9.1 Anhang A Kristallografischer Teil

Kationen

Umsetzungen chiraler Kationen mit Kupferiodid

Umsetzungen chiraler Kationen mit Silberiodid

Nebenprodukte bei Umsetzungen chiraler Kationen mit Silberiodid

Zwischenprodukte bei der Sandmeyer-Reaktion von Paratoluidin

Kationen (R)-(1-Cyclohexylethyl)dimethylammoniumiodid ($C_{10}H_{22}NI$)

Table 1. Crystal data and structure refinement for (R)-(1-Cyclohexylethyl)dimethylammoniumiodid

Diffractometer type	CCD	
Empirical formula	C_{10} H_{22} I N	
Formula weight	283.19	
Temperature	173(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 860.25(9) pm	α= 90°.
	b = 967.40(9) pm	β= 90°.
	c = 1512.83(15) pm	γ = 90°.
Volume	1.2590(2) nm^3	
Z	4	
Density (calculated)	1.494 g/cm^3	
Absorption coefficient	2.503 mm^{-1}	
F(000)	568	
Crystal size	0.30 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.50 to 29.99°.	
Index ranges	-11<=h<=11, -13<=k<=13, -21<=l<=21	
Reflections collected	14202	
Independent reflections	3606 [R(int) = 0.0568]	
Completeness to theta = 29.99°	99.1 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3606 / 0 / 109	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0976	
R indices (all data)	R1 = 0.0610, wR2 = 0.1063	
Absolute structure parameter[99]	0.01(6)	
Largest diff. peak and hole	1.485 and -0.972 e.$Å^{-3}$	
Absorption correction	sadabs	
Effective transmission (min. / max.)	0.4268 / 0.6948	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (R)-(1-Cyclohexylethyl)dimethylammoniumiodid.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	2554(1)	3942(1)	8965(1)	39(1)
N(1)	2364(5)	13219(4)	11257(2)	34(1)
C(1)	2521(15)	10435(5)	10440(3)	68(2)
C(2)	3202(13)	9111(7)	10096(5)	102(4)
C(3)	2628(13)	7850(5)	10594(4)	62(2)
C(4)	3000(9)	8040(7)	11546(5)	70(2)
C(5)	2320(10)	9356(6)	11930(4)	56(2)
C(6)	2781(6)	10641(5)	11407(3)	36(1)
C(7)	1957(6)	11897(5)	11770(3)	36(1)
C(8)	2172(8)	12149(6)	12752(3)	54(2)
C(9)	1161(6)	14317(6)	11377(4)	46(2)
C(10)	3939(6)	13784(6)	11439(4)	43(1)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (R)-(1-Cyclohexylethyl)dimethyl-ammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	36(1)	47(1)	33(1)	9(1)	4(1)	2(1)
N(1)	40(2)	34(2)	29(2)	-1(1)	4(2)	-2(2)
C(1)	142(6)	37(3)	25(2)	2(2)	20(6)	9(6)
C(2)	214(11)	36(3)	56(4)	-8(3)	52(5)	-4(4)
C(3)	92(5)	36(3)	56(3)	-4(2)	10(5)	-12(5)
C(4)	95(6)	38(3)	76(5)	13(3)	-8(4)	1(3)
C(5)	89(5)	38(2)	40(3)	9(2)	-3(4)	-7(4)
C(6)	34(3)	37(2)	38(2)	2(2)	1(2)	-2(2)
C(7)	38(2)	41(3)	29(2)	4(2)	4(2)	-10(2)
C(8)	90(5)	49(3)	25(2)	-3(2)	6(3)	-10(3)
C(9)	41(3)	46(4)	51(4)	-5(3)	4(2)	8(2)
C(10)	37(2)	49(4)	43(3)	2(3)	1(2)	-10(2)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (R)-(1-Cyclohexylethyl)dimethylammoniumiodid.

