Tabelle 1. Kristall- und Verfeinerungsdaten für mja191 (M. Jochem AK Detert)

Substanzkode	mja191	
Summenformel	$C_{40}H_{57}BrCl_2N_3NaO_8$	
Molekülformel	$C_{39}H_{55}N_3NaO_8$,CH_2Cl_2, Br	
Formelgewicht	881.68	
Temperatur	120(2) K	
Wellenlänge, Strahlungsart	0.71073Å, MoKα	
Diffraktometer	STOE IPDS 2T	
Kristallsystem	Triclinic	
Raumgruppenname, Nummer	P -1, (2)	
Gitterkonstanten	a = 13.0218(6) Å	α = 74.897(4)°
	b = 13.4232(6) Å	β = 74.232(4)°
	c = 14.0528(7) Å	γ = 63.961(3)°
Volumen	2095.43(19) $Å^3$	
Reflexanzahl und	23375	
Messbereich für Gitterkonstanten	2.10° <=Θ<= 28.57°	
Z	2	
Dichte (berechnet)	1.397 Mg/m^3	
Absorptionskoeffizient	1.173 mm^{-1}	
Methode der Absorptionskorrektur	None	
F(000)	924	
Kristallgröße, Form und Farbe	0.360 x 0.210 x 0.210 mm^3, farbloser Block	
Theta Bereich der Messung	2.539 bis 27.992°.	
Index Bereich	-17<=h<=17, -17<=k<=17, -18<=l<=17	
Zahl der Reflexe:		
gemessen	17904	
unabhängig	9891 [R_{int} = 0.0324]	
beobachtet [I>2sigma(I)]	7662	
Vollständigkeit bei Θ_{max}= 25.2°	99.4 %	
Verfeinerungsmethode	Full-matrix least-squares on F^2	
Reflexe / Restraints / Parameter	9891 / 0 / 499	
Fitgüte für F^2	1.125	
Abschließende R Werte [I>2sigma(I)]	R1 = 0.0529, wR2 = 0.1049	
R Wert (alle Daten)	R1 = 0.0798, wR2 = 0.1193	
Maximum und Minimum der diff. Map	0.500 und -0.456 $e.Å^{-3}$	

