

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3** (cont.).

	x	y	z	U(eq)
H(10W)	3055	273	-609	80
H(10\$)	2796	-135	-780	80
H(10)	1898	163	-762	80
H(10\$)	4061	258	-1787	80
H(10)	4096	-83	-1409	80
H(10A)	4304	319	-1195	80
H(11A)	3012	751	-1260	90
H(11B)	1834	626	-1255	90
H(11C)	2090	953	-1957	93
H(11D)	3061	712	-2103	93
H(11E)	526	800	-2158	80
H(11F)	474	412	-1882	80
H(11G)	243	442	-2479	80
H(11H)	1512	430	-3041	80
H(11I)	2653	553	-2875	80
H(11J)	1727	841	-2862	80
H(114)	7184	-1299	-4647	80
H(115)	8146	-873	-4177	80
H(116)	9437	-1070	-3608	80
H(117)	9765	-1693	-3508	80
H(118)	8803	-2119	-3978	80
H(119)	7512	-1922	-4548	80
H(120)	-4023	-1094	-6022	80
H(121)	-5584	-981	-5623	80
H(122)	-5681	-528	-5001	80
H(123)	-4217	-188	-4778	80
H(124)	-2655	-300	-5176	80
H(125)	-2558	-753	-5798	80

Table S11. Crystal data and structure refinement for 4.

Identification code	4	
Empirical formula	$C_{137}H_{200}Na_3Nb_2O_{20}$	
Formula weight	2421.76	
Temperature	143(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	$a = 33.504(4)$ Å	$\alpha = 90^\circ$.
	$b = 13.289(2)$ Å	$\beta = 108.08(2)^\circ$.
	$c = 31.235(4)$ Å	$\gamma = 90^\circ$.
Volume	$13220(3)$ Å ³	
Z	4	
Density (calculated)	1.217 Mg/m ³	
Absorption coefficient	0.247 mm ⁻¹	
F(000)	5188	
Crystal size	0.33 x 0.27 x 0.20 mm ³	
Theta range for data collection	1.68 to 25.03°	
Index ranges	$-35 < h < 36$, $-15 < k < 15$, $-37 < l < 37$	
Reflections collected	72872	
Independent reflections	20855 [R(int) = 0.0532]	
Absorption correction	None	
Refinement method	Full-matrix-block least-squares on F ²	
Data / restraints / parameters	20855 / 171 / 1488	
Goodness-of-fit on F ²	1.062	
Final R indices [I > 2sigma(I)]	R1 = 0.0590, wR2 = 0.1647	
R indices (all data)	R1 = 0.0839, wR2 = 0.1796	
Extinction coefficient	0.00340(18)	
Largest diff. peak and hole	0.881 and -0.785 e.Å ⁻³	

Table S12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Nb(1)	3003(1)	-4590(1)	-4522(1)	32
Nb(2)	1961(1)	-4285(1)	-5473(1)	32
O(1)	3311(1)	-5310(2)	-4924(1)	36
O(2)	3341(1)	-3404(2)	-4529(1)	37
O(3)	2827(1)	-3948(2)	-3997(1)	34
O(4)	2908(1)	-5945(2)	-4295(1)	36
O(5)	2167(1)	-4883(2)	-5989(1)	34
O(6)	1947(1)	-2966(2)	-5758(1)	36
O(7)	1619(1)	-3646(2)	-5082(1)	33
O(8)	1718(1)	-5621(2)	-5403(1)	35
C(1)	3712(1)	-5662(3)	-4748(1)	32
C(2)	3789(1)	-6642(3)	-4592(1)	33
C(3)	4199(1)	-7018(3)	-4458(1)	36
C(4)	4541(1)	-6431(3)	-4473(1)	35
C(5)	4456(1)	-5441(3)	-4609(1)	34
C(6)	4054(1)	-5027(3)	-4742(1)	32
C(7)	3995(1)	-3920(3)	-4877(1)	35
C(8)	3721(1)	-3002(3)	-4318(1)	33
C(9)	4058(1)	-3216(3)	-4481(1)	33
C(10)	4447(1)	-2767(3)	-4256(1)	37
C(11)	4509(1)	-2128(3)	-3891(1)	36
C(12)	4163(1)	-1957(3)	-3736(1)	36
C(13)	3772(1)	-2390(3)	-3943(1)	33
C(14)	3405(1)	-2249(3)	-3757(1)	34
C(15)	3111(1)	-3927(3)	-3575(1)	33
C(16)	3382(1)	-3096(3)	-3437(1)	32
C(17)	3649(1)	-3048(3)	-2997(1)	36
C(18)	3664(1)	-3803(3)	-2679(1)	36
C(19)	3404(1)	-4629(3)	-2829(1)	37
C(20)	3131(1)	-4707(3)	-3269(1)	33
C(21)	2867(1)	-5656(3)	-3407(1)	40
C(22)	3141(1)	-6575(3)	-3968(1)	36
C(23)	3119(1)	-6506(3)	-3532(1)	36
C(24)	3340(1)	-7196(3)	-3210(1)	44
C(25)	3588(1)	-7955(3)	-3310(1)	44
C(26)	3607(1)	-7991(3)	-3750(1)	41
C(27)	3391(1)	-7312(3)	-4082(1)	36
C(28)	3437(1)	-7336(3)	-4551(1)	37
C(29)	4979(1)	-6891(3)	-4389(1)	39
C(30)	4927(1)	-1599(3)	-3662(1)	44
C(31)	3963(1)	-3690(3)	-2198(1)	42
C(32)	3817(2)	-8726(4)	-2954(2)	57
C(33)	5018(1)	-7187(4)	-4846(2)	59
C(34)	5041(1)	-7842(4)	-4094(2)	70
C(35)	5328(1)	-6145(4)	-4157(2)	72
C(36)	5025(1)	-1581(5)	-3152(2)	73
C(37)	4901(2)	-530(4)	-3832(2)	90
C(38)	5294(1)	-2123(5)	-3763(2)	77
C(39)	4417(1)	-3648(4)	-2209(1)	54
C(40)	3854(2)	-2708(4)	-1996(2)	63

Table S12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4** (cont).

	x	y	z	U(eq)
C(41)	3926(1)	-4559(4)	-1895(1)	54
C(42A)	3460(4)	-9461(9)	-2888(4)	81
C(43A)	4102(4)	-9376(10)	-3112(4)	82
C(44A)	4014(3)	-8216(9)	-2519(4)	70
C(42B)	3694(4)	-9763(8)	-3101(4)	79
C(43B)	4330(3)	-8671(10)	-2910(4)	86
C(44B)	3809(5)	-8520(10)	-2476(4)	90
C(45)	1893(1)	-4980(3)	-6409(1)	32
C(46)	1659(1)	-5872(3)	-6536(1)	36
C(47)	1397(1)	-5990(3)	-6978(1)	38
C(48)	1347(1)	-5237(3)	-7302(1)	40
C(49)	1565(1)	-4348(3)	-7166(1)	37
C(50)	1836(1)	-4190(3)	-6730(1)	36
C(51)	2049(1)	-3188(3)	-6616(1)	36
C(52)	1712(1)	-2359(3)	-6087(1)	34
C(53)	1762(1)	-2394(3)	-6516(1)	36
C(54)	1525(1)	-1748(3)	-6844(1)	37
C(55)	1237(1)	-1070(3)	-6769(1)	37
C(56)	1192(1)	-1070(3)	-6334(1)	36
C(57)	1421(1)	-1705(3)	-5993(1)	34
C(58)	1361(1)	-1717(3)	-5532(1)	35
C(59)	1201(1)	-3446(3)	-5266(1)	31
C(60)	1060(1)	-2527(3)	-5473(1)	33
C(61)	627(1)	-2327(3)	-5625(1)	34
C(62)	332(1)	-3004(3)	-5578(1)	34
C(63)	478(1)	-3933(3)	-5388(1)	35
C(64)	905(1)	-4182(3)	-5241(1)	32
C(65)	1034(1)	-5240(3)	-5074(1)	34
C(66)	1344(1)	-6071(3)	-5626(1)	34
C(67)	1004(1)	-5957(3)	-5460(1)	32
C(68)	633(1)	-6467(3)	-5680(1)	37
C(69)	589(1)	-7070(3)	-6053(1)	36
C(70)	932(1)	-7136(3)	-6214(1)	37
C(71)	1310(1)	-6646(3)	-6008(1)	35
C(72)	1674(1)	-6708(3)	-6201(1)	37
C(73)	1056(1)	-5438(4)	-7785(1)	46
C(74)	971(1)	-342(3)	-7131(1)	42
C(75)	-138(1)	-2749(3)	-5687(1)	41
C(76)	185(1)	-7683(3)	-6270(1)	42
C(77)	1231(2)	-6342(5)	-7982(2)	71
C(78)	613(1)	-5686(4)	-7782(2)	57
C(79)	1033(2)	-4516(4)	-8089(2)	67
C(80)	506(1)	-442(4)	-7167(2)	58
C(81)	1007(2)	-570(4)	-7597(2)	67
C(82)	1115(2)	724(4)	-6999(2)	60
C(83)	-408(1)	-3559(4)	-5995(2)	68
C(84)	-242(1)	-2713(4)	-5247(1)	51
C(85)	-241(1)	-1720(4)	-5919(2)	58
C(86)	253(2)	-8744(4)	-6066(2)	65
C(87)	-198(1)	-7215(4)	-6181(2)	60

