2)-O(2)#7	2.485(4)
O(1C)-Na(4)	2.475(7)	Na(2)-Na(4)	3.161(9)
O(2C)-Na(2)	2.434(4)	Na(2)-Na(1)#8	3.892(5)
O(2C)-Na(4)	2.603(8)	Na(3)-Na(4)	1.383(9)
Na(1)-O(1)#3	2.301(4)	Na(3)-O(2W)	2.269(7)
Na(1)-O(4)#6	2.306(4)	Na(3)-O(6)#1	2.447(6)
Na(1)-O(1LM)	2.373(4)	Na(3)-O(1LM)	2.520(6)
Na(1)-O(3)#7	2.380(4)	Na(4)-O(2)#7	2.611(8)
Na(1)-O(2)#7	2.882(4)	Na(4)-O(2W)	2.646(9)
Na(1)-S(1)#7	3.143(3)	Na(4)-C(15)#1	2.804(8)
Na(1)-Na(4)	3.389(7)	Na(4)-O(1W)	2.854(12)
Na(1)-Na(3)	3.570(5)	O(1LM)-C(1LM)	1.412(7)
Na(1)-Na(2)#8	3.892(5)	O(2LM)-O(3W)	1.085(16)
Na(1)-Na(2)	4.078(4)	O(2LM)-C(2LM)	1.42(2)
Na(2)-O(5)#5	2.362(4)		

Table 4

Bond angles in [°].

atom	angle	atom	angle
O(32)-Cu(1)-O(11)	174.53(14)	C(23)-N(22)-Cu(1)	125.1(3)
O(32)-Cu(1)-N(22)	93.86(15)	N(24)-C(23)-N(22)	112.2(4)
O(11)-Cu(1)-N(22)	91.08(16)	N(24)-C(23)-C(31)	123.5(4)
O(32)-Cu(1)-O(2C)	85.54(15)	N(22)-C(23)-C(31)	124.3(4)
O(11)-Cu(1)-O(2C)	89.46(16)	C(23)-N(24)-N(25)	103.9(3)
N(22)-Cu(1)-O(2C)	178.10(13)	C(21)-N(25)-N(24)	110.2(3)
O(32)-Cu(1)-Na(2)	45.85(12)	C(21)-N(25)-C(41)	133.3(4)
O(11)-Cu(1)-Na(2)	128.69(13)	N(24)-N(25)-C(41)	116.5(3)
N(22)-Cu(1)-Na(2)	132.11(11)	O(11)-C(11)-C(12)	126.3(4)
O(2C)-Cu(1)-Na(2)	46.52(11)	O(11)-C(11)-C(16)	118.0(4)
C(32)-C(31)-C(36)	119.0(4)	C(12)-C(11)-C(16)	115.6(4)
C(32)-C(31)-C(23)	122.9(4)	C(11)-O(11)-Cu(1)	129.9(3)
C(36)-C(31)-C(23)	118.0(4)	C(13)-C(12)-C(11)	119.9(4)
O(32)-C(32)-C(31)	123.5(4)	C(13)-C(12)-C(21)	121.7(4)
O(32)-C(32)-C(33)	118.0(4)	C(11)-C(12)-C(21)	118.4(4)
C(31)-C(32)-C(33)	118.5(4)	C(14)-C(13)-C(12)	122.2(5)
C(32)-O(32)-Cu(1)	129.4(3)	C(13)-C(14)-C(15)	118.6(5)
C(32)-O(32)-Na(2)	125.2(3)	C(16)-C(15)-C(14)	120.9(5)
Cu(1)-O(32)-Na(2)	99.58(16)	C(16)-C(15)-Na(4)#1	91.4(4)
C(34)-C(33)-C(32)	121.5(4)	C(14)-C(15)-Na(4)#1	94.7(4)
C(33)-C(34)-C(35)	119.8(4)	C(15)-C(16)-C(11)	122.7(5)
C(36)-C(35)-C(34)	120.2(5)	C(42)-C(41)-C(46)	120.1(4)
C(35)-C(36)-C(31)	121.1(4)	C(42)-C(41)-N(25)	116.5(3)
N(25)-C(21)-N(22)	107.5(4)	C(46)-C(41)-N(25)	123.2(4)
N(25)-C(21)-C(12)	126.7(4)	C(43)-C(42)-C(41)	119.4(4)
N(22)-C(21)-C(12)	125.8(4)	C(42)-C(43)-C(44)	121.3(4)
C(21)-N(22)-C(23)	106.2(4)	C(42)-C(43)-S(1)	117.9(3)
C(21)-N(22)-Cu(1)	127.5(3)	C(44)-C(43)-S(1)	120.7(3)