Tabelle 2. Endkoordinaten und äquivalente Auslenkungsparameter (Å^2) für mja191

$U_{äq}=(1/3)*\Sigma\Sigma_{ij}a_i^*a_j^*\ \mathbf{a}_i\mathbf{a}_j$

Atom	x	y	z	$U_{äq}$
Na1	0.27317(10)	0.35569(9)	0.28485(8)	0.0268(2)
Br1	0.25070(3)	0.43480(3)	0.78237(2)	0.03321(9)
C1	0.7522(3)	0.2109(2)	0.3975(2)	0.0260(6)
C2	0.8599(3)	0.1453(3)	0.4239(2)	0.0316(7)
C3	0.8767(3)	0.1324(3)	0.5203(3)	0.0366(7)
C4	0.7835(3)	0.1827(3)	0.5916(2)	0.0360(7)
C5	0.6745(3)	0.2467(3)	0.5661(2)	0.0327(7)
C6	0.6559(3)	0.2632(2)	0.4690(2)	0.0255(6)
O7	0.73301(18)	0.21951(17)	0.30296(15)	0.0287(4)
C8	0.8108(3)	0.2516(3)	0.2189(2)	0.0311(6)
C9	0.8004(3)	0.2220(3)	0.1273(2)	0.0338(7)
O10	0.8440(2)	0.1046(2)	0.12768(19)	0.0455(6)
C11	0.9667(4)	0.0521(4)	0.1175(4)	0.0735(14)
N12	0.5463(2)	0.3277(2)	0.44070(18)	0.0251(5)
C13	0.5452(3)	0.4211(2)	0.3561(2)	0.0256(6)
C14	0.5157(2)	0.4111(2)	0.2620(2)	0.0263(6)
O15	0.39443(18)	0.47210(16)	0.25468(15)	0.0269(4)
C16	0.4464(3)	0.3576(3)	0.5226(2)	0.0285(6)
C17	0.3320(3)	0.3965(2)	0.4897(2)	0.0267(6)
O18	0.32518(18)	0.31101(16)	0.45109(15)	0.0260(4)
C19	0.3573(3)	0.5856(2)	0.2195(2)	0.0257(6)
C20	0.2433(3)	0.6394(2)	0.2007(2)	0.0270(6)
C21	0.2037(3)	0.7523(3)	0.1584(2)	0.0323(7)
C22	0.2721(3)	0.8130(3)	0.1390(2)	0.0340(7)
C23	0.3826(3)	0.7611(3)	0.1634(2)	0.0299(6)
C24	0.4254(3)	0.6467(2)	0.2021(2)	0.0283(6)
C25	0.2994(2)	0.2267(2)	0.5191(2)	0.0243(6)
C26	0.3040(3)	0.1403(2)	0.4773(2)	0.0251(6)
C27	0.2696(3)	0.0579(2)	0.5410(2)	0.0278(6)
C28	0.2331(3)	0.0596(2)	0.6439(2)	0.0298(6)
C29	0.2347(3)	0.1417(2)	0.6853(2)	0.0274(6)
C30	0.2686(3)	0.2256(2)	0.6220(2)	0.0274(6)
C31	0.4554(3)	0.8273(3)	0.1521(3)	0.0359(7)
C32	0.2035(3)	0.1421(3)	0.7971(2)	0.0355(7)
N33	0.1701(2)	0.5771(2)	0.22704(18)	0.0267(5)
N34	0.3450(2)	0.1422(2)	0.37106(18)	0.0264(5)
C35	0.0750(3)	0.6218(3)	0.3107(2)	0.0301(6)
C36	0.0009(3)	0.5551(2)	0.3534(2)	0.0304(6)
O37	0.07391(18)	0.44067(17)	0.38556(16)	0.0298(5)
C38	0.0127(3)	0.3688(3)	0.4088(2)	0.0335(7)
C39	0.0223(3)	0.3258(3)	0.3168(3)	0.0347(7)
O40	0.14172(18)	0.25630(17)	0.28238(16)	0.0306(5)
C41	0.1722(3)	0.1421(3)	0.3306(2)	0.0310(6)
C42	0.3024(3)	0.0865(2)	0.3236(2)	0.0285(6)
C43	0.4731(3)	0.1029(2)	0.3484(2)	0.0280(6)
C44	0.5211(3)	0.1184(2)	0.2371(2)	0.0300(6)
O45	0.45796(18)	0.23122(17)	0.19416(15)	0.0282(4)
C46	0.4706(3)	0.2446(3)	0.0884(2)	0.0322(7)
C47	0.4113(3)	0.3674(3)	0.0485(2)	0.0328(7)

Atom	x	y	z	$U_{äq}$
O48	0.29551(18)	0.40845(17)	0.10223(15)	0.0291(4)
C49	0.2295(3)	0.5218(2)	0.0607(2)	0.0311(6)
C50	0.1291(3)	0.5746(3)	0.1402(2)	0.0306(6)
C1L	0.1872(3)	0.2719(3)	0.0282(3)	0.0446(8)
Cl1	0.24439(12)	0.12351(9)	0.05282(8)	0.0649(3)
Cl2	0.03476(10)	0.33474(11)	0.05888(8)	0.0648(3)