Table S12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4** (cont).

	x	y	z	U(eq)
C(88)	90(1)	-7770(4)	-6780(1)	52
C(89)	2487(1)	-4362(3)	-5001(1)	37
Na(1)	2183(1)	-3287(1)	-4438(1)	38
O(9)	2365(1)	-1585(2)	-4476(1)	50
C(90)	2512(2)	-1385(5)	-4854(2)	87
C(91)	2883(2)	-732(4)	-4693(2)	67
C(92)	2785(2)	-120(4)	-4339(2)	74
C(93)	2459(2)	-710(4)	-4193(2)	86
O(10)	1827(1)	-3519(4)	-3925(1)	85
C(94)	2030(2)	-3632(10)	-3468(2)	181
C(95)	1728(3)	-3615(12)	-3262(3)	258
C(96)	1339(3)	-3723(14)	-3596(3)	292
C(97)	1389(2)	-3607(6)	-3990(2)	86
Na(2)	2882(1)	-4799(1)	-5628(1)	42
O(11)	3111(1)	-3240(2)	-5819(1)	50
C(98)	3323(2)	-2805(5)	-6106(2)	79
C(99)	3124(2)	-1789(5)	-6253(2)	87
C(100)	2917(2)	-1528(4)	-5901(2)	65
C(101)	3028(1)	-2387(4)	-5578(2)	58
O(12)	3243(1)	-5670(4)	-6027(1)	90
C(102)	3205(4)	-6564(8)	-6160(5)	274
C(103)	3524(4)	-6862(11)	-6334(6)	323
C(104)	3854(3)	-6290(10)	-6065(5)	278
C(105)	3668(2)	-5524(8)	-5968(3)	161
Na(3)	2264(1)	-6381(1)	-4833(1)	42
O(13)	1996(1)	-7071(3)	-4295(1)	64
C(106)	1915(2)	-8532(5)	-5238(2)	88
C(107)	1816(2)	-9070(5)	-5651(2)	101
C(108)	2220(2)	-9143(5)	-5757(2)	93
C(109)	2515(2)	-8282(5)	-5459(2)	80
O(14)	2270(1)	-7881(3)	-5210(1)	65
C(110)	1669(2)	-6723(6)	-4134(2)	111
C(111)	1680(2)	-7312(7)	-3729(3)	139
C(112)	2071(2)	-7880(5)	-3617(2)	92
C(113)	2178(1)	-7915(4)	-4029(2)	64
O(15)	-26(1)	-1013(3)	-1876(1)	57
C(114)	279(1)	-272(4)	-1642(2)	55
C(115)	703(1)	-762(4)	-1540(1)	48
C(116)	626(1)	-1591(4)	-1888(2)	48
C(117)	183(1)	-1907(3)	-1929(2)	47
O(16)	3579(1)	-5305(4)	-162(2)	108
C(118)	3721(3)	-5816(7)	-445(3)	127
C(119)	4075(3)	-5276(11)	-537(3)	190
C(120)	4219(3)	-4652(9)	-144(3)	166
C(121)	3941(2)	-4851(6)	120(2)	98
O(17)	4326(2)	-95(5)	1549(2)	141
C(122)	4328(2)	838(4)	1822(2)	75
C(123)	4756(3)	1236(6)	1895(2)	118
C(124)	5010(2)	501(6)	1890(3)	97
C(125)	4809(2)	-334(6)	1701(3)	120

Table S12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4** (cont).

	x	y	z	U(eq)
O(18)	686(2)	-4873(6)	160(3)	166
C(126)	1067(2)	-5560(6)	245(4)	151
C(127)	1388(2)	-5082(5)	438(3)	106
C(128)	1318(2)	-4203(7)	640(3)	129
C(129)	852(2)	-3980(6)	508(2)	103
O(19)	2422(4)	4787(9)	-2209(5)	307
C(130)	2730(4)	4086(12)	-1912(6)	315
C(131)	2444(5)	3412(12)	-1842(5)	284
C(132)	2386(6)	3067(10)	-2268(5)	336
C(133)	2176(3)	3894(10)	-2465(4)	227
O(20)	2756(3)	-11539(12)	-2523(6)	383
C(134)	2435(6)	-11428(13)	-2930(7)	497
C(135)	2374(4)	-10442(12)	-2924(5)	264
C(136)	2506(4)	-10018(11)	-2550(5)	286
C(137)	2807(5)	-10632(13)	-2239(5)	359

Table S13. Bond lengths [Å] and angles [°] for 4.