	x	y	z	U(eq)
H(1)	2349	12983	10661	41
H(1A)	2986	11221	10115	81
H(1B)	1389	10439	10322	81
H(2A)	4349	9158	10143	122
H(2B)	2934	9013	9463	122
H(3A)	1491	7746	10514	74
H(3B)	3143	7007	10365	74
H(4A)	4144	8059	11620	83
H(4B)	2597	7239	11883	83
H(5A)	2677	9459	12549	67
H(5B)	1172	9279	11938	67
H(6)	3922	10785	11497	43
H(7)	821	11735	11677	43
H(8A)	1589	12975	12927	82
H(8B)	3278	12285	12880	82
H(8C)	1786	11349	13083	82
H(9A)	130	13930	11256	69
H(9B)	1367	15080	10967	69
H(9C)	1197	14661	11986	69
H(10A)	4717	13058	11347	64
H(10B)	3989	14109	12052	64
H(10C)	4148	14557	11037	64

Kationen (S)-(1-Cyclohexylethyl)dimethylammoniumiodid ($C_{10}H_{22}NI$)

Table 1. Crystal data and structure refinement for (S)-(1-Cyclohexylethyl)dimethylammoniumiodid

Diffractometer type	CCD	
Empirical formula	C_{10} H_{22} I N	
Formula weight	283.19	
Temperature	173(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 858.01(7) pm	α= 90°.
	b = 965.63(8) pm	β= 90°.
	c = 1513.03(11) pm	γ = 90°.
Volume	1.25358(17) nm^3	
Z	4	
Density (calculated)	1.500 g/cm^3	
Absorption coefficient	2.514 mm^{-1}	
F(000)	568	
Crystal size	0.40 x 0.07 x 0.05 mm^3	
Theta range for data collection	2.50 to 27.54°.	
Index ranges	-11<=h<=11, -12<=k<=12, -19<=l<=19	
Reflections collected	12492	
Independent reflections	2887 [R(int) = 0.0360]	
Completeness to theta = 27.54°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2887 / 0 / 109	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0264, wR2 = 0.0510	
R indices (all data)	R1 = 0.0379, wR2 = 0.0543	
Absolute structure parameter[99]	0.03(4)	
Largest diff. peak and hole	0.728 and -0.417 e.$Å^{-3}$	
Absorption correction	sadabs	
Effective transmission (min. / max.)	0.4782 / 0.6942	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-Cyclohexylethyl)dimethylammoniumiodid.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	7435(1)	6050(1)	1026(1)	36(1)
N(1)	7642(4)	-3220(3)	-1261(2)	29(1)
C(1)	7453(12)	-430(4)	-441(2)	60(1)
C(2)	6782(7)	896(5)	-95(3)	78(2)
C(3)	7388(10)	2143(4)	-594(3)	61(1)
C(4)	6982(6)	1958(5)	-1564(3)	62(2)
C(5)	7700(7)	649(4)	-1926(2)	47(1)
C(6)	7201(5)	-645(4)	-1414(2)	32(1)
C(7)	8051(4)	-1901(4)	-1768(2)	29(1)
C(8)	7876(5)	-2143(4)	-2758(2)	43(1)
C(9)	8833(5)	-4327(5)	-1384(3)	40(1)
C(10)	6048(4)	-3772(4)	-1451(3)	38(1)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (S)-(1-Cyclohexylethyl)dimethyl-ammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	35(1)	43(1)	31(1)	8(1)	4(1)	2(1)
N(1)	34(2)	29(1)	24(1)	0(1)	3(2)	-1(2)
C(1)	124(4)	32(2)	24(2)	0(1)	17(4)	-7(5)
C(2)	151(6)	37(3)	45(3)	-5(2)	41(3)	-5(3)
C(3)	96(4)	30(2)	56(2)	-7(2)	16(5)	0(4)
C(4)	89(4)	38(2)	58(3)	6(2)	-8(3)	8(2)
C(5)	74(3)	32(2)	34(2)	8(2)	0(3)	-7(3)
C(6)	32(2)	32(2)	34(2)	3(1)	2(2)	-4(2)
C(7)	32(2)	30(2)	25(2)	1(2)	2(1)	-7(2)
C(8)	69(3)	37(2)	24(2)	1(2)	0(2)	-10(2)
C(9)	41(2)	34(3)	45(3)	0(2)	5(2)	7(2)
C(10)	37(2)	35(3)	44(2)	1(2)	0(2)	-9(2)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (S)-(1-Cyclohexylethyl)dimethylammoniumiodid.