Tabelle 3. Anisotrope Auslenkunsparameter ($Å^2$) für mja191. Die anisotropen Auslenkungsparameter haben die Form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na1	0.0275(6)	0.0271(6)	0.0242(6)	-0.0015(5)	-0.0042(5)	-0.0110(5)
Br1	0.03539(17)	0.03303(16)	0.03303(17)	-0.00225(12)	-0.00495(13)	-0.01764(13)
C1	0.0291(15)	0.0263(14)	0.0262(14)	-0.0003(11)	-0.0063(12)	-0.0156(12)
C2	0.0290(16)	0.0293(15)	0.0317(16)	-0.0011(12)	-0.0042(13)	-0.0101(13)
C3	0.0330(17)	0.0387(18)	0.0361(18)	0.0016(14)	-0.0119(14)	-0.0134(14)
C4	0.0400(19)	0.0399(18)	0.0289(16)	-0.0003(14)	-0.0116(14)	-0.0163(15)
C5	0.0343(17)	0.0363(17)	0.0283(16)	-0.0047(13)	-0.0057(13)	-0.0148(14)
C6	0.0270(15)	0.0248(14)	0.0259(14)	-0.0008(11)	-0.0052(12)	-0.0129(12)
O7	0.0299(11)	0.0319(11)	0.0245(10)	-0.0026(9)	-0.0029(9)	-0.0147(9)
C8	0.0295(16)	0.0326(16)	0.0282(15)	-0.0027(13)	0.0000(13)	-0.0140(13)
C9	0.0385(18)	0.0316(16)	0.0279(16)	0.0008(13)	-0.0046(13)	-0.0148(14)
O10	0.0612(17)	0.0350(13)	0.0402(14)	-0.0082(11)	0.0010(12)	-0.0238(12)
C11	0.066(3)	0.046(2)	0.088(4)	-0.025(2)	-0.001(3)	-0.002(2)
N12	0.0254(12)	0.0270(12)	0.0218(12)	-0.0004(10)	-0.0035(10)	-0.0118(10)
C13	0.0269(15)	0.0251(14)	0.0265(15)	-0.0019(11)	-0.0047(12)	-0.0130(12)
C14	0.0248(14)	0.0259(14)	0.0280(15)	-0.0021(12)	-0.0066(12)	-0.0101(12)
O15	0.0273(11)	0.0230(10)	0.0288(11)	0.0010(8)	-0.0080(9)	-0.0099(8)
C16	0.0311(16)	0.0325(15)	0.0241(14)	-0.0070(12)	-0.0021(12)	-0.0149(13)
C17	0.0285(15)	0.0235(14)	0.0284(15)	-0.0051(11)	-0.0033(12)	-0.0111(12)
O18	0.0299(11)	0.0255(10)	0.0245(10)	-0.0010(8)	-0.0055(8)	-0.0140(9)
C19	0.0302(15)	0.0252(14)	0.0196(13)	-0.0023(11)	-0.0013(11)	-0.0118(12)
C20	0.0281(15)	0.0261(14)	0.0253(14)	-0.0027(11)	-0.0034(12)	-0.0110(12)
C21	0.0313(16)	0.0261(15)	0.0337(17)	-0.0004(13)	-0.0069(13)	-0.0080(13)
C22	0.0392(18)	0.0236(15)	0.0325(17)	0.0007(12)	-0.0035(14)	-0.0111(13)
C23	0.0375(17)	0.0286(15)	0.0233(14)	-0.0032(12)	-0.0006(12)	-0.0160(13)
C24	0.0294(15)	0.0291(15)	0.0244(14)	-0.0037(12)	-0.0015(12)	-0.0122(12)
C25	0.0218(14)	0.0239(13)	0.0264(14)	-0.0005(11)	-0.0031(11)	-0.0110(11)
C26	0.0251(14)	0.0252(14)	0.0234(14)	-0.0007(11)	-0.0068(11)	-0.0090(11)
C27	0.0299(15)	0.0237(14)	0.0299(15)	-0.0010(12)	-0.0083(12)	-0.0110(12)
C28	0.0294(16)	0.0267(15)	0.0299(16)	0.0009(12)	-0.0042(13)	-0.0119(12)
C29	0.0271(15)	0.0260(14)	0.0245(14)	-0.0009(11)	-0.0035(12)	-0.0087(12)
C30	0.0264(15)	0.0272(14)	0.0284(15)	-0.0047(12)	-0.0058(12)	-0.0099(12)
C31	0.0444(19)	0.0308(16)	0.0329(17)	-0.0030(13)	-0.0003(14)	-0.0203(15)
C32	0.0429(19)	0.0337(17)	0.0274(16)	-0.0022(13)	-0.0031(14)	-0.0165(15)
N33	0.0260(13)	0.0287(12)	0.0242(12)	-0.0024(10)	-0.0051(10)	-0.0106(10)
N34	0.0268(13)	0.0293(13)	0.0230(12)	-0.0044(10)	-0.0021(10)	-0.0124(10)
C35	0.0276(15)	0.0302(15)	0.0299(16)	-0.0064(12)	-0.0033(12)	-0.0095(12)
C36	0.0257(15)	0.0295(15)	0.0314(16)	-0.0046(12)	-0.0037(12)	-0.0077(12)
O37	0.0261(11)	0.0290(11)	0.0307(11)	-0.0019(9)	-0.0046(9)	-0.0097(9)
C38	0.0276(16)	0.0350(16)	0.0339(17)	-0.0028(13)	-0.0001(13)	-0.0137(13)
C39	0.0291(16)	0.0360(17)	0.0403(18)	-0.0022(14)	-0.0092(14)	-0.0147(14)
O40	0.0299(11)	0.0298(11)	0.0308(11)	-0.0014(9)	-0.0076(9)	-0.0114(9)
C41	0.0370(17)	0.0301(15)	0.0301(16)	-0.0039(13)	-0.0086(13)	-0.0160(13)
C42	0.0318(16)	0.0259(14)	0.0284(15)	-0.0028(12)	-0.0074(12)	-0.0117(12)
C43	0.0280(15)	0.0259(14)	0.0260(15)	-0.0002(12)	-0.0047(12)	-0.0092(12)
C44	0.0287(16)	0.0254(14)	0.0308(16)	-0.0037(12)	-0.0020(13)	-0.0085(12)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O45	0.0321(11)	0.0257(10)	0.0238(10)	-0.0033(8)	-0.0047(9)	-0.0093(9)
C46	0.0327(17)	0.0326(16)	0.0249(15)	-0.0067(12)	-0.0028(13)	-0.0075(13)
C47	0.0311(16)	0.0327(16)	0.0254(15)	-0.0014(12)	0.0009(13)	-0.0097(13)
O48	0.0308(11)	0.0262(10)	0.0243(10)	-0.0016(8)	-0.0026(9)	-0.0089(9)
C49	0.0358(17)	0.0279(15)	0.0255(15)	-0.0009(12)	-0.0079(13)	-0.0094(13)
C50	0.0319(16)	0.0284(15)	0.0279(15)	-0.0012(12)	-0.0091(13)	-0.0085(13)
C1L	0.048(2)	0.046(2)	0.043(2)	-0.0024(16)	-0.0056(17)	-0.0255(18)
Cl1	0.1116(10)	0.0442(5)	0.0470(6)	0.0010(4)	-0.0272(6)	-0.0354(6)
Cl2	0.0477(6)	0.1003(9)	0.0467(6)	0.0086(6)	-0.0173(5)	-0.0359(6)