Nb(1)-C(89)	1.925(4)	C(29)-C(35)	1.531(6)	O(9)-C(93)	1.435(6)
Nb(1)-O(2)	1.944(3)	C(29)-C(34)	1.539(6)	O(9)-C(90)	1.437(6)
Nb(1)-O(4)	1.996(3)	C(30)-C(37)	1.510(7)	C(90)-C(91)	1.470(7)
Nb(1)-O(1)	2.086(2)	C(30)-C(36)	1.523(6)	C(91)-C(92)	1.490(7)
Nb(1)-O(3)	2.089(2)	C(30)-C(38)	1.529(6)	C(92)-C(93)	1.526(7)
Nb(1)-Na(1)	3.3251(14)	C(31)-C(41)	1.523(6)	O(10)-C(94)	1.387(7)
Nb(1)-Na(3)	3.3526(16)	C(31)-C(39)	1.532(5)	O(10)-C(97)	1.420(5)
Nb(1)-Na(2)	3.3622(15)	C(31)-C(40)	1.542(6)	C(94)-C(95)	1.358(9)
Nb(2)-C(89)	1.919(3)	C(32)-C(42B)	1.470(12)	C(95)-C(96)	1.400(12)
Nb(2)-O(6)	1.960(3)	C(32)-C(44A)	1.479(11)	C(96)-C(97)	1.302(9)
Nb(2)-O(8)	1.992(3)	C(32)-C(43A)	1.479(11)	Na(2)-O(12)	2.299(4)
Nb(2)-O(7)	2.094(2)	C(32)-C(44B)	1.528(13)	Na(2)-O(11)	2.348(4)
Nb(2)-O(5)	2.097(2)	C(32)-C(42A)	1.606(11)	O(11)-C(98)	1.429(5)
Nb(2)-Na(2)	3.3399(14)	C(32)-C(43B)	1.683(12)	O(11)-C(101)	1.436(5)
Nb(2)-Na(1)	3.3566(15)	C(45)-C(46)	1.407(5)	C(98)-C(99)	1.514(8)
Nb(2)-Na(3)	3.3942(17)	C(45)-C(50)	1.423(5)	C(99)-C(100)	1.510(8)
O(1)-C(1)	1.369(4)	C(46)-C(47)	1.396(5)	C(100)-C(101)	1.493(7)
O(1)-Na(2)	2.325(3)	C(46)-C(72)	1.517(5)	O(12)-C(102)	1.253(9)
O(2)-C(8)	1.349(4)	C(47)-C(48)	1.396(6)	O(12)-C(105)	1.393(7)
O(3)-C(15)	1.368(4)	C(48)-C(49)	1.385(6)	C(102)-C(103)	1.398(10)
O(3)-Na(1)	2.340(3)	C(48)-C(73)	1.544(5)	C(102)-C(105)	2.025(13)
O(4)-C(22)	1.364(4)	C(49)-C(50)	1.399(5)	C(103)-C(104)	1.388(15)
O(4)-Na(3)	2.359(3)	C(50)-C(51)	1.500(6)	C(104)-C(105)	1.278(10)
O(5)-C(45)	1.355(4)	C(51)-C(53)	1.523(5)	Na(3)-O(14)	2.318(4)
O(5)-Na(2)	2.312(3)	C(52)-C(53)	1.400(5)	Na(3)-O(13)	2.326(3)
O(6)-C(52)	1.352(4)	C(52)-C(57)	1.403(5)	O(13)-C(113)	1.417(6)
O(7)-C(59)	1.366(4)	C(53)-C(54)	1.383(5)	O(13)-C(110)	1.419(6)
O(7)-Na(1)	2.342(3)	C(54)-C(55)	1.392(5)	C(106)-C(107)	1.420(9)
O(8)-C(66)	1.369(4)	C(55)-C(56)	1.413(5)	C(106)-O(14)	1.451(6)
O(8)-Na(3)	2.347(3)	C(55)-C(74)	1.544(5)	C(107)-C(108)	1.495(9)
C(1)-C(2)	1.387(5)	C(56)-C(57)	1.388(5)	C(108)-C(109)	1.605(8)
C(1)-C(6)	1.418(5)	C(57)-C(58)	1.515(5)	C(109)-O(14)	1.399(6)
C(2)-C(3)	1.398(5)	C(58)-C(60)	1.524(5)	C(110)-C(111)	1.479(8)
C(2)-C(28)	1.533(5)	C(59)-C(60)	1.394(5)	C(111)-C(112)	1.457(8)
C(3)-C(4)	1.399(5)	C(59)-C(64)	1.411(5)	C(112)-C(113)	1.438(7)
C(4)-C(5)	1.385(5)	C(60)-C(61)	1.406(5)	O(15)-C(117)	1.414(5)
C(4)-C(29)	1.535(5)	C(61)-C(62)	1.378(5)	O(15)-C(114)	1.443(5)
C(5)-C(6)	1.394(5)	C(62)-C(63)	1.391(5)	C(114)-C(115)	1.506(6)
C(6)-C(7)	1.527(6)	C(62)-C(75)	1.539(5)	C(115)-C(116)	1.512(6)
C(7)-C(9)	1.513(5)	C(63)-C(64)	1.401(5)	C(116)-C(117)	1.509(5)
C(8)-C(13)	1.392(5)	C(64)-C(65)	1.514(5)	O(16)-C(118)	1.316(8)
C(8)-C(9)	1.404(5)	C(65)-C(67)	1.514(5)	O(16)-C(121)	1.397(7)
C(9)-C(10)	1.408(5)	C(66)-C(71)	1.392(5)	C(118)-C(119)	1.490(12)
C(10)-C(11)	1.387(5)	C(66)-C(67)	1.399(5)	C(119)-C(120)	1.436(13)
C(11)-C(12)	1.404(5)	C(67)-C(68)	1.395(5)	C(120)-C(121)	1.446(10)
C(11)-C(30)	1.532(5)	C(68)-C(69)	1.382(5)	O(17)-C(122)	1.506(8)
C(12)-C(13)	1.393(5)	C(69)-C(70)	1.392(5)	O(17)-C(125)	1.568(8)
C(13)-C(14)	1.526(5)	C(69)-C(76)	1.546(5)	C(122)-C(123)	1.478(8)
C(14)-C(16)	1.523(5)	C(70)-C(71)	1.391(5)	C(123)-C(124)	1.299(9)
C(15)-C(20)	1.397(5)	C(71)-C(72)	1.520(5)	C(124)-C(125)	1.337(9)
C(15)-C(16)	1.409(5)	C(73)-C(78)	1.522(6)	O(18)-C(126)	1.526(9)
C(16)-C(17)	1.389(5)	C(73)-C(79)	1.537(7)	O(18)-C(129)	1.588(10)
C(17)-C(18)	1.401(5)	C(73)-C(77)	1.546(6)	C(126)-C(127)	1.232(10)

Table S13. Bond lengths [Å] and angles [°] for 4 (cont.).