O(1)-S(1)-O(3)	111.6(2)	S(2)-O(5)-Na(2)#5	145.8(2)
O(1)-S(1)-O(2)	114.9(2)	S(2)-O(6)-Na(3)#1	136.9(3)
O(3)-S(1)-O(2)	112.3(2)	O(1C)-C(1C)-O(2C)	121.6(4)
O(1)-S(1)-C(43)	104.6(2)	O(1C)-C(1C)-O(3C)	120.1(4)
O(3)-S(1)-C(43)	105.26(19)	O(2C)-C(1C)-O(3C)	118.3(4)
O(2)-S(1)-C(43)	107.39(19)	O(1C)-C(1C)-Na(4)	58.4(3)
O(1)-S(1)-Na(1)#2	131.13(14)	O(2C)-C(1C)-Na(4)	64.3(3)
O(3)-S(1)-Na(1)#2	46.21(14)	O(3C)-C(1C)-Na(4)	169.1(4)
O(2)-S(1)-Na(1)#2	66.16(15)	C(1C)-O(1C)-Na(1)	124.0(3)
C(43)-S(1)-Na(1)#2	122.21(15)	C(1C)-O(1C)-Na(3)	116.7(3)
S(1)-O(1)-Na(1)#3	143.0(2)	Na(1)-O(1C)-Na(3)	98.04(17)
S(1)-O(2)-Na(2)#2	119.3(2)	C(1C)-O(1C)-Na(4)	96.5(3)
S(1)-O(2)-Na(4)#2	158.0(3)	Na(1)-O(1C)-Na(4)	90.27(19)
Na(2)#2-O(2)-Na(4)#2	76.6(2)	Na(3)-O(1C)-Na(4)	32.8(2)
S(1)-O(2)-Na(1)#2	86.04(17)	C(1C)-O(2C)-Cu(1)	127.3(3)
Na(2)#2-O(2)-Na(1)#2	98.61(12)	C(1C)-O(2C)-Na(2)	126.4(3)
Na(4)#2-O(2)-Na(1)#2	76.01(19)	Cu(1)-O(2C)-Na(2)	97.48(16)
S(1)-O(3)-Na(1)#2	107.55(18)	C(1C)-O(2C)-Na(4)	89.3(3)
S(1)-O(3)-Na(2)#3	130.5(2)	Cu(1)-O(2C)-Na(4)	131.9(2)
Na(1)#2-O(3)-Na(2)#3	107.05(13)	Na(2)-O(2C)-Na(4)	77.7(2)
C(45)-C(44)-C(43)	118.8(4)	O(1)#3-Na(1)-O(1C)	87.81(16)
C(44)-C(45)-C(46)	121.0(4)	O(1)#3-Na(1)-O(4)#6	90.53(15)
C(45)-C(46)-C(41)	119.4(4)	O(1C)-Na(1)-O(4)#6	111.11(14)
C(45)-C(46)-S(2)	118.3(3)	O(1)#3-Na(1)-O(1LM)	167.02(17)
C(41)-C(46)-S(2)	122.3(3)	O(1C)-Na(1)-O(1LM)	81.85(16)
O(6)-S(2)-O(5)	114.2(2)	O(4)#6-Na(1)-O(1LM)	100.49(17)
O(6)-S(2)-O(4)	111.0(2)	O(1)#3-Na(1)-O(3)#7	83.98(14)
O(5)-S(2)-O(4)	114.0(2)	O(1C)-Na(1)-O(3)#7	142.54(14)
O(6)-S(2)-C(46)	106.3(2)	O(4)#6-Na(1)-O(3)#7	105.46(14)
O(5)-S(2)-C(46)	105.7(2)	O(1LM)-Na(1)-O(3)#7	99.49(15)
O(4)-S(2)-C(46)	104.7(2)	O(1)#3-Na(1)-O(2)#7	90.19(13)
S(2)-O(4)-Na(1)#4	134.3(2)	O(1C)-Na(1)-O(2)#7	89.66(13)

O(4)#6-Na(1)-O(2)#7	159.23(13)	Na(3)-Na(1)-Na(2)#8	153.66(9)
O(1LM)-Na(1)-O(2)#7	81.96(14)	O(1)#3-Na(1)-Na(2)	62.12(12)
O(3)#7-Na(1)-O(2)#7	54.00(11)	O(1C)-Na(1)-Na(2)	66.46(11)
O(1)#3-Na(1)-S(1)#7	85.69(11)	O(4)#6-Na(1)-Na(2)	152.32(11)
O(1C)-Na(1)-S(1)#7	116.81(12)	O(1LM)-Na(1)-Na(2)	106.21(14)
O(4)#6-Na(1)-S(1)#7	131.69(12)	O(3)#7-Na(1)-Na(2)	77.47(10)
O(1LM)-Na(1)-S(1)#7	91.97(12)	O(2)#7-Na(1)-Na(2)	37.06(8)
O(3)#7-Na(1)-S(1)#7	26.24(8)	S(1)#7-Na(1)-Na(2)	55.29(6)
O(2)#7-Na(1)-S(1)#7	27.79(7)	Na(4)-Na(1)-Na(2)	49.02(15)
O(1)#3-Na(1)-Na(4)	106.76(19)	Na(3)-Na(1)-Na(2)	70.90(9)
O(1C)-Na(1)-Na(4)	46.91(14)	Na(2)#8-Na(1)-Na(2)	93.99(7)
O(4)#6-Na(1)-Na(4)	149.57(17)	O(5)#5-Na(2)-O(1W)	72.6(2)
O(1LM)-Na(1)-Na(4)	60.34(19)	O(5)#5-Na(2)-O(32)	99.65(15)
O(3)#7-Na(1)-Na(4)	101.19(15)	O(1W)-Na(2)-O(32)	95.0(2)
O(2)#7-Na(1)-Na(4)	48.39(15)	O(5)#5-Na(2)-O(2C)	151.87(15)
S(1)#7-Na(1)-Na(4)	75.66(14)	O(1W)-Na(2)-O(2C)	84.3(2)
O(1)#3-Na(1)-Na(3)	122.55(15)	O(32)-Na(2)-O(2C)	65.87(14)
O(1C)-Na(1)-Na(3)	42.24(11)	O(5)#5-Na(2)-O(3)#3	99.70(14)
O(4)#6-Na(1)-Na(3)	127.33(13)	O(1W)-Na(2)-O(3)#3	172.2(2)
O(1LM)-Na(1)-Na(3)	44.79(14)	O(32)-Na(2)-O(3)#3	87.61(13)
O(3)#7-Na(1)-Na(3)	116.75(12)	O(2C)-Na(2)-O(3)#3	103.43(14)
O(2)#7-Na(1)-Na(3)	68.42(11)	O(5)#5-Na(2)-O(2)#7	96.80(14)
S(1)#7-Na(1)-Na(3)	93.77(10)	O(1W)-Na(2)-O(2)#7	88.4(2)
Na(4)-Na(1)-Na(3)	22.73(15)	O(32)-Na(2)-O(2)#7	163.47(14)
O(1)#3-Na(1)-Na(2)#8	62.80(12)	O(2C)-Na(2)-O(2)#7	98.50(15)
O(1C)-Na(1)-Na(2)#8	150.29(12)	O(3)#3-Na(2)-O(2)#7	91.15(14)
O(4)#6-Na(1)-Na(2)#8	75.49(11)	O(5)#5-Na(2)-Na(4)	122.18(16)
O(1LM)-Na(1)-Na(2)#8	126.50(13)	O(1W)-Na(2)-Na(4)	60.0(2)
O(3)#7-Na(1)-Na(2)#8	37.16(9)	O(32)-Na(2)-Na(4)	114.90(16)
O(2)#7-Na(1)-Na(2)#8	86.42(10)	O(2C)-Na(2)-Na(4)	53.56(15)
S(1)#7-Na(1)-Na(2)#8	60.08(7)	O(3)#3-Na(2)-Na(4)	125.25(17)
Na(4)-Na(1)-Na(2)#8	134.60(15)	O(2)#7-Na(2)-Na(4)	53.49(16)