Tabelle 4. Koordinaten und isotrope Auslenkungsparameter der Wasserstoffatome ($Å^2$) für mja191.

Atom	x	y	z	U(iso)
H2	0.923	0.109	0.375	0.038
H3	0.952	0.089	0.537	0.044
H4	0.794	0.174	0.658	0.043
H5	0.611	0.280	0.616	0.039
H8A	0.892	0.211	0.231	0.037
H8B	0.790	0.333	0.210	0.037
H9A	0.717	0.256	0.121	0.041
H9B	0.843	0.255	0.068	0.041
H11A	0.994	-0.024	0.103	0.110
H11B	0.989	0.048	0.180	0.110
H11C	1.002	0.096	0.062	0.110
H13A	0.623	0.425	0.339	0.031
H13B	0.488	0.493	0.378	0.031
H14A	0.563	0.439	0.202	0.032
H14B	0.538	0.331	0.261	0.032
H16A	0.446	0.418	0.551	0.034
H16B	0.455	0.291	0.576	0.034
H17A	0.268	0.418	0.547	0.032
H17B	0.322	0.464	0.437	0.032
H21	0.128	0.789	0.142	0.039
H22	0.244	0.890	0.109	0.041
H24	0.502	0.610	0.217	0.034
H27	0.271	-0.001	0.514	0.033
H28	0.207	0.004	0.686	0.036
H30	0.270	0.282	0.649	0.033
H31A	0.538	0.777	0.144	0.054
H31B	0.433	0.862	0.212	0.054
H31C	0.442	0.886	0.093	0.054
H32A	0.268	0.143	0.820	0.053
H32B	0.189	0.075	0.832	0.053
H32C	0.133	0.209	0.812	0.053
H35A	0.025	0.700	0.287	0.036
H35B	0.109	0.623	0.365	0.036
H36A	-0.058	0.587	0.411	0.037
H36B	-0.040	0.559	0.302	0.037
H38A	-0.070	0.411	0.436	0.040
H38B	0.045	0.305	0.461	0.040
H39A	-0.026	0.282	0.332	0.042

Atom	x	y	z	U(iso)
H39B	-0.007	0.390	0.263	0.042
H41A	0.147	0.102	0.298	0.037
H41B	0.133	0.139	0.402	0.037
H42A	0.324	0.007	0.356	0.034
H42B	0.340	0.088	0.252	0.034
H43A	0.508	0.022	0.377	0.034
H43B	0.496	0.145	0.381	0.034
H44A	0.605	0.103	0.226	0.036
H44B	0.513	0.065	0.205	0.036
H46A	0.435	0.201	0.072	0.039
H46B	0.554	0.217	0.058	0.039
H47A	0.454	0.410	0.057	0.039
H47B	0.411	0.378	-0.024	0.039
H49A	0.200	0.522	0.002	0.037
H49B	0.279	0.565	0.038	0.037
H50A	0.082	0.652	0.112	0.037
H50B	0.079	0.531	0.162	0.037
H1LA	0.221	0.299	0.067	0.054
H1LB	0.212	0.297	-0.044	0.054

Tabelle 5. Bindungslängen [Å] und -winkel [°] für mja191.