C(18)-C(19)	1.390(6)	C(74)-C(82)	1.511(6)	C(127)-C(128)	1.382(9)
C(18)-C(31)	1.532(5)	C(74)-C(81)	1.527(6)	C(128)-C(129)	1.514(8)
C(19)-C(20)	1.399(5)	C(74)-C(80)	1.533(6)	O(19)-C(130)	1.484(14)
C(20)-C(21)	1.524(5)	C(75)-C(84)	1.523(5)	O(19)-C(133)	1.521(13)
C(21)-C(23)	1.532(5)	C(75)-C(85)	1.535(6)	C(130)-C(131)	1.377(14)
C(22)-C(23)	1.389(5)	C(75)-C(83)	1.538(6)	C(130)-C(132)	1.898(15)
C(22)-C(27)	1.405(5)	C(76)-C(87)	1.524(6)	C(131)-C(132)	1.364(18)
C(23)-C(24)	1.392(6)	C(76)-C(88)	1.530(6)	C(131)-C(133)	1.979(16)
C(24)-C(25)	1.404(6)	C(76)-C(86)	1.535(6)	C(132)-C(133)	1.345(14)
C(25)-C(26)	1.396(6)	C(89)-Na(1)	2.698(4)	O(20)-C(134)	1.395(16)
C(25)-C(32)	1.532(6)	C(89)-Na(2)	2.745(4)	O(20)-C(137)	1.475(17)
C(26)-C(27)	1.395(5)	C(89)-Na(3)	2.876(4)	C(134)-C(135)	1.326(16)
C(27)-C(28)	1.522(5)	Na(1)-O(10)	2.297(3)	C(135)-C(136)	1.249(18)
C(29)-C(33)	1.526(6)	Na(1)-O(9)	2.354(4)	C(136)-C(137)	1.421(14)
C(89)-Nb(1)-O(2)	104.46(14)	C(33)-C(29)-C(34)	108.2(4)	O(9)-Na(1)-C(89)	108.62(12)
C(89)-Nb(1)-O(4)	102.39(14)	C(35)-C(29)-C(34)	107.9(4)	O(10)-Na(1)-Nb(1)	127.29(12)
O(2)-Nb(1)-O(4)	153.11(10)	C(4)-C(29)-C(34)	112.0(3)	O(3)-Na(1)-Nb(1)	38.55(6)
C(89)-Nb(1)-O(1)	95.58(12)	C(37)-C(30)-C(36)	108.9(5)	O(7)-Na(1)-Nb(1)	106.95(8)
O(2)-Nb(1)-O(1)	88.10(10)	C(37)-C(30)-C(38)	108.5(4)	O(9)-Na(1)-Nb(1)	105.23(8)
O(4)-Nb(1)-O(1)	87.86(10)	C(36)-C(30)-C(38)	107.3(4)	C(89)-Na(1)-Nb(1)	35.37(8)
C(89)-Nb(1)-O(3)	98.14(12)	C(37)-C(30)-C(11)	108.8(3)	O(10)-Na(1)-Nb(2)	127.62(11)
O(2)-Nb(1)-O(3)	89.08(10)	C(36)-C(30)-C(11)	111.3(3)	O(3)-Na(1)-Nb(2)	107.85(8)
O(4)-Nb(1)-O(3)	88.58(10)	C(38)-C(30)-C(11)	111.9(4)	O(7)-Na(1)-Nb(2)	38.14(6)
O(1)-Nb(1)-O(3)	166.27(9)	C(41)-C(31)-C(18)	112.4(4)	O(9)-Na(1)-Nb(2)	108.31(9)
C(89)-Nb(1)-Na(1)	54.25(10)	C(41)-C(31)-C(39)	108.3(3)	C(89)-Na(1)-Nb(2)	34.85(8)
O(2)-Nb(1)-Na(1)	94.40(8)	C(18)-C(31)-C(39)	109.5(3)	Nb(1)-Na(1)-Nb(2)	70.12(3)
O(4)-Nb(1)-Na(1)	102.46(7)	C(41)-C(31)-C(40)	108.1(4)	C(93)-O(9)-C(90)	106.9(4)
O(1)-Nb(1)-Na(1)	149.39(7)	C(18)-C(31)-C(40)	108.6(3)	C(93)-O(9)-Na(1)	139.2(3)
O(3)-Nb(1)-Na(1)	44.28(7)	C(39)-C(31)-C(40)	109.9(4)	C(90)-O(9)-Na(1)	112.3(3)
C(89)-Nb(1)-Na(3)	58.87(13)	C(42B)-C(32)-C(44A)	136.0(7)	O(9)-C(90)-C(91)	107.4(5)
O(2)-Nb(1)-Na(3)	162.23(8)	C(42B)-C(32)-C(43A)	59.8(7)	C(90)-C(91)-C(92)	102.6(4)
O(4)-Nb(1)-Na(3)	43.81(7)	C(44A)-C(32)-C(43A)	115.0(8)	C(91)-C(92)-C(93)	106.5(4)
O(1)-Nb(1)-Na(3)	87.63(7)	C(42B)-C(32)-C(44B)	112.6(8)	O(9)-C(93)-C(92)	105.8(4)
O(3)-Nb(1)-Na(3)	98.92(7)	C(44A)-C(32)-C(44B)	32.6(6)	C(94)-O(10)-C(97)	107.1(4)
Na(1)-Nb(1)-Na(3)	80.76(4)	C(43A)-C(32)-C(44B)	129.8(8)	C(94)-O(10)-Na(1)	122.5(3)
C(89)-Nb(1)-Na(2)	54.72(10)	C(42B)-C(32)-C(25)	111.8(5)	C(97)-O(10)-Na(1)	130.4(3)
O(2)-Nb(1)-Na(2)	86.61(8)	C(44A)-C(32)-C(25)	109.9(6)	C(95)-C(94)-O(10)	106.5(6)
O(4)-Nb(1)-Na(2)	107.99(8)	C(43A)-C(32)-C(25)	112.2(6)	C(94)-C(95)-C(96)	107.7(8)
O(1)-Nb(1)-Na(2)	43.04(7)	C(44B)-C(32)-C(25)	115.7(6)	C(97)-C(96)-C(95)	109.2(7)
O(3)-Nb(1)-Na(2)	150.08(7)	C(42B)-C(32)-C(42A)	47.4(6)	C(96)-C(97)-O(10)	107.7(6)
Na(1)-Nb(1)-Na(2)	106.57(4)	C(44A)-C(32)-C(42A)	107.3(8)	O(12)-Na(2)-O(5)	110.53(13)
Na(3)-Nb(1)-Na(2)	78.53(4)	C(43A)-C(32)-C(42A)	105.7(8)	O(12)-Na(2)-O(1)	95.26(13)
C(89)-Nb(2)-O(6)	106.47(14)	C(44B)-C(32)-C(42A)	75.0(8)	O(5)-Na(2)-O(1)	133.57(11)
C(89)-Nb(2)-O(8)	100.20(14)	C(25)-C(32)-C(42A)	106.0(5)	O(12)-Na(2)-O(11)	92.23(15)
O(6)-Nb(2)-O(8)	153.33(10)	C(42B)-C(32)-C(43B)	104.3(7)	O(5)-Na(2)-O(11)	106.80(11)
C(89)-Nb(2)-O(7)	96.43(12)	C(44A)-C(32)-C(43B)	75.6(7)	O(1)-Na(2)-O(11)	110.13(11)
O(6)-Nb(2)-O(7)	87.85(10)	C(43A)-C(32)-C(43B)	46.0(6)	O(12)-Na(2)-C(89)	160.69(17)
O(8)-Nb(2)-O(7)	88.99(10)	C(44B)-C(32)-C(43B)	103.9(8)	O(5)-Na(2)-C(89)	72.67(10)
C(89)-Nb(2)-O(5)	97.29(12)	C(25)-C(32)-C(43B)	107.3(5)	O(1)-Na(2)-C(89)	71.26(10)
O(6)-Nb(2)-O(5)	87.51(10)	C(42A)-C(32)-C(43B)	143.0(7)	O(11)-Na(2)-C(89)	105.24(13)
O(8)-Nb(2)-O(5)	89.37(10)	O(5)-C(45)-C(46)	120.2(3)	O(12)-Na(2)-Nb(2)	147.79(12)
O(7)-Nb(2)-O(5)	166.26(9)	O(5)-C(45)-C(50)	121.0(3)	O(5)-Na(2)-Nb(2)	38.39(6)

Table S13. Bond lengths [Å] and angles [°] for **4** (cont.).