O(5)#5-Na(2)-Cu(1)	120.09(13)	O(1C)-Na(3)-O(1LM)	76.58(17)
O(1W)-Na(2)-Cu(1)	76.5(2)	O(6)#1-Na(3)-O(1LM)	82.67(19)
O(32)-Na(2)-Cu(1)	34.57(8)	Na(4)-Na(3)-Na(1)	71.3(3)
O(2C)-Na(2)-Cu(1)	36.00(10)	O(2W)-Na(3)-Na(1)	128.42(18)
O(3)#3-Na(2)-Cu(1)	109.31(11)	O(1C)-Na(3)-Na(1)	39.72(11)
O(2)#7-Na(2)-Cu(1)	132.33(12)	O(6)#1-Na(3)-Na(1)	116.93(17)
Na(4)-Na(2)-Cu(1)	80.34(14)	O(1LM)-Na(3)-Na(1)	41.56(11)
O(5)#5-Na(2)-Na(1)#8	67.98(11)	Na(3)-Na(4)-O(1C)	71.6(3)
O(1W)-Na(2)-Na(1)#8	136.70(19)	Na(3)-Na(4)-O(2C)	110.5(4)
O(32)-Na(2)-Na(1)#8	108.43(12)	O(1C)-Na(4)-O(2C)	51.26(16)
O(2C)-Na(2)-Na(1)#8	138.26(12)	Na(3)-Na(4)-O(2)#7	131.1(5)
O(3)#3-Na(2)-Na(1)#8	35.78(8)	O(1C)-Na(4)-O(2)#7	92.6(2)
O(2)#7-Na(2)-Na(1)#8	79.25(11)	O(2C)-Na(4)-O(2)#7	91.2(2)
Na(4)-Na(2)-Na(1)#8	131.54(14)	Na(3)-Na(4)-O(2W)	59.1(3)
Cu(1)-Na(2)-Na(1)#8	139.91(8)	O(1C)-Na(4)-O(2W)	80.6(2)
O(5)#5-Na(2)-Na(1)	137.91(12)	O(2C)-Na(4)-O(2W)	74.3(2)
O(1W)-Na(2)-Na(1)	113.2(2)	O(2)#7-Na(4)-O(2W)	165.3(3)
O(32)-Na(2)-Na(1)	120.28(11)	Na(3)-Na(4)-C(15)#1	96.7(4)
O(2C)-Na(2)-Na(1)	66.11(11)	O(1C)-Na(4)-C(15)#1	167.3(4)
O(3)#3-Na(2)-Na(1)	71.33(11)	O(2C)-Na(4)-C(15)#1	140.5(3)
O(2)#7-Na(2)-Na(1)	44.34(9)	O(2)#7-Na(4)-C(15)#1	91.7(2)
Na(4)-Na(2)-Na(1)	54.06(14)	O(2W)-Na(4)-C(15)#1	97.7(2)
Cu(1)-Na(2)-Na(1)	101.27(7)	Na(3)-Na(4)-O(1W)	150.7(4)
Na(1)#8-Na(2)-Na(1)	86.01(7)	O(1C)-Na(4)-O(1W)	122.7(3)
Na(4)-Na(3)-O(2W)	89.4(4)	O(2C)-Na(4)-O(1W)	72.6(3)
Na(4)-Na(3)-O(1C)	75.7(3)	O(2)#7-Na(4)-O(1W)	76.7(3)
O(2W)-Na(3)-O(1C)	89.85(19)	O(2W)-Na(4)-O(1W)	95.9(3)
Na(4)-Na(3)-O(6)#1	163.1(3)	C(15)#1-Na(4)-O(1W)	69.9(2)
O(2W)-Na(3)-O(6)#1	95.4(3)	Na(3)-Na(4)-C(1C)	88.8(3)
O(1C)-Na(3)-O(6)#1	120.5(2)	O(1C)-Na(4)-C(1C)	25.17(13)
Na(4)-Na(3)-O(1LM)	97.4(4)	O(2C)-Na(4)-C(1C)	26.37(13)
O(2W)-Na(3)-O(1LM)	162.7(2)	O(2)#7-Na(4)-C(1C)	94.9(2)