Na1-O48	2.450(2)	C27-H27	0.9500
Na1-O18	2.459(2)	C28-C29	1.384(4)
Na1-O45	2.474(2)	C28-H28	0.9500
Na1-O37	2.507(2)	C29-C30	1.398(4)
Na1-O15	2.564(2)	C29-C32	1.513(4)
Na1-O40	2.602(2)	C30-H30	0.9500
Na1-N34	2.648(3)	C31-H31A	0.9800
Na1-N33	2.669(3)	C31-H31B	0.9800
C1-C2	1.381(4)	C31-H31C	0.9800
C1-O7	1.384(3)	C32-H32A	0.9800
C1-C6	1.409(4)	C32-H32B	0.9800
C2-C3	1.385(5)	C32-H32C	0.9800
C2-H2	0.9500	N33-C50	1.472(4)
C3-C4	1.380(5)	N33-C35	1.483(4)
C3-H3	0.9500	N34-C42	1.462(4)
C4-C5	1.388(5)	N34-C43	1.479(4)
C4-H4	0.9500	C35-C36	1.502(4)
C5-C6	1.395(4)	C35-H35A	0.9900
C5-H5	0.9500	C35-H35B	0.9900
C6-N12	1.410(4)	C36-O37	1.434(4)
O7-C8	1.440(3)	C36-H36A	0.9900
C8-C9	1.498(4)	C36-H36B	0.9900
C8-H8A	0.9900	O37-C38	1.429(4)
C8-H8B	0.9900	C38-C39	1.502(5)
C9-O10	1.420(4)	C38-H38A	0.9900
C9-H9A	0.9900	C38-H38B	0.9900
C9-H9B	0.9900	C39-O40	1.440(4)
O10-C11	1.418(5)	C39-H39A	0.9900
C11-H11A	0.9800	C39-H39B	0.9900
C11-H11B	0.9800	O40-C41	1.427(4)
C11-H11C	0.9800	C41-C42	1.508(4)
N12-C16	1.465(4)	C41-H41A	0.9900
N12-C13	1.484(4)	C41-H41B	0.9900
C13-C14	1.525(4)	C42-H42A	0.9900
C13-H13A	0.9900	C42-H42B	0.9900
C13-H13B	0.9900	C43-C44	1.514(4)
C14-O15	1.443(3)	C43-H43A	0.9900
C14-H14A	0.9900	C43-H43B	0.9900
C14-H14B	0.9900	C44-O45	1.426(3)
O15-C19	1.375(3)	C44-H44A	0.9900
C16-C17	1.506(4)	C44-H44B	0.9900
C16-H16A	0.9900	O45-C46	1.422(4)
C16-H16B	0.9900	C46-C47	1.505(4)
C17-O18	1.436(3)	C46-H46A	0.9900
C17-H17A	0.9900	C46-H46B	0.9900
C17-H17B	0.9900	C47-O48	1.420(4)
O18-C25	1.379(3)	C47-H47A	0.9900
C19-C24	1.392(4)	C47-H47B	0.9900
C19-C20	1.403(4)	O48-C49	1.434(3)
C20-C21	1.389(4)	C49-C50	1.504(4)
C20-N33	1.445(4)	C49-H49A	0.9900
C21-C22	1.384(4)	C49-H49B	0.9900
C21-H21	0.9500	C50-H50A	0.9900
C22-C23	1.392(5)	C50-H50B	0.9900
C22-H22	0.9500	C1L-Cl2	1.758(4)
C23-C24	1.394(4)	C1L-Cl1	1.767(4)
C23-C31	1.515(4)	C1L-H1LA	0.9900
C24-H24	0.9500	C1L-H1LB	0.9900
C25-C30	1.390(4)		
C25-C26	1.402(4)	O48-Na1-O18	156.97(9)
C26-C27	1.387(4)	O48-Na1-O45	66.41(7)
C26-N34	1.441(4)	O18-Na1-O45	99.47(8)
C27-C28	1.397(4)	O48-Na1-O37	117.34(8)