	x	y	z	U(eq)
H(1)	7656	-2989	-665	35
H(1A)	6979	-1214	-117	72
H(1B)	8587	-441	-320	72
H(2A)	7050	992	539	94
H(2B)	5632	864	-144	94
H(3A)	8531	2218	-521	73
H(3B)	6902	2999	-363	73
H(4A)	5835	1915	-1632	74
H(4B)	7367	2764	-1904	74
H(5A)	8850	731	-1903	56
H(5B)	7395	543	-2554	56
H(6)	6060	-787	-1515	39
H(7)	9185	-1730	-1662	35
H(8A)	7550	-3101	-2864	65
H(8B)	8876	-1973	-3051	65
H(8C)	7089	-1509	-2996	65
H(9A)	9874	-3943	-1276	60
H(9B)	8776	-4682	-1990	60
H(9C)	8633	-5082	-966	60
H(10A)	5273	-3045	-1343	58
H(10B)	5836	-4564	-1064	58
H(10C)	5990	-4068	-2069	58

Kationen (S)-(1-Cyclohexylethyl)methylammoniumiodid ($C_9H_{20}NI$)

Table 1. Crystal data and structure refinement for (S)-(1-Cyclohexylethyl)methylammoniumiodid

Diffractometer type	CCD	
Empirical formula	$C_9 H_{20} I N$	
Formula weight	269.16	
Temperature	213(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1	
Unit cell dimensions	a = 825.37(8) pm	α= 90°.
	b = 839.43(8) pm	β= 111.547(2)°.
	c = 921.64(9) pm	γ = 90°.
Volume	0.59393(10) nm3	
Z	2	
Density (calculated)	1.505 g/cm^3	
Absorption coefficient	2.649 mm^{-1}	
F(000)	268	
Crystal size	0.45 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.38 to 30.04°.	
Index ranges	-11<=h<=11, -11<=k<=11, -12<=l<=12	
Reflections collected	7011	
Independent reflections	3418 [R(int) = 0.0584]	
Completeness to theta = 30.04°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3418 / 1 / 101	
Goodness-of-fit on F^2	1.083	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0948	
R indices (all data)	R1 = 0.0509, wR2 = 0.1007	
Absolute structure parameter[99]	0.00(11)	
Largest diff. peak and hole	1.036 and -0.662 e.Å^{-3}	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^{2}x 10^{-1}) for (S)-(1-Cyclohexylethyl)methylammoniumiodid.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	7252(1)	3123	5852(1)	36(1)
N(1)	2761(6)	2374(6)	4430(6)	35(1)
C(1)	-801(8)	4761(8)	1946(10)	39(2)
C(2)	17218(8)	4878(8)	1459(9)	37(1)
C(3)	16313(10)	3642(9)	145(9)	42(2)
C(4)	-3067(11)	2026(11)	656(12)	51(2)
C(5)	-1082(10)	1876(9)	1156(11)	46(2)
C(6)	-161(6)	3001(14)	2468(5)	24(1)
C(7)	1814(7)	2869(9)	2996(7)	33(2)
C(8)	2628(7)	3150(30)	1830(7)	56(2)
C(9)	2332(9)	2732(12)	5853(7)	57(3)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (S)-(1-Cyclohexylethyl)methyl-ammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	28(1)	30(1)	46(1)	0(1)	9(1)	2(1)
N(1)	23(2)	37(2)	40(3)	1(2)	7(2)	0(2)
C(1)	18(3)	27(3)	61(5)	5(3)	3(3)	-3(2)
C(2)	32(3)	30(3)	43(4)	-1(3)	5(3)	2(2)
C(3)	33(3)	47(4)	41(4)	-11(3)	6(3)	-4(3)
C(4)	34(4)	46(5)	74(7)	-34(5)	20(4)	-14(3)
C(5)	32(3)	34(4)	64(5)	-20(3)	9(4)	5(3)
C(6)	24(2)	17(3)	30(2)	3(3)	7(2)	4(3)
C(7)	27(2)	29(6)	42(3)	3(2)	12(2)	3(2)
C(8)	32(2)	92(5)	47(3)	-12(10)	19(2)	-8(10)
C(9)	44(3)	92(11)	32(3)	-6(4)	11(3)	7(4)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (S)-(1-Cyclohexylethyl)methylammoniumiodid.