C(89)-Nb(2)-Na(2)	55.26(10)	C(46)-C(45)-C(50)	118.8(3)	O(1)-Na(2)-Nb(2)	104.44(8)
O(6)-Nb(2)-Na(2)	90.53(7)	C(47)-C(46)-C(45)	119.8(4)	O(11)-Na(2)-Nb(2)	104.22(9)
O(8)-Nb(2)-Na(2)	105.09(7)	C(47)-C(46)-C(72)	118.3(4)	C(89)-Na(2)-Nb(2)	35.06(7)
O(7)-Nb(2)-Na(2)	149.77(7)	C(45)-C(46)-C(72)	121.8(3)	O(12)-Na(2)-Nb(1)	133.02(12)
O(5)-Nb(2)-Na(2)	43.22(7)	C(46)-C(47)-C(48)	122.3(4)	O(5)-Na(2)-Nb(1)	106.29(8)
C(89)-Nb(2)-Na(1)	53.48(10)	C(49)-C(48)-C(47)	117.1(3)	O(1)-Na(2)-Nb(1)	37.77(6)
O(6)-Nb(2)-Na(1)	92.93(8)	C(49)-C(48)-C(73)	124.0(4)	O(11)-Na(2)-Nb(1)	104.13(9)
O(8)-Nb(2)-Na(1)	102.90(8)	C(47)-C(48)-C(73)	118.8(4)	C(89)-Na(2)-Nb(1)	34.92(8)
O(7)-Nb(2)-Na(1)	43.68(6)	C(48)-C(49)-C(50)	123.2(4)	Nb(2)-Na(2)-Nb(1)	69.87(3)
O(5)-Nb(2)-Na(1)	149.58(6)	C(49)-C(50)-C(45)	118.7(4)	C(98)-O(11)-C(101)	103.0(4)
Na(2)-Nb(2)-Na(1)	106.36(4)	C(49)-C(50)-C(51)	118.8(4)	C(98)-O(11)-Na(2)	141.4(3)
C(89)-Nb(2)-Na(3)	57.86(13)	C(45)-C(50)-C(51)	122.4(3)	C(101)-O(11)-Na(2)	115.6(2)
O(6)-Nb(2)-Na(3)	164.11(7)	C(50)-C(51)-C(53)	112.3(3)	O(11)-C(98)-C(99)	107.0(4)
O(8)-Nb(2)-Na(3)	42.45(7)	O(6)-C(52)-C(53)	119.5(3)	C(100)-C(99)-C(98)	104.1(4)
O(7)-Nb(2)-Na(3)	96.17(8)	O(6)-C(52)-C(57)	119.3(3)	C(101)-C(100)-C(99)	104.0(4)
O(5)-Nb(2)-Na(3)	91.80(8)	C(53)-C(52)-C(57)	121.2(3)	O(11)-C(101)-C(100)	107.2(4)
Na(2)-Nb(2)-Na(3)	78.26(4)	C(54)-C(53)-C(52)	118.5(3)	C(102)-O(12)-C(105)	99.7(6)
Na(1)-Nb(2)-Na(3)	79.71(4)	C(54)-C(53)-C(51)	122.1(3)	C(102)-O(12)-Na(2)	130.0(5)
C(1)-O(1)-Nb(1)	121.7(2)	C(52)-C(53)-C(51)	119.3(4)	C(105)-O(12)-Na(2)	123.1(4)
C(1)-O(1)-Na(2)	136.1(2)	C(53)-C(54)-C(55)	123.0(3)	O(12)-C(102)-C(103)	112.8(8)
Nb(1)-O(1)-Na(2)	99.19(10)	C(54)-C(55)-C(56)	116.7(4)	O(12)-C(102)-C(105)	42.7(4)
C(8)-O(2)-Nb(1)	141.3(2)	C(54)-C(55)-C(74)	123.7(3)	C(103)-C(102)-C(105)	72.5(6)
C(15)-O(3)-Nb(1)	119.0(2)	C(56)-C(55)-C(74)	119.6(3)	C(104)-C(103)-C(102)	99.9(9)
C(15)-O(3)-Na(1)	143.0(2)	C(57)-C(56)-C(55)	122.6(3)	C(105)-C(104)-C(103)	103.0(8)
Nb(1)-O(3)-Na(1)	97.16(10)	C(56)-C(57)-C(52)	118.0(3)	C(104)-C(105)-O(12)	114.3(8)
C(22)-O(4)-Nb(1)	134.6(2)	C(56)-C(57)-C(58)	122.1(3)	C(104)-C(105)-C(102)	76.8(7)
C(22)-O(4)-Na(3)	124.6(2)	C(52)-C(57)-C(58)	119.9(3)	O(12)-C(105)-C(102)	37.6(4)
Nb(1)-O(4)-Na(3)	100.35(11)	C(57)-C(58)-C(60)	114.2(3)	O(14)-Na(3)-O(13)	95.39(14)
C(45)-O(5)-Nb(2)	119.60(19)	O(7)-C(59)-C(60)	121.4(3)	O(14)-Na(3)-O(8)	96.45(11)
C(45)-O(5)-Na(2)	140.0(2)	O(7)-C(59)-C(64)	119.3(3)	O(13)-Na(3)-O(8)	109.48(11)
Nb(2)-O(5)-Na(2)	98.38(10)	C(60)-C(59)-C(64)	119.4(3)	O(14)-Na(3)-O(4)	115.02(12)
C(52)-O(6)-Nb(2)	143.6(2)	C(59)-C(60)-C(61)	119.2(3)	O(13)-Na(3)-O(4)	93.13(11)
C(59)-O(7)-Nb(2)	120.6(2)	C(59)-C(60)-C(58)	122.3(3)	O(8)-Na(3)-O(4)	139.40(12)
C(59)-O(7)-Na(1)	140.4(2)	C(61)-C(60)-C(58)	118.5(3)	O(14)-Na(3)-C(89)	131.76(12)
Nb(2)-O(7)-Na(1)	98.18(9)	C(62)-C(61)-C(60)	122.7(4)	O(13)-Na(3)-C(89)	132.82(13)
C(66)-O(8)-Nb(2)	132.4(2)	C(61)-C(62)-C(63)	117.1(3)	O(8)-Na(3)-C(89)	69.28(10)
C(66)-O(8)-Na(3)	124.9(2)	C(61)-C(62)-C(75)	123.3(4)	O(4)-Na(3)-C(89)	70.63(10)
Nb(2)-O(8)-Na(3)	102.60(10)	C(63)-C(62)-C(75)	119.4(3)	O(14)-Na(3)-Nb(1)	129.47(10)
O(1)-C(1)-C(2)	121.0(3)	C(62)-C(63)-C(64)	122.6(4)	O(13)-Na(3)-Nb(1)	119.08(10)
O(1)-C(1)-C(6)	119.4(3)	C(63)-C(64)-C(59)	118.8(4)	O(8)-Na(3)-Nb(1)	104.21(8)
C(2)-C(1)-C(6)	119.6(3)	C(63)-C(64)-C(65)	119.0(3)	O(4)-Na(3)-Nb(1)	35.84(7)
C(1)-C(2)-C(3)	119.9(3)	C(59)-C(64)-C(65)	122.2(3)	C(89)-Na(3)-Nb(1)	34.95(7)
C(1)-C(2)-C(28)	122.1(3)	C(67)-C(65)-C(64)	111.7(3)	O(14)-Na(3)-Nb(2)	117.06(10)
C(3)-C(2)-C(28)	118.0(4)	O(8)-C(66)-C(71)	119.6(3)	O(13)-Na(3)-Nb(2)	129.57(10)
C(2)-C(3)-C(4)	122.0(4)	O(8)-C(66)-C(67)	119.2(3)	O(8)-Na(3)-Nb(2)	34.95(7)
C(5)-C(4)-C(3)	116.7(3)	C(71)-C(66)-C(67)	121.2(3)	O(4)-Na(3)-Nb(2)	104.95(8)
C(5)-C(4)-C(29)	121.6(3)	C(68)-C(67)-C(66)	117.9(3)	C(89)-Na(3)-Nb(2)	34.39(7)
C(3)-C(4)-C(29)	121.4(4)	C(68)-C(67)-C(65)	121.8(3)	Nb(1)-Na(3)-Nb(2)	69.34(4)
C(4)-C(5)-C(6)	123.6(3)	C(66)-C(67)-C(65)	120.1(3)	C(113)-O(13)-C(110)	106.8(4)
C(5)-C(6)-C(1)	118.1(4)	C(69)-C(68)-C(67)	122.8(3)	C(113)-O(13)-Na(3)	123.0(3)
C(5)-C(6)-C(7)	119.5(3)	C(68)-C(69)-C(70)	117.2(3)	C(110)-O(13)-Na(3)	129.9(3)
C(1)-C(6)-C(7)	122.3(3)	C(68)-C(69)-C(76)	121.6(3)	C(107)-C(106)-O(14)	108.2(5)
C(9)-C(7)-C(6)	113.3(3)	C(70)-C(69)-C(76)	121.1(3)	C(106)-C(107)-C(108)	105.1(5)

Table S13. Bond lengths [Å] and angles [°] for 4 (cont.)