O(2W)-Na(4)-C(1C)	73.4(2)	O(2C)-Na(4)-Na(1)	77.73(17)
C(15)#1-Na(4)-C(1C)	165.2(3)	O(2)#7-Na(4)-Na(1)	55.61(14)
O(1W)-Na(4)-C(1C)	98.8(3)	O(2W)-Na(4)-Na(1)	121.9(3)
Na(3)-Na(4)-Na(2)	155.3(4)	C(15)#1-Na(4)-Na(1)	133.9(2)
O(1C)-Na(4)-Na(2)	83.8(2)	O(1W)-Na(4)-Na(1)	122.3(3)
O(2C)-Na(4)-Na(2)	48.78(16)	C(1C)-Na(4)-Na(1)	59.93(15)
O(2)#7-Na(4)-Na(2)	49.90(16)	Na(2)-Na(4)-Na(1)	76.92(16)
O(2W)-Na(4)-Na(2)	116.0(3)	C(1LM)-O(1LM)-Na(1)	119.0(3)
C(15)#1-Na(4)-Na(2)	108.0(3)	C(1LM)-O(1LM)-Na(3)	129.6(4)
O(1W)-Na(4)-Na(2)	46.39(18)	Na(1)-O(1LM)-Na(3)	93.66(18)
C(1C)-Na(4)-Na(2)	67.25(18)	Na(2)-O(1W)-Na(4)	73.6(3)
Na(3)-Na(4)-Na(1)	86.0(4)	Na(3)-O(2W)-Na(4)	31.5(2)
O(1C)-Na(4)-Na(1)	42.83(13)	O(3W)-O(2LM)-C(2LM)	65.5(13)

Symmetry transformations used to generate equivalent atoms:

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

#4 x,y,z-1 #5 -x,-y,-z #6 x,y,z+1 #7 x-1,y,z+1

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

Crystal structure $\text{Na}_3[\text{Cu}(\text{DSA})(\text{HCO}_3)] \cdot (\text{H}_2\text{O})_{25/6} \cdot 3 \text{ MeOH}$

Table 1

Operator	Dr. Volker Huch	
Diffractometer	Bruker X8 Area	
Identification code	sh3031	
Empirical formula	$\text{C}_{24} \text{H}_{32.33} \text{Cu N}_3 \text{Na}_3 \text{O}_{18.17} \text{S}_2$	
Formula weight	850.17 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	$a = 11.9315(7) \text{ Å}$	$\alpha = 90^\circ$
	$b = 21.6062(12) \text{ Å}$	$\beta = 105.147(2)^\circ$
	$c = 14.9654(8) \text{ Å}$	$\gamma = 90^\circ$
Volume	$3724.0(4) \text{ Å}^3$	
Z	4	
Density (calculated)	1.516 mg/m^3	
Absorption coefficient	0.810 mm^{-1}	
F(000)	1747	
Crystal size	$0.29 \times 0.19 \times 0.19 \text{ mm}^3$	
Theta range for data collection	$1.77 \text{ to } 27.00^\circ$	
Index ranges	$-15 \leq h \leq 14, -26 \leq k \leq 27, -16 \leq l \leq 19$	
Reflections collected	32384	
Independent reflections	8119 [R(int) = 0.0504]	
Completeness to theta = 27.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8614 and 0.7991	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8119 / 2 / 466	
Goodness-of-fit on F^2	1.025	

Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0750$, $wR_2 = 0.2131$
R indices (all data)	$R_1 = 0.1021$, $wR_2 = 0.2372$
Largest diff. peak and hole	2.555 and -0.780 e.Å ⁻³

Table 2

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for the crystal structure $\text{Na}_3[\text{Cu}(\text{DSA})(\text{HCO}_3)] \cdot (\text{H}_2\text{O})_{25/6} \cdot 3 \text{ MeOH}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	$U(\text{eq})$
Cu(1)	1253(1)	5768(1)	1836(1)	18(1)
C(1C)	2592(5)	5117(2)	3495(4)	24(1)
O(1C)	3022(3)	5098(2)	4349(3)	28(1)
O(2C)	2989(9)	4685(4)	2869(5)	119(4)
O(3C)	1812(3)	5517(2)	3136(2)	23(1)
C(11)	3240(5)	6226(3)	1239(4)	23(1)
O(11)	2740(3)	6120(2)	1915(2)	31(1)
C(16)	4454(5)	6265(3)	1481(4)	34(1)
C(15)	5059(5)	6391(3)	827(4)	31(1)
C(14)	4471(5)	6468(3)	-89(4)	28(1)
C(13)	3283(5)	6426(3)	-359(4)	24(1)
C(12)	2638(4)	6305(2)	291(3)	18(1)
C(21)	1384(4)	6218(2)	0(3)	16(1)
N(22)	756(4)	5978(2)	542(3)	17(1)
C(23)	-353(4)	5913(2)	-10(3)	16(1)
N(24)	-451(4)	6111(2)	-861(3)	18(1)
N(25)	645(4)	6314(2)	-841(3)	17(1)
C(31)	-1309(4)	5648(2)	287(3)	18(1)
C(32)	-1212(4)	5465(2)	1204(3)	18(1)
O(32)	-245(3)	5508(2)	1896(2)	20(1)
C(33)	-2213(5)	5215(2)	1416(4)	21(1)
C(34)	-3238(5)	5138(3)	740(4)	25(1)