O18-Na1-O37	80.92(8)	N12-C13-C14	114.5(2)
O45-Na1-O37	165.98(8)	N12-C13-H13A	108.6
O48-Na1-O15	80.03(7)	C14-C13-H13A	108.6
O18-Na1-O15	79.65(7)	N12-C13-H13B	108.6
O45-Na1-O15	80.35(7)	C14-C13-H13B	108.6
O37-Na1-O15	113.35(8)	H13A-C13-H13B	107.6
O48-Na1-O40	89.82(8)	O15-C14-C13	113.8(2)
O18-Na1-O40	110.93(8)	O15-C14-H14A	108.8
O45-Na1-O40	98.68(8)	C13-C14-H14A	108.8
O37-Na1-O40	68.44(7)	O15-C14-H14B	108.8
O15-Na1-O40	169.33(8)	C13-C14-H14B	108.8
O48-Na1-N34	121.19(8)	H14A-C14-H14B	107.7
O18-Na1-N34	62.89(7)	C19-O15-C14	117.3(2)
O45-Na1-N34	65.90(8)	C19-O15-Na1	125.06(17)
O37-Na1-N34	102.54(8)	C14-O15-Na1	117.02(16)
O15-Na1-N34	122.41(8)	N12-C16-C17	113.0(2)
O40-Na1-N34	65.85(7)	N12-C16-H16A	109.0
O48-Na1-N33	67.56(8)	C17-C16-H16A	109.0
O18-Na1-N33	111.61(8)	N12-C16-H16B	109.0
O45-Na1-N33	124.44(8)	C17-C16-H16B	109.0
O37-Na1-N33	67.36(8)	H16A-C16-H16B	107.8
O15-Na1-N33	62.53(7)	O18-C17-C16	112.0(2)
O40-Na1-N33	110.57(8)	O18-C17-H17A	109.2
N34-Na1-N33	169.63(9)	C16-C17-H17A	109.2
C2-C1-O7	121.3(3)	O18-C17-H17B	109.2
C2-C1-C6	120.7(3)	C16-C17-H17B	109.2
O7-C1-C6	117.8(3)	H17A-C17-H17B	107.9
C1-C2-C3	120.8(3)	C25-O18-C17	117.8(2)
C1-C2-H2	119.6	C25-O18-Na1	117.35(16)
C3-C2-H2	119.6	C17-O18-Na1	119.32(16)
C4-C3-C2	119.4(3)	O15-C19-C24	124.0(3)
C4-C3-H3	120.3	O15-C19-C20	115.8(2)
C2-C3-H3	120.3	C24-C19-C20	120.2(3)
C3-C4-C5	120.0(3)	C21-C20-C19	118.3(3)
C3-C4-H4	120.0	C21-C20-N33	122.0(3)
C5-C4-H4	120.0	C19-C20-N33	119.6(3)
C4-C5-C6	121.7(3)	C22-C21-C20	121.6(3)
C4-C5-H5	119.1	C22-C21-H21	119.2
C6-C5-H5	119.1	C20-C21-H21	119.2
C5-C6-C1	117.3(3)	C21-C22-C23	119.9(3)
C5-C6-N12	123.1(3)	C21-C22-H22	120.0
C1-C6-N12	119.6(3)	C23-C22-H22	120.0
C1-O7-C8	116.8(2)	C22-C23-C24	119.2(3)
O7-C8-C9	108.3(2)	C22-C23-C31	121.4(3)
O7-C8-H8A	110.0	C24-C23-C31	119.5(3)
C9-C8-H8A	110.0	C19-C24-C23	120.6(3)
O7-C8-H8B	110.0	C19-C24-H24	119.7
C9-C8-H8B	110.0	C23-C24-H24	119.7
H8A-C8-H8B	108.4	O18-C25-C30	123.8(3)
O10-C9-C8	114.0(3)	O18-C25-C26	115.3(3)
O10-C9-H9A	108.7	C30-C25-C26	120.9(3)
C8-C9-H9A	108.7	C27-C26-C25	118.0(3)
O10-C9-H9B	108.7	C27-C26-N34	124.1(3)
C8-C9-H9B	108.7	C25-C26-N34	117.9(2)
H9A-C9-H9B	107.6	C26-C27-C28	121.2(3)
C11-O10-C9	112.6(3)	C26-C27-H27	119.4
O10-C11-H11A	109.5	C28-C27-H27	119.4
O10-C11-H11B	109.5	C29-C28-C27	120.4(3)
H11A-C11-H11B	109.5	C29-C28-H28	119.8
O10-C11-H11C	109.5	C27-C28-H28	119.8
H11A-C11-H11C	109.5	C28-C29-C30	118.9(3)
H11B-C11-H11C	109.5	C28-C29-C32	122.0(3)
C6-N12-C16	116.3(2)	C30-C29-C32	119.0(3)
C6-N12-C13	114.0(2)	C25-C30-C29	120.4(3)
C16-N12-C13	114.4(2)	C25-C30-H30	119.8