O(2)-C(8)-C(13)	119.6(3)	C(71)-C(70)-C(69)	122.5(4)	C(107)-C(108)-C(109)	105.2(5)
O(2)-C(8)-C(9)	119.0(3)	C(70)-C(71)-C(66)	118.2(3)	O(14)-C(109)-C(108)	103.5(5)
C(13)-C(8)-C(9)	121.4(3)	C(70)-C(71)-C(72)	121.2(3)	C(109)-O(14)-C(106)	110.5(5)
C(8)-C(9)-C(10)	117.3(3)	C(66)-C(71)-C(72)	120.5(3)	C(109)-O(14)-Na(3)	135.1(3)
C(8)-C(9)-C(7)	120.0(3)	C(46)-C(72)-C(71)	112.1(3)	C(106)-O(14)-Na(3)	114.0(3)
C(10)-C(9)-C(7)	122.8(3)	C(78)-C(73)-C(79)	108.4(4)	O(13)-C(110)-C(111)	108.3(5)
C(11)-C(10)-C(9)	123.2(3)	C(78)-C(73)-C(48)	110.7(3)	C(112)-C(111)-C(110)	105.1(5)
C(10)-C(11)-C(12)	117.1(3)	C(79)-C(73)-C(48)	111.1(4)	C(113)-C(112)-C(111)	105.0(5)
C(10)-C(11)-C(30)	123.1(3)	C(78)-C(73)-C(77)	109.0(4)	O(13)-C(113)-C(112)	108.5(5)
C(12)-C(11)-C(30)	119.8(3)	C(79)-C(73)-C(77)	109.0(4)	C(117)-O(15)-C(114)	109.6(3)
C(13)-C(12)-C(11)	122.0(4)	C(48)-C(73)-C(77)	108.6(3)	O(15)-C(114)-C(115)	106.5(4)
C(8)-C(13)-C(12)	119.0(3)	C(82)-C(74)-C(81)	109.4(4)	C(114)-C(115)-C(116)	103.0(3)
C(8)-C(13)-C(14)	119.2(3)	C(82)-C(74)-C(80)	109.4(4)	C(117)-C(116)-C(115)	102.0(3)
C(12)-C(13)-C(14)	121.8(3)	C(81)-C(74)-C(80)	107.0(4)	O(15)-C(117)-C(116)	105.4(4)
C(16)-C(14)-C(13)	111.6(3)	C(82)-C(74)-C(55)	109.0(4)	C(118)-O(16)-C(121)	102.9(6)
O(3)-C(15)-C(20)	121.0(3)	C(81)-C(74)-C(55)	112.0(3)	O(16)-C(118)-C(119)	110.8(8)
O(3)-C(15)-C(16)	120.1(3)	C(80)-C(74)-C(55)	110.0(3)	C(120)-C(119)-C(118)	100.9(6)
C(20)-C(15)-C(16)	118.9(3)	C(84)-C(75)-C(85)	108.4(4)	C(119)-C(120)-C(121)	106.1(7)
C(17)-C(16)-C(15)	119.6(4)	C(84)-C(75)-C(83)	109.3(4)	O(16)-C(121)-C(120)	107.9(7)
C(17)-C(16)-C(14)	118.0(3)	C(85)-C(75)-C(83)	109.0(4)	C(122)-O(17)-C(125)	99.9(5)
C(15)-C(16)-C(14)	122.4(3)	C(84)-C(75)-C(62)	108.1(3)	C(123)-C(122)-O(17)	102.4(5)
C(16)-C(17)-C(18)	122.7(4)	C(85)-C(75)-C(62)	111.6(3)	C(124)-C(123)-C(122)	109.7(6)
C(19)-C(18)-C(17)	116.4(3)	C(83)-C(75)-C(62)	110.4(3)	C(123)-C(124)-C(125)	112.8(6)
C(19)-C(18)-C(31)	124.0(4)	C(87)-C(76)-C(88)	107.8(3)	C(124)-C(125)-O(17)	107.3(5)
C(17)-C(18)-C(31)	119.6(4)	C(87)-C(76)-C(86)	108.9(4)	C(126)-O(18)-C(129)	103.3(6)
C(18)-C(19)-C(20)	122.8(4)	C(88)-C(76)-C(86)	108.6(4)	C(127)-C(126)-O(18)	109.4(7)
C(15)-C(20)-C(19)	119.6(4)	C(87)-C(76)-C(69)	112.2(3)	C(126)-C(127)-C(128)	114.4(6)
C(15)-C(20)-C(21)	121.4(3)	C(88)-C(76)-C(69)	111.6(3)	C(127)-C(128)-C(129)	110.3(6)
C(19)-C(20)-C(21)	119.0(4)	C(86)-C(76)-C(69)	107.8(3)	C(128)-C(129)-O(18)	98.9(6)
C(20)-C(21)-C(23)	111.3(3)	Nb(2)-C(89)-Nb(1)	173.9(2)	C(130)-O(19)-C(133)	89.8(10)
O(4)-C(22)-C(23)	120.1(3)	Nb(2)-C(89)-Na(1)	91.68(12)	C(131)-C(130)-O(19)	97.1(11)
O(4)-C(22)-C(27)	119.1(3)	Nb(1)-C(89)-Na(1)	90.38(13)	C(131)-C(130)-C(132)	45.9(8)
C(23)-C(22)-C(27)	120.7(4)	Nb(2)-C(89)-Na(2)	89.67(13)	O(19)-C(130)-C(132)	84.4(8)
C(22)-C(23)-C(24)	119.2(4)	Nb(1)-C(89)-Na(2)	90.36(12)	C(132)-C(131)-C(130)	87.7(10)
C(22)-C(23)-C(21)	119.9(4)	Na(1)-C(89)-Na(2)	160.03(18)	C(132)-C(131)-C(133)	42.7(6)
C(24)-C(23)-C(21)	120.8(3)	Nb(2)-C(89)-Na(3)	87.75(14)	C(130)-C(131)-C(133)	76.1(9)
C(23)-C(24)-C(25)	122.1(4)	Nb(1)-C(89)-Na(3)	86.18(14)	C(133)-C(132)-C(131)	93.9(11)
C(26)-C(25)-C(24)	117.1(4)	Na(1)-C(89)-Na(3)	101.75(12)	C(133)-C(132)-C(130)	79.7(9)
C(26)-C(25)-C(32)	121.7(4)	Na(2)-C(89)-Na(3)	98.21(13)	C(131)-C(132)-C(130)	46.4(7)
C(24)-C(25)-C(32)	121.2(4)	O(10)-Na(1)-O(3)	97.06(12)	C(132)-C(133)-O(19)	106.1(10)
C(27)-C(26)-C(25)	122.5(4)	O(10)-Na(1)-O(7)	96.68(11)	C(132)-C(133)-C(131)	43.4(8)
C(26)-C(27)-C(22)	118.5(4)	O(3)-Na(1)-O(7)	141.19(11)	O(19)-C(133)-C(131)	74.3(7)
C(26)-C(27)-C(28)	121.2(4)	O(10)-Na(1)-O(9)	111.34(15)	C(134)-O(20)-C(137)	112.0(14)
C(22)-C(27)-C(28)	120.3(4)	O(3)-Na(1)-O(9)	100.62(11)	C(135)-C(134)-O(20)	99.8(13)
C(27)-C(28)-C(2)	112.1(3)	O(7)-Na(1)-O(9)	107.76(11)	C(136)-C(135)-C(134)	116.6(13)
C(33)-C(29)-C(35)	109.5(4)	O(10)-Na(1)-C(89)	140.00(16)	C(135)-C(136)-C(137)	110.6(13)
C(33)-C(29)-C(4)	107.2(3)	O(3)-Na(1)-C(89)	73.67(10)	C(136)-C(137)-O(20)	97.6(11)
C(35)-C(29)-C(4)	111.9(3)	O(7)-Na(1)-C(89)	72.51(10)		