C(35)	-3328(5)	5308(3)	-172(4)	31(1)
C(36)	-2368(5)	5562(3)	-384(4)	27(1)
C(41)	808(4)	6517(2)	-1719(3)	16(1)
C(42)	744(4)	6062(2)	-2383(3)	15(1)
C(43)	883(5)	6230(2)	-3245(3)	18(1)
S(1)	721(1)	5643(1)	-4103(1)	17(1)
O(1)	-456(4)	5418(2)	-4231(2)	26(1)
O(2)	922(3)	5939(2)	-4916(2)	20(1)
O(3)	1563(4)	5160(2)	-3716(2)	27(1)
C(44)	1079(5)	6841(2)	-3445(4)	24(1)
C(45)	1100(5)	7290(2)	-2780(4)	24(1)
C(46)	937(5)	7138(2)	-1917(3)	18(1)
S(2)	852(1)	7752(1)	-1139(1)	19(1)
O(4)	-202(4)	7636(2)	-852(3)	27(1)
O(5)	791(4)	8315(2)	-1683(3)	26(1)
O(6)	1888(4)	7719(2)	-393(3)	28(1)
Na(1)	2594(2)	6193(1)	-5432(2)	26(1)
Na(2)	-7(2)	5663(1)	3504(1)	20(1)
Na(3)	-2244(2)	5630(1)	-5253(2)	38(1)
O(1LM)	3881(4)	6425(2)	-6361(3)	30(1)
C(1LM)	4281(7)	7050(4)	-6326(6)	54(2)
O(2LM)	-1592(3)	6293(2)	3738(3)	28(1)
C(2LM)	-2457(7)	6448(3)	2922(5)	46(2)
O(1W)	3912(7)	6250(6)	-4025(5)	124(4)
O(3W)	-4274(5)	5565(3)	-5948(4)	62(2)
O(3LM)	-2120(8)	7625(4)	1460(6)	110(3)
O(6W)	-2413(13)	7685(6)	4934(11)	115(5)
O(5W)	-2445(10)	6575(4)	-4405(9)	140(4)
O(2W)	4101(13)	5436(7)	7227(11)	82(4)
C(3LA)	-2399(14)	7840(8)	586(10)	50(4)
C(3LB)	-2188(16)	8085(8)	2234(11)	60(4)

Table 3

Bond length in [Å].

atom	bond length	atom	bond length
Cu(1)-O(32)	1.898(4)	C(31)-C(32)	1.404(7)
Cu(1)-O(11)	1.905(4)	C(31)-C(36)	1.405(7)
Cu(1)-N(22)	1.926(4)	C(32)-O(32)	1.337(6)
Cu(1)-O(3C)	1.961(4)	C(32)-C(33)	1.420(7)
Cu(1)-Na(2)	3.241(2)	O(32)-Na(2)	2.373(4)
C(1C)-O(1C)	1.246(6)	C(33)-C(34)	1.379(8)
C(1C)-O(3C)	1.281(6)	C(34)-C(35)	1.390(8)
C(1C)-O(2C)	1.486(9)	C(35)-C(36)	1.380(8)
C(1C)-Na(1)#1	2.824(6)	C(41)-C(42)	1.384(7)
O(1C)-Na(3)#2	2.412(5)	C(41)-C(46)	1.393(7)
O(1C)-Na(1)#1	2.459(5)	C(42)-C(43)	1.391(7)
O(3C)-Na(2)	2.396(4)	C(43)-C(44)	1.387(7)
O(3C)-Na(1)#1	2.559(4)	C(43)-S(1)	1.779(5)
C(11)-O(11)	1.323(6)	S(1)-O(2)	1.450(3)
C(11)-C(16)	1.400(8)	S(1)-O(1)	1.452(4)
C(11)-C(12)	1.422(7)	S(1)-O(3)	1.459(4)
C(16)-C(15)	1.387(8)	S(1)-Na(2)#2	3.144(2)
C(15)-C(14)	1.378(8)	O(1)-Na(3)	2.322(5)
C(14)-C(13)	1.372(8)	O(1)-Na(2)#2	2.573(4)
C(13)-C(12)	1.414(7)	O(2)-Na(1)	2.384(4)
C(12)-C(21)	1.457(7)	O(2)-Na(2)#3	2.409(4)
C(21)-N(22)	1.343(6)	O(3)-Na(3)#4	2.571(4)
C(21)-N(25)	1.351(6)	O(3)-Na(2)#2	2.648(5)
N(22)-C(23)	1.371(6)	C(44)-C(45)	1.384(7)
C(23)-N(24)	1.319(6)	C(45)-C(46)	1.395(7)
C(23)-C(31)	1.447(7)	C(46)-S(2)	1.785(5)
N(24)-N(25)	1.372(6)	S(2)-O(6)	1.435(4)
N(25)-C(41)	1.446(6)	S(2)-O(4)	1.452(4)

S(2)-O(5)	1.456(4)	Na(2)-S(1)#2	3.144(2)
S(2)-Na(1)#5	3.080(3)	Na(2)-Na(1)#1	3.300(3)
O(5)-Na(2)#6	2.451(4)	Na(2)-Na(3)#1	3.632(3)
O(5)-Na(1)#5	2.675(5)	Na(3)-O(2LM)#3	2.357(5)
O(6)-Na(1)#5	2.503(4)	Na(3)-O(3W)	2.377(6)
Na(1)-O(1W)	2.280(7)	Na(3)-O(1C)#2	2.412(5)
Na(1)-O(1LM)	2.378(5)	Na(3)-O(5W)	2.449(8)
Na(1)-O(1C)#3	2.459(5)	Na(3)-O(3)#4	2.571(4)
Na(1)-O(6)#6	2.503(4)	Na(3)-Na(2)#3	3.632(3)
Na(1)-O(3C)#3	2.559(4)	Na(3)-Na(1)#4	4.117(3)
Na(1)-O(5)#6	2.675(5)	O(1LM)-C(1LM)	1.428(8)
Na(1)-C(1C)#3	2.824(6)	O(2LM)-C(2LM)	1.417(8)
Na(1)-S(2)#6	3.080(3)	O(2LM)-Na(3)#1	2.357(5)
Na(1)-Na(2)#3	3.300(3)	O(3LM)-C(3LA)	1.346(13)
Na(1)-Na(3)#4	4.117(3)	O(3LM)-C(3LB)	1.545(14)
Na(2)-O(2)#1	2.409(4)	O(6W)-C(3LA)#5	1.49(2)
Na(2)-O(2LM)	2.430(5)	O(5W)-C(3LA)#6	1.265(18)
Na(2)-O(5)#5	2.451(4)	C(3LA)-O(5W)#5	1.265(18)
Na(2)-O(1)#2	2.573(4)	C(3LA)-O(6W)#6	1.49(2)
Na(2)-O(3)#2	2.648(5)		