C29-C30-H30	119.8	O40-C41-H41B	110.0
C23-C31-H31A	109.5	C42-C41-H41B	110.0
C23-C31-H31B	109.5	H41A-C41-H41B	108.3
H31A-C31-H31B	109.5	N34-C42-C41	112.2(2)
C23-C31-H31C	109.5	N34-C42-H42A	109.2
H31A-C31-H31C	109.5	C41-C42-H42A	109.2
H31B-C31-H31C	109.5	N34-C42-H42B	109.2
C29-C32-H32A	109.5	C41-C42-H42B	109.2
C29-C32-H32B	109.5	H42A-C42-H42B	107.9
H32A-C32-H32B	109.5	N34-C43-C44	113.0(2)
C29-C32-H32C	109.5	N34-C43-H43A	109.0
H32A-C32-H32C	109.5	C44-C43-H43A	109.0
H32B-C32-H32C	109.5	N34-C43-H43B	109.0
C20-N33-C50	112.6(2)	C44-C43-H43B	109.0
C20-N33-C35	108.8(2)	H43A-C43-H43B	107.8
C50-N33-C35	113.7(2)	O45-C44-C43	108.4(2)
C20-N33-Na1	116.46(18)	O45-C44-H44A	110.0
C50-N33-Na1	98.17(17)	C43-C44-H44A	110.0
C35-N33-Na1	106.87(17)	O45-C44-H44B	110.0
C26-N34-C42	115.8(2)	C43-C44-H44B	110.0
C26-N34-C43	109.9(2)	H44A-C44-H44B	108.4
C42-N34-C43	112.9(2)	C46-O45-C44	112.3(2)
C26-N34-Na1	107.14(17)	C46-O45-Na1	117.39(17)
C42-N34-Na1	106.74(17)	C44-O45-Na1	122.33(17)
C43-N34-Na1	103.41(16)	O45-C46-C47	108.6(2)
N33-C35-C36	114.0(2)	O45-C46-H46A	110.0
N33-C35-H35A	108.8	C47-C46-H46A	110.0
C36-C35-H35A	108.8	O45-C46-H46B	110.0
N33-C35-H35B	108.8	C47-C46-H46B	110.0
C36-C35-H35B	108.8	H46A-C46-H46B	108.3
H35A-C35-H35B	107.7	O48-C47-C46	108.7(2)
O37-C36-C35	108.9(2)	O48-C47-H47A	109.9
O37-C36-H36A	109.9	C46-C47-H47A	109.9
C35-C36-H36A	109.9	O48-C47-H47B	109.9
O37-C36-H36B	109.9	C46-C47-H47B	109.9
C35-C36-H36B	109.9	H47A-C47-H47B	108.3
H36A-C36-H36B	108.3	C47-O48-C49	111.8(2)
C38-O37-C36	111.4(2)	C47-O48-Na1	115.59(17)
C38-O37-Na1	111.87(17)	C49-O48-Na1	118.55(17)
C36-O37-Na1	118.93(17)	O48-C49-C50	108.7(2)
O37-C38-C39	110.5(3)	O48-C49-H49A	109.9
O37-C38-H38A	109.6	C50-C49-H49A	109.9
C39-C38-H38A	109.6	O48-C49-H49B	109.9
O37-C38-H38B	109.6	C50-C49-H49B	109.9
C39-C38-H38B	109.6	H49A-C49-H49B	108.3
H38A-C38-H38B	108.1	N33-C50-C49	111.1(3)
O40-C39-C38	110.0(3)	N33-C50-H50A	109.4
O40-C39-H39A	109.7	C49-C50-H50A	109.4
C38-C39-H39A	109.7	N33-C50-H50B	109.4
O40-C39-H39B	109.7	C49-C50-H50B	109.4
C38-C39-H39B	109.7	H50A-C50-H50B	108.0
H39A-C39-H39B	108.2	Cl2-C1L-Cl1	113.6(2)
C41-O40-C39	112.1(2)	Cl2-C1L-H1LA	108.8
C41-O40-Na1	117.57(17)	Cl1-C1L-H1LA	108.8
C39-O40-Na1	109.03(17)	Cl2-C1L-H1LB	108.8
O40-C41-C42	108.7(2)	Cl1-C1L-H1LB	108.8
O40-C41-H41A	110.0	H1LA-C1L-H1LB	107.7
C42-C41-H41A	110.0		

Tabelle 6. Torsionswinkel [°] für mja191.