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Nb(1)	23	42	26	-4	3	0
Nb(2)	24	42	25	-4	3	2
O(1)	27	47	30	-5	3	2
O(2)	30	47	29	-4	6	2
O(3)	26	47	27	-4	3	1
O(4)	30	44	33	-1	9	-1
O(5)	29	41	28	-4	4	4
O(6)	33	44	31	-3	10	3
O(7)	24	44	29	-3	4	1
O(8)	28	43	31	-5	4	2
C(1)	26	43	25	-5	5	3
C(2)	27	40	32	-9	8	-6
C(3)	33	33	41	-3	11	0
C(4)	29	41	32	-3	7	1
C(5)	29	41	30	-3	9	-2
C(6)	28	41	27	-4	8	-1
C(7)	28	48	27	-1	8	-3
C(8)	27	32	34	4	3	-1
C(9)	32	30	33	3	7	0
C(10)	33	39	37	1	9	1
C(11)	34	33	38	1	6	-2
C(12)	35	35	34	-3	6	0
C(13)	34	34	30	0	7	2
C(14)	35	33	31	-3	4	4
C(15)	30	44	23	-4	7	4
C(16)	29	38	27	-2	7	5
C(17)	32	40	31	-8	5	0
C(18)	36	44	24	-3	6	8
C(19)	39	40	30	2	11	6
C(20)	31	35	33	-3	11	2
C(21)	44	42	35	-1	15	-1
C(22)	30	36	41	-5	9	-8
C(23)	35	36	38	-6	12	-6
C(24)	51	42	39	-4	15	-8
C(25)	46	35	46	2	8	-3
C(26)	41	32	49	-6	11	-5
C(27)	29	36	40	-5	9	-8
C(28)	33	35	42	-9	9	-5
C(29)	28	42	44	8	7	5
C(30)	36	43	49	-4	8	-8
C(31)	46	49	25	-2	1	6
C(32)	75	41	49	2	12	4
C(33)	51	71	57	5	22	17
C(34)	38	88	85	43	20	19
C(35)	30	65	110	-24	6	1
C(36)	51	105	56	-21	6	-25
C(37)	60	61	125	19	-6	-24
C(38)	38	101	87	-42	11	-17
C(39)	44	68	38	-5	-4	-5
C(40)	74	69	36	-17	2	16
C(41)	49	75	32	2	3	0
C(42A)	87	68	84	38	19	-16
C(43A)	94	68	89	33	36	36
C(44A)	79	60	48	-2	-16	14
C(42B)	116	49	60	11	9	10
C(43B)	76	77	82	14	-9	11
C(44B)	130	63	61	4	8	16
C(45)	22	45	27	-7	4	5
C(46)	31	42	31	-5	7	9
C(47)	29	49	33	-11	6	3
C(48)	31	55	30	-9	4	8

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4 (cont.).

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(49)	32	51	28	-4	8	6
C(50)	27	51	30	-5	11	5
C(51)	33	45	30	-1	11	1
C(52)	33	35	31	1	7	-4
C(53)	31	44	35	-8	12	-8
C(54)	38	45	29	-2	13	-2
C(55)	40	37	32	-1	8	-2
C(56)	36	37	37	-4	12	1
C(57)	34	35	32	-6	10	-4
C(58)	36	37	34	-5	12	0
C(59)	26	41	24	-3	5	2
C(60)	34	37	27	-5	10	3
C(61)	34	41	28	0	10	9
C(62)	29	45	26	-2	6	6
C(63)	28	49	29	-5	9	-1
C(64)	29	42	23	-2	6	1
C(65)	29	42	29	0	8	0
C(66)	34	32	31	1	5	2
C(67)	30	32	28	2	3	3
C(68)	32	42	34	6	8	2
C(69)	35	35	35	3	5	-2
C(70)	40	33	33	-3	3	4
C(71)	33	36	32	0	3	6
C(72)	37	39	33	-4	6	6
C(73)	37	64	31	-12	3	6
C(74)	51	36	39	4	13	4
C(75)	30	56	36	1	8	8
C(76)	41	43	38	-1	5	-8
C(77)	65	98	40	-30	1	23
C(78)	42	76	43	-21	-3	-3
C(79)	60	97	29	8	-9	5
C(80)	53	60	55	16	6	7
C(81)	88	70	43	11	20	29
C(82)	69	45	59	8	12	2
C(83)	29	95	68	-28	1	2
C(84)	40	70	46	6	20	14
C(85)	40	81	53	21	15	25
C(86)	64	56	62	2	1	-22
C(87)	41	69	65	-19	9	-18
C(88)	48	55	45	-7	4	-16
C(89)	37	43	34	-6	15	2
Na(1)	33	46	33	-4	7	1
O(9)	51	46	53	-4	14	-2
C(90)	124	76	79	-9	57	-30
C(91)	58	71	71	29	17	8
C(92)	77	54	74	0	-3	-16
C(93)	92	62	123	-21	59	-2
O(10)	49	166	42	7	18	2
C(94)	99	384	67	31	34	78
C(95)	151	534	112	117	75	120
C(96)	80	649	167	136	69	32
C(97)	58	140	62	-7	23	0
Na(2)	30	57	35	-3	6	3
O(11)	46	58	49	3	17	0
C(98)	88	94	74	4	52	-4
C(99)	126	70	71	14	37	-18
C(100)	67	49	69	2	6	-7
C(101)	61	61	55	-1	25	6
O(12)	76	121	77	-36	28	20
C(102)	311	174	475	-152	324	-111
C(103)	335	275	469	-225	285	-63
C(104)	150	305	400	-128	115	82

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4** (cont.).

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(105)	50	281	140	-118	12	22
Na(3)	37	47	36	4	3	-8
O(13)	60	72	65	24	25	-1
C(106)	91	59	91	8	-6	-26
C(107)	125	75	92	2	17	-25
C(108)	108	87	60	-22	-10	44
C(109)	92	69	65	-4	3	17
O(14)	69	48	62	-7	-2	-13
C(110)	87	145	118	69	56	47
C(111)	123	201	125	103	87	83
C(112)	103	100	85	39	45	26
C(113)	55	64	73	13	16	-7
O(15)	41	59	65	-2	7	3
C(114)	65	43	55	-4	16	0
C(115)	46	54	39	5	6	-10
C(116)	46	52	47	1	16	1
C(117)	53	43	43	-3	13	-3
O(16)	95	106	119	-7	26	-4
C(118)	171	119	96	-3	50	40
C(119)	152	344	102	15	80	48
C(120)	122	228	146	32	39	-64
C(121)	67	118	97	6	11	-13
O(17)	140	169	118	-28	46	-48
C(122)	84	66	73	3	21	17
C(123)	177	102	85	-48	54	-81
C(124)	44	108	123	-29	0	-11
C(125)	137	110	134	38	72	72
O(18)	128	160	192	55	24	-16
C(126)	104	99	283	53	111	22
C(127)	45	86	169	-36	6	-1
C(128)	53	220	101	-37	8	9
C(129)	89	147	71	11	24	19
O(19)	325	204	345	-28	35	-18
C(130)	164	341	344	-2	-62	-75
C(131)	319	317	251	33	140	8
C(132)	415	210	335	-132	48	5
C(133)	157	332	175	-118	28	18
O(20)	158	413	499	51	-12	108
C(134)	445	356	579	-87	-1	-187
C(135)	173	366	256	146	72	86
C(136)	134	513	244	152	107	27
C(137)	218	594	263	235	72	-101

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 4.

	x	y	z	U(eq)
H(3)	4247	-7693	-4354	43
H(5)	4685	-5021	-4612	40
H(7A)	4197	-3740	-5039	42
H(7B)	3708	-3824	-5088	42
H(10)	4679	-2910	-4360	44
H(12)	4197	-1532	-3482	43
H(14A)	3436	-1598	-3596	41
H(14B)	3139	-2228	-4010	41
H(17)	3828	-2481	-2907	43
H(19)	3412	-5163	-2624	44
H(21A)	2618	-5504	-3669	48
H(21B)	2767	-5878	-3156	48
H(24)	3321	-7151	-2913	52
H(26)	3774	-8497	-3826	49
H(28A)	3168	-7127	-4773	45
H(28B)	3497	-8034	-4624	45
H(33A)	4975	-6592	-5040	88
H(33B)	4806	-7696	-4986	88
H(33C)	5299	-7463	-4806	88
H(34A)	4840	-8360	-4250	105
H(34B)	4995	-7678	-3807	105
H(34C)	5328	-8094	-4037	105
H(35A)	5602	-6469	-4104	108
H(35B)	5295	-5933	-3870	108
H(35C)	5309	-5556	-4351	108
H(36A)	4824	-1140	-3072	109
H(36B)	5310	-1328	-3013	109
H(36C)	5002	-2264	-3043	109
H(37A)	4869	-534	-4155	135
H(37B)	5158	-169	-3669	135
H(37C)	4658	-194	-3782	135
H(38A)	5299	-2835	-3681	116
H(38B)	5558	-1804	-3589	116
H(38C)	5260	-2065	-4085	116
H(39A)	4479	-4258	-2353	80
H(39B)	4609	-3605	-1900	80
H(39C)	4454	-3056	-2379	80
H(40A)	3895	-2134	-2174	95
H(40B)	4037	-2637	-1684	95
H(40C)	3561	-2731	-2000	95
H(41A)	3637	-4597	-1884	81
H(41B)	4118	-4449	-1591	81
H(41C)	3998	-5191	-2015	81
H(42A)	3593	-10049	-2711	122
H(42B)	3277	-9682	-3183	122
H(42C)	3293	-9101	-2729	122
H(43A)	4282	-8955	-3233	123
H(43B)	3935	-9828	-3348	123
H(43C)	4277	-9774	-2859	123
H(44A)	4139	-8720	-2287	105
H(44B)	3801	-7832	-2434	105
H(44C)	4234	-7758	-2548	105
H(42D)	3887	-10235	-2898	119
H(42E)	3706	-9857	-3408	119
H(42F)	3407	-9887	-3096	119
H(43D)	4442	-8011	-2792	129
H(43E)	4364	-8771	-3208	129
H(43F)	4482	-9199	-2705	129
H(44D)	3948	-9073	-2278	135