Table 4

Bond angles in [°].

atom	angle	atom	angle
O(32)-Cu(1)-O(11)	171.23(17)	C(11)-O(11)-Cu(1)	128.4(3)
O(32)-Cu(1)-N(22)	94.08(16)	C(15)-C(16)-C(11)	121.6(5)
O(11)-Cu(1)-N(22)	90.31(17)	C(14)-C(15)-C(16)	120.1(5)
O(32)-Cu(1)-O(3C)	87.27(15)	C(13)-C(14)-C(15)	120.2(5)
O(11)-Cu(1)-O(3C)	88.75(16)	C(14)-C(13)-C(12)	121.2(5)
N(22)-Cu(1)-O(3C)	176.79(17)	C(13)-C(12)-C(11)	118.9(5)
O(32)-Cu(1)-Na(2)	46.45(11)	C(13)-C(12)-C(21)	121.3(5)
O(11)-Cu(1)-Na(2)	126.27(12)	C(11)-C(12)-C(21)	119.7(4)
N(22)-Cu(1)-Na(2)	135.12(13)	N(22)-C(21)-N(25)	106.9(4)
O(3C)-Cu(1)-Na(2)	47.36(11)	N(22)-C(21)-C(12)	124.1(4)
O(1C)-C(1C)-O(3C)	120.8(5)	N(25)-C(21)-C(12)	128.9(4)
O(1C)-C(1C)-O(2C)	120.8(6)	C(21)-N(22)-C(23)	106.2(4)
O(3C)-C(1C)-O(2C)	118.4(5)	C(21)-N(22)-Cu(1)	128.6(3)
O(1C)-C(1C)-Na(1)#1	60.4(3)	C(23)-N(22)-Cu(1)	125.2(3)
O(3C)-C(1C)-Na(1)#1	64.9(3)	N(24)-C(23)-N(22)	112.1(4)
O(2C)-C(1C)-Na(1)#1	157.3(6)	N(24)-C(23)-C(31)	123.2(4)
C(1C)-O(1C)-Na(3)#2	118.7(4)	N(22)-C(23)-C(31)	124.7(4)
C(1C)-O(1C)-Na(1)#1	93.5(3)	C(23)-N(24)-N(25)	103.8(4)
Na(3)#2-O(1C)-Na(1)#1	115.37(18)	C(21)-N(25)-N(24)	110.9(4)
C(1C)-O(3C)-Cu(1)	128.7(3)	C(21)-N(25)-C(41)	133.2(4)
C(1C)-O(3C)-Na(2)	126.4(3)	N(24)-N(25)-C(41)	115.5(4)
Cu(1)-O(3C)-Na(2)	95.61(15)	C(32)-C(31)-C(36)	119.4(5)
C(1C)-O(3C)-Na(1)#1	88.1(3)	C(32)-C(31)-C(23)	122.8(5)
Cu(1)-O(3C)-Na(1)#1	128.90(18)	C(36)-C(31)-C(23)	117.8(5)
Na(2)-O(3C)-Na(1)#1	83.45(13)	O(32)-C(32)-C(31)	124.8(5)
O(11)-C(11)-C(16)	117.1(5)	O(32)-C(32)-C(33)	117.3(4)
O(11)-C(11)-C(12)	124.9(5)	C(31)-C(32)-C(33)	117.8(5)
C(16)-C(11)-C(12)	118.0(5)	C(32)-O(32)-Cu(1)	128.1(3)