O7-C1-C2-C3	-176.5(3)	N34-C26-C27-C28	178.6(3)
C6-C1-C2-C3	-2.2(5)	C26-C27-C28-C29	-2.5(5)
C1-C2-C3-C4	2.2(5)	C27-C28-C29-C30	2.8(5)
C2-C3-C4-C5	-0.8(5)	C27-C28-C29-C32	-175.9(3)
C3-C4-C5-C6	-0.7(5)	O18-C25-C30-C29	174.9(3)
C4-C5-C6-C1	0.7(4)	C26-C25-C30-C29	-3.9(4)
C4-C5-C6-N12	-180.0(3)	C28-C29-C30-C25	0.4(4)
C2-C1-C6-C5	0.7(4)	C32-C29-C30-C25	179.1(3)
O7-C1-C6-C5	175.2(2)	C21-C20-N33-C50	60.0(4)
C2-C1-C6-N12	-178.6(3)	C19-C20-N33-C50	-121.1(3)
O7-C1-C6-N12	-4.1(4)	C21-C20-N33-C35	-66.9(4)
C2-C1-O7-C8	-53.2(4)	C19-C20-N33-C35	112.0(3)
C6-C1-O7-C8	132.3(3)	C21-C20-N33-Na1	172.3(2)
C1-O7-C8-C9	162.7(3)	C19-C20-N33-Na1	-8.8(3)
O7-C8-C9-O10	-68.2(3)	C27-C26-N34-C42	26.7(4)
C8-C9-O10-C11	-69.6(4)	C25-C26-N34-C42	-153.7(3)
C5-C6-N12-C16	-12.7(4)	C27-C26-N34-C43	-102.7(3)
C1-C6-N12-C16	166.5(2)	C25-C26-N34-C43	76.9(3)
C5-C6-N12-C13	123.6(3)	C27-C26-N34-Na1	145.6(3)
C1-C6-N12-C13	-57.1(3)	C25-C26-N34-Na1	-34.8(3)
C6-N12-C13-C14	116.7(3)	C20-N33-C35-C36	-173.1(3)
C16-N12-C13-C14	-106.1(3)	C50-N33-C35-C36	60.6(3)
N12-C13-C14-O15	95.2(3)	Na1-N33-C35-C36	-46.6(3)
C13-C14-O15-C19	81.1(3)	N33-C35-C36-O37	56.7(3)
C13-C14-O15-Na1	-107.2(2)	C35-C36-O37-C38	-168.7(2)
C6-N12-C16-C17	-163.6(2)	C35-C36-O37-Na1	-36.3(3)
C13-N12-C16-C17	60.2(3)	C36-O37-C38-C39	88.6(3)
N12-C16-C17-O18	60.9(3)	Na1-O37-C38-C39	-47.3(3)
C16-C17-O18-C25	79.5(3)	O37-C38-C39-O40	64.2(3)
C16-C17-O18-Na1	-127.3(2)	C38-C39-O40-C41	86.8(3)
C14-O15-C19-C24	-7.9(4)	C38-C39-O40-Na1	-45.2(3)
Na1-O15-C19-C24	-178.9(2)	C39-O40-C41-C42	-157.9(2)
C14-O15-C19-C20	171.8(2)	Na1-O40-C41-C42	-30.4(3)
Na1-O15-C19-C20	0.8(3)	C26-N34-C42-C41	63.0(3)
O15-C19-C20-C21	-175.5(3)	C43-N34-C42-C41	-169.1(2)
C24-C19-C20-C21	4.2(4)	Na1-N34-C42-C41	-56.1(3)
O15-C19-C20-N33	5.5(4)	O40-C41-C42-N34	59.5(3)
C24-C19-C20-N33	-174.8(3)	C26-N34-C43-C44	-171.7(2)
C19-C20-C21-C22	-2.9(5)	C42-N34-C43-C44	57.4(3)
N33-C20-C21-C22	176.0(3)	Na1-N34-C43-C44	-57.5(2)
C20-C21-C22-C23	-1.0(5)	N34-C43-C44-O45	50.0(3)
C21-C22-C23-C24	3.5(5)	C43-C44-O45-C46	-161.7(2)
C21-C22-C23-C31	-174.3(3)	C43-C44-O45-Na1	-13.7(3)
O15-C19-C24-C23	178.0(3)	C44-O45-C46-C47	-174.5(3)
C20-C19-C24-C23	-1.7(4)	Na1-O45-C46-C47	35.8(3)
C22-C23-C24-C19	-2.2(4)	O45-C46-C47-O48	-52.9(3)
C31-C23-C24-C19	175.7(3)	C46-C47-O48-C49	-173.4(2)
C17-O18-C25-C30	6.6(4)	C46-C47-O48-Na1	46.8(3)
Na1-O18-C25-C30	-147.2(2)	C47-O48-C49-C50	-157.8(3)
C17-O18-C25-C26	-174.5(2)	Na1-O48-C49-C50	-19.4(3)
Na1-O18-C25-C26	31.7(3)	C20-N33-C50-C49	59.3(3)
O18-C25-C26-C27	-174.7(3)	C35-N33-C50-C49	-176.4(2)
C30-C25-C26-C27	4.2(4)	Na1-N33-C50-C49	-63.9(2)
O18-C25-C26-N34	5.6(4)	O48-C49-C50-N33	60.8(3)
C30-C25-C26-N34	-175.4(3)		
C25-C26-C27-C28	-1.0(4)		