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4 (cont.).

	x	y	z	U(eq)
H(44E)	3517	-8467	-2476	135
H(44F)	3956	-7888	-2367	135
H(47)	1248	-6604	-7060	45
H(49)	1529	-3820	-7380	44
H(51A)	2142	-2958	-6870	43
H(51B)	2301	-3265	-6349	43
H(54)	1561	-1768	-7134	44
H(56)	997	-617	-6272	44
H(58A)	1254	-1052	-5476	42
H(58B)	1637	-1819	-5302	42
H(61)	533	-1699	-5767	41
H(63)	280	-4418	-5358	42
H(65A)	1326	-5231	-4869	40
H(65B)	850	-5482	-4901	40
H(68)	400	-6396	-5570	44
H(70)	906	-7530	-6475	45
H(72A)	1942	-6668	-5952	45
H(72B)	1665	-7366	-6352	45
H(77A)	1225	-6946	-7803	107
H(77B)	1521	-6201	-7972	107
H(77C)	1058	-6454	-8294	107
H(78A)	432	-5797	-8091	86
H(78B)	503	-5124	-7649	86
H(78C)	620	-6295	-7603	86
H(79A)	844	-4661	-8392	101
H(79B)	1314	-4364	-8105	101
H(79C)	927	-3937	-7963	101
H(80A)	338	4	-7405	88
H(80B)	466	-254	-6879	88
H(80C)	415	-1139	-7239	88
H(81A)	925	-1270	-7677	100
H(81B)	1297	-467	-7593	100
H(81C)	821	-119	-7819	100
H(82A)	954	1189	-7233	89
H(82B)	1414	783	-6967	89
H(82C)	1069	890	-6712	89
H(83A)	-357	-4212	-5842	101
H(83B)	-335	-3598	-6275	101
H(83C)	-706	-3383	-6065	101
H(84A)	-173	-3361	-5092	76
H(84B)	-542	-2576	-5310	76
H(84C)	-78	-2179	-5055	76
H(85A)	-544	-1600	-6001	87
H(85B)	-155	-1712	-6191	87
H(85C)	-91	-1192	-5712	87
H(86A)	322	-8699	-5738	97
H(86B)	484	-9072	-6142	97
H(86C)	-5	-9140	-6188	97
H(87A)	-223	-6510	-6277	90
H(87B)	-165	-7252	-5859	90
H(87C)	-451	-7584	-6351	90
H(88A)	-167	-8163	-6907	78
H(88B)	324	-8106	-6846	78
H(88C)	52	-7096	-6914	78
H(90A)	2291	-1045	-5096	104
H(90B)	2588	-2022	-4974	104
H(91A)	2917	-302	-4939	81
H(91B)	3142	-1133	-4566	81
H(92A)	2672	546	-4461	89

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **4** (cont.).

	x	y	z	U(eq)
H(92B)	3042	-14	-4080	89
H(93A)	2572	-906	-3873	104
H(93B)	2203	-300	-4234	104
H(94A)	2185	-4278	-3408	80
H(94B)	2233	-3076	-3355	80
H(95A)	1738	-2971	-3100	80
H(95B)	1772	-4172	-3042	80
H(96A)	1223	-4399	-3575	80
H(96B)	1140	-3214	-3552	80
H(97A)	1241	-2995	-4138	80
H(97B)	1273	-4194	-4184	80
H(98A)	3294	-3241	-6371	95
H(98B)	3626	-2726	-5941	95
H(99A)	3339	-1282	-6259	105
H(99B)	2914	-1829	-6556	105
H(10A)	3027	-886	-5750	78
H(10B)	2609	-1472	-6038	78
H(10C)	3280	-2220	-5322	69
H(10D)	2793	-2535	-5458	69
H(10E)	2930	-6645	-6396	80
H(10F)	3207	-7011	-5906	80
H(10G)	3582	-7592	-6293	80
H(10H)	3458	-6686	-6657	80
H(10I)	4012	-6662	-5790	80
H(10J)	4049	-6090	-6232	80
H(10K)	3698	-4952	-6159	80
H(10L)	3810	-5337	-5651	80
H(10M)	1987	-9008	-4981	106
H(10N)	1671	-8126	-5227	106
H(10O)	1602	-8705	-5892	121
H(10P)	1707	-9749	-5617	121
H(10Q)	2175	-9026	-6081	112
H(10R)	2349	-9815	-5675	112
H(10S)	2779	-8570	-5258	96
H(10T)	2582	-7763	-5653	96
H(11A)	1394	-6810	-4369	134
H(11B)	1708	-5999	-4057	134
H(11C)	1677	-6861	-3477	166
H(11D)	1436	-7771	-3793	166
H(11E)	2293	-7539	-3377	111
H(11F)	2031	-8568	-3515	111
H(11G)	2487	-7901	-3960	77
H(11H)	2071	-8544	-4194	77
H(11I)	226	-63	-1360	66
H(11J)	262	331	-1833	66
H(11K)	797	-1041	-1231	58
H(11L)	916	-280	-1575	58
H(11M)	647	-1336	-2178	57
H(11N)	826	-2154	-1782	57
H(11O)	46	-2212	-2228	56
H(11P)	182	-2402	-1693	56
H(11Q)	3491	-5916	-731	152
H(11R)	3817	-6488	-317	152
H(11S)	4296	-5747	-560	228
H(11T)	3978	-4869	-815	228
H(12A)	4206	-3933	-230	199
H(12B)	4512	-4821	30	199
H(12C)	4080	-5303	375	117
H(12D)	3869	-4215	244	117

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4 (cont.).

	x	y	z	U(eq)
H(12E)	4112	1324	1655	90
H(12F)	4281	674	2112	90
H(12G)	4753	1725	1654	142
H(12H)	4854	1590	2188	142
H(12I)	5182	349	2203	117
H(12J)	5202	714	1722	117
H(12K)	4873	-894	1921	145
H(12L)	4897	-531	1438	145
H(12M)	1039	-6138	434	181
H(12N)	1085	-5825	-44	181
H(12O)	1534	-4916	216	127
H(12P)	1577	-5518	671	127
H(12Q)	1464	-3638	545	154
H(12R)	1433	-4269	971	154
H(12S)	783	-3312	363	123
H(12T)	744	-4026	768	123
H(13A)	2916	3774	-2066	80
H(13B)	2900	4411	-1629	80
H(13C)	2568	2910	-1603	80
H(13D)	2192	3731	-1799	80
H(13E)	2653	2967	-2336	80
H(13F)	2213	2449	-2338	80
H(13G)	1887	3891	-2445	80
H(13H)	2162	3924	-2786	80
H(13I)	2526	-11633	-3190	80
H(13J)	2181	-11811	-2933	80
H(13K)	2509	-10122	-3130	80
H(13L)	2068	-10313	-3048	80
H(13M)	2269	-9881	-2434	80
H(13N)	2636	-9366	-2585	80
H(13O)	2733	-10757	-1961	80
H(13P)	3094	-10350	-2161	80