C(32)-O(32)-Na(2)	130.3(3)	C(45)-C(44)-C(43)	119.0(5)
Cu(1)-O(32)-Na(2)	98.13(15)	C(44)-C(45)-C(46)	121.3(5)
C(34)-C(33)-C(32)	121.2(5)	C(41)-C(46)-C(45)	118.2(4)
C(33)-C(34)-C(35)	121.0(5)	C(41)-C(46)-S(2)	123.3(4)
C(36)-C(35)-C(34)	118.4(5)	C(45)-C(46)-S(2)	118.5(4)
C(35)-C(36)-C(31)	122.2(5)	O(6)-S(2)-O(4)	113.5(2)
C(42)-C(41)-C(46)	121.3(4)	O(6)-S(2)-O(5)	112.5(2)
C(42)-C(41)-N(25)	116.2(4)	O(4)-S(2)-O(5)	112.9(2)
C(46)-C(41)-N(25)	122.3(4)	O(6)-S(2)-C(46)	106.7(2)
C(41)-C(42)-C(43)	118.9(4)	O(4)-S(2)-C(46)	105.5(2)
C(44)-C(43)-C(42)	121.0(5)	O(5)-S(2)-C(46)	104.9(2)
C(44)-C(43)-S(1)	121.0(4)	O(6)-S(2)-Na(1)#5	53.29(16)
C(42)-C(43)-S(1)	117.9(4)	O(4)-S(2)-Na(1)#5	125.77(16)
O(2)-S(1)-O(1)	113.8(2)	O(5)-S(2)-Na(1)#5	60.23(17)
O(2)-S(1)-O(3)	113.7(2)	C(46)-S(2)-Na(1)#5	128.68(18)
O(1)-S(1)-O(3)	110.8(2)	S(2)-O(5)-Na(2)#6	130.8(2)
O(2)-S(1)-C(43)	106.3(2)	S(2)-O(5)-Na(1)#5	91.57(19)
O(1)-S(1)-C(43)	104.7(2)	Na(2)#6-O(5)-Na(1)#5	80.03(12)
O(3)-S(1)-C(43)	106.9(2)	S(2)-O(6)-Na(1)#5	99.4(2)
O(2)-S(1)-Na(2)#2	138.77(15)	O(1W)-Na(1)-O(1LM)	97.7(3)
O(1)-S(1)-Na(2)#2	53.95(16)	O(1W)-Na(1)-O(2)	98.5(3)
O(3)-S(1)-Na(2)#2	56.99(18)	O(1LM)-Na(1)-O(2)	163.89(16)
C(43)-S(1)-Na(2)#2	114.86(17)	O(1W)-Na(1)-O(1C)#3	93.3(3)
S(1)-O(1)-Na(3)	135.4(2)	O(1LM)-Na(1)-O(1C)#3	86.35(16)
S(1)-O(1)-Na(2)#2	98.9(2)	O(2)-Na(1)-O(1C)#3	92.45(15)
Na(3)-O(1)-Na(2)#2	121.07(17)	O(1W)-Na(1)-O(6)#6	94.7(3)
S(1)-O(2)-Na(1)	135.2(2)	O(1LM)-Na(1)-O(6)#6	95.08(16)
S(1)-O(2)-Na(2)#3	125.4(2)	O(2)-Na(1)-O(6)#6	83.85(14)
Na(1)-O(2)-Na(2)#3	87.03(13)	O(1C)#3-Na(1)-O(6)#6	171.55(16)
S(1)-O(3)-Na(3)#4	122.0(2)	O(1W)-Na(1)-O(3C)#3	144.8(3)
S(1)-O(3)-Na(2)#2	95.5(2)	O(1LM)-Na(1)-O(3C)#3	77.33(14)
Na(3)#4-O(3)-Na(2)#2	88.18(14)	O(2)-Na(1)-O(3C)#3	89.30(14)

O(1C)#3-Na(1)-O(3C)#3	51.87(13)	O(1W)-Na(1)-Na(3)#4	85.0(3)
O(6)#6-Na(1)-O(3C)#3	120.31(14)	O(1LM)-Na(1)-Na(3)#4	118.02(13)
O(1W)-Na(1)-O(5)#6	149.3(3)	O(2)-Na(1)-Na(3)#4	63.37(10)
O(1LM)-Na(1)-O(5)#6	91.80(15)	O(1C)#3-Na(1)-Na(3)#4	31.96(10)
O(2)-Na(1)-O(5)#6	74.35(13)	O(6)#6-Na(1)-Na(3)#4	146.69(13)
O(1C)#3-Na(1)-O(5)#6	116.49(14)	O(3C)#3-Na(1)-Na(3)#4	67.93(10)
O(6)#6-Na(1)-O(5)#6	55.20(12)	O(5)#6-Na(1)-Na(3)#4	116.05(11)
O(3C)#3-Na(1)-O(5)#6	65.84(12)	C(1C)#3-Na(1)-Na(3)#4	50.89(11)
O(1W)-Na(1)-C(1C)#3	117.9(3)	S(2)#6-Na(1)-Na(3)#4	133.65(8)
O(1LM)-Na(1)-C(1C)#3	75.30(16)	Na(2)#3-Na(1)-Na(3)#4	69.17(6)
O(2)-Na(1)-C(1C)#3	96.81(16)	O(32)-Na(2)-O(3C)	67.89(13)
O(1C)#3-Na(1)-C(1C)#3	26.13(14)	O(32)-Na(2)-O(2)#1	158.90(16)
O(6)#6-Na(1)-C(1C)#3	146.74(16)	O(3C)-Na(2)-O(2)#1	92.67(14)
O(3C)#3-Na(1)-C(1C)#3	26.95(14)	O(32)-Na(2)-O(2LM)	109.46(15)
O(5)#6-Na(1)-C(1C)#3	92.78(15)	O(3C)-Na(2)-O(2LM)	153.26(16)
O(1W)-Na(1)-S(2)#6	121.2(3)	O(2)#1-Na(2)-O(2LM)	83.99(14)
O(1LM)-Na(1)-S(2)#6	97.15(13)	O(32)-Na(2)-O(5)#5	87.58(14)
O(2)-Na(1)-S(2)#6	74.60(10)	O(3C)-Na(2)-O(5)#5	71.91(14)
O(1C)#3-Na(1)-S(2)#6	144.21(13)	O(2)#1-Na(2)-O(5)#5	78.21(13)
O(6)#6-Na(1)-S(2)#6	27.36(9)	O(2LM)-Na(2)-O(5)#5	81.45(15)
O(3C)#3-Na(1)-S(2)#6	94.00(11)	O(32)-Na(2)-O(1)#2	104.90(14)
O(5)#6-Na(1)-S(2)#6	28.19(8)	O(3C)-Na(2)-O(1)#2	82.58(14)
C(1C)#3-Na(1)-S(2)#6	120.94(13)	O(2)#1-Na(2)-O(1)#2	79.49(13)
O(1W)-Na(1)-Na(2)#3	143.1(3)	O(2LM)-Na(2)-O(1)#2	122.48(15)
O(1LM)-Na(1)-Na(2)#3	117.44(13)	O(5)#5-Na(2)-O(1)#2	145.00(16)
O(2)-Na(1)-Na(2)#3	46.80(10)	O(32)-Na(2)-O(3)#2	97.18(13)
O(1C)#3-Na(1)-Na(2)#3	78.68(11)	O(3C)-Na(2)-O(3)#2	130.18(15)
O(6)#6-Na(1)-Na(2)#3	93.31(12)	O(2)#1-Na(2)-O(3)#2	101.91(13)
O(3C)#3-Na(1)-Na(2)#3	46.16(10)	O(2LM)-Na(2)-O(3)#2	76.25(14)
O(5)#6-Na(1)-Na(2)#3	47.01(9)	O(5)#5-Na(2)-O(3)#2	157.53(16)
C(1C)#3-Na(1)-Na(2)#3	65.12(13)	O(1)#2-Na(2)-O(3)#2	54.60(13)
S(2)#6-Na(1)-Na(2)#3	68.07(6)	O(32)-Na(2)-S(1)#2	101.14(11)

O(3C)-Na(2)-S(1)#2	106.09(11)	Na(1)#1-Na(2)-Na(3)#1	118.96(8)
O(2)#1-Na(2)-S(1)#2	91.88(10)	O(1)-Na(3)-O(2LM)#3	98.14(16)
O(2LM)-Na(2)-S(1)#2	100.54(12)	O(1)-Na(3)-O(3W)	158.8(2)
O(5)#5-Na(2)-S(1)#2	169.68(12)	O(2LM)#3-Na(3)-O(3W)	102.95(19)
O(1)#2-Na(2)-S(1)#2	27.14(9)	O(1)-Na(3)-O(1C)#2	85.65(15)
O(3)#2-Na(2)-S(1)#2	27.52(9)	O(2LM)#3-Na(3)-O(1C)#2	174.55(19)
O(32)-Na(2)-Cu(1)	35.42(9)	O(3W)-Na(3)-O(1C)#2	73.15(18)
O(3C)-Na(2)-Cu(1)	37.03(9)	O(1)-Na(3)-O(5W)	91.2(3)
O(2)#1-Na(2)-Cu(1)	123.48(12)	O(2LM)#3-Na(3)-O(5W)	85.3(3)
O(2LM)-Na(2)-Cu(1)	127.34(12)	O(3W)-Na(3)-O(5W)	92.9(3)
O(5)#5-Na(2)-Cu(1)	64.93(10)	O(1C)#2-Na(3)-O(5W)	98.6(3)
O(1)#2-Na(2)-Cu(1)	107.33(11)	O(1)-Na(3)-O(3)#4	83.34(15)
O(3)#2-Na(2)-Cu(1)	128.31(10)	O(2LM)#3-Na(3)-O(3)#4	79.03(15)
S(1)#2-Na(2)-Cu(1)	119.82(7)	O(3W)-Na(3)-O(3)#4	98.3(2)
O(32)-Na(2)-Na(1)#1	112.74(12)	O(1C)#2-Na(3)-O(3)#4	97.60(16)
O(3C)-Na(2)-Na(1)#1	50.39(10)	O(5W)-Na(3)-O(3)#4	162.5(3)
O(2)#1-Na(2)-Na(1)#1	46.16(10)	O(1)-Na(3)-Na(2)#3	70.68(11)
O(2LM)-Na(2)-Na(1)#1	113.91(12)	O(2LM)#3-Na(3)-Na(2)#3	41.41(11)
O(5)#5-Na(2)-Na(1)#1	52.97(11)	O(3W)-Na(3)-Na(2)#3	125.31(18)
O(1)#2-Na(2)-Na(1)#1	92.30(11)	O(1C)#2-Na(3)-Na(2)#3	137.89(14)
O(3)#2-Na(2)-Na(1)#1	140.86(11)	O(5W)-Na(3)-Na(2)#3	115.7(2)
S(1)#2-Na(2)-Na(1)#1	117.71(7)	O(3)#4-Na(3)-Na(2)#3	46.79(11)
Cu(1)-Na(2)-Na(1)#1	77.32(6)	O(1)-Na(3)-Na(1)#4	77.46(12)
O(32)-Na(2)-Na(3)#1	127.42(12)	O(2LM)#3-Na(3)-Na(1)#4	144.39(14)
O(3C)-Na(2)-Na(3)#1	161.24(12)	O(3W)-Na(3)-Na(1)#4	83.96(16)
O(2)#1-Na(2)-Na(3)#1	73.34(11)	O(1C)#2-Na(3)-Na(1)#4	32.66(11)
O(2LM)-Na(2)-Na(3)#1	39.92(10)	O(5W)-Na(3)-Na(1)#4	129.7(3)
O(5)#5-Na(2)-Na(3)#1	115.84(12)	O(3)#4-Na(3)-Na(1)#4	65.38(11)
O(1)#2-Na(2)-Na(3)#1	82.59(11)	Na(2)#3-Na(3)-Na(1)#4	106.38(8)
O(3)#2-Na(2)-Na(3)#1	45.03(10)	C(1LM)-O(1LM)-Na(1)	116.0(4)
S(1)#2-Na(2)-Na(3)#1	63.01(6)	C(2LM)-O(2LM)-Na(3)#1	114.1(4)
Cu(1)-Na(2)-Na(3)#1	161.23(8)	C(2LM)-O(2LM)-Na(2)	115.3(4)

Na(3)#1-O(2LM)-Na(2)	98.67(16)	O(5W)#5-C(3LA)-O(3LM)	109.5(13)
C(3LA)-O(3LM)-C(3LB)	117.3(12)	O(5W)#5-C(3LA)-O(6W)#6	140.6(13)
C(3LA)#6-O(5W)-Na(3)	144.8(10)	O(3LM)-C(3LA)-O(6W)#6	109.4(13)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 -x,-y+1,-z #3 x,y,z-1 #4 -x,-y+1,-z-1

#5 x,-y+3/2,z+1/2 #6 x,-y+3/2,z-1/2