	x	y	z	U(eq)
H(1A)	3860	2745	4640	42
H(1B)	2820	1295	4376	42
H(1C)	-237	5496	2811	46
H(1D)	-468	5071	1069	46
H(2A)	16831	5956	1081	45
H(2B)	16892	4669	2362	45
H(3A)	15049	3690	-128	51
H(3B)	16560	3911	-788	51
H(4A)	-3630	1279	-199	62
H(4B)	-3405	1730	1534	62
H(5A)	-728	780	1490	56
H(5B)	-744	2112	264	56
H(6)	-495	2723	3363	29
H(7)	1969	3999	3327	39
H(8A)	3883	3052	2329	83
H(8B)	2333	4207	1394	83
H(8C)	2201	2363	1003	83
H(9A)	3193	2238	6761	85
H(9B)	1187	2314	5706	85
H(9C)	2341	3876	6008	85

Kationen (+)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)trimethylammoniumiodid ($C_{12}H_{20}NOI$)

Table 1. Crystal data and structure refinement for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)trimethyl-ammoniumiodid

Diffractometer type	CAD 4	
Empirical formula	C_{12} H_{20} I N O	
Formula weight	321.19	
Temperature	293(2) K	
Wavelength	71.069 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 941.2(2) pm	α= 90°.
	b = 1213.7(3) pm	β= 90°.
	c = 1236.9(3) pm	γ = 90°.
Volume	1.4130(6) nm^3	
Z	4	
Density (calculated)	1.510 g/cm^3	
Absorption coefficient	2.246 mm^{-1}	
F(000)	640	
Crystal size	0.30 x 0.30 x 0.20 mm^3	
Theta range for data collection	2.35 to 24.96°.	
Index ranges	-11<=h<=11, -14<=k<=14, -14<=l<=14	
Reflections collected	2908	
Independent reflections	2502 [R(int) = 0.0308]	
Completeness to theta = 24.96°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2502 / 0 / 128	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0298, wR2 = 0.0737	
R indices (all data)	R1 = 0.0396, wR2 = 0.0807	
Absolute structure parameter[99]	0.00(4)	
Extinction coefficient	0.0069(9)	
Largest diff. peak and hole	0.430 and -0.562 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)trimethylammoniumiodid. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	3752(1)	-268(1)	1353(1)	61(1)
O(1)	10283(3)	-1103(3)	950(3)	63(1)
N(1)	7542(4)	-2327(3)	1784(3)	45(1)
C(1)	9748(6)	1132(5)	520(4)	62(2)
C(2)	9546(7)	2268(6)	363(5)	75(2)
C(3)	8588(8)	2829(5)	947(6)	79(2)
C(4)	7789(7)	2305(6)	1706(5)	73(2)
C(5)	7953	1183	1872	55
C(6)	8949(5)	593(4)	1278(4)	46(1)
C(7)	9113(5)	-639(4)	1498(4)	48(1)
C(8)	7774(5)	-1246(4)	1162(4)	42(1)
C(9)	7710(6)	-1402(5)	-68(4)	61(1)
C(10)	8771(6)	-3106(5)	1730(5)	66(1)
C(11)	6255(6)	-2915(4)	1337(4)	64(1)
C(12)	7227(7)	-2075(5)	2934(4)	63(1)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)trimethylammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	40(1)	47(1)	97(1)	-1(1)	-1(1)	3(1)
O(1)	35(2)	72(2)	81(2)	-25(2)	7(2)	1(2)
N(1)	35(2)	47(2)	54(2)	-4(2)	-5(2)	3(2)
C(1)	52(3)	81(4)	52(3)	-7(3)	-5(2)	-4(3)
C(2)	70(4)	84(4)	71(4)	25(3)	-19(3)	-15(4)
C(3)	76(4)	62(3)	100(4)	9(3)	-31(4)	-5(4)
C(4)	67(4)	61(3)	91(4)	-17(3)	-10(3)	12(3)
C(5)	49	55	60	-6	4	7
C(6)	39(2)	59(2)	39(2)	-1(2)	-4(2)	-6(2)
C(7)	36(2)	58(3)	50(3)	-11(2)	-3(2)	3(2)
C(8)	32(2)	50(2)	44(3)	-3(2)	-4(2)	4(2)
C(9)	64(3)	74(3)	44(3)	3(3)	-11(2)	-14(3)
C(10)	48(3)	65(3)	86(3)	-3(3)	-7(3)	24(3)
C(11)	51(3)	56(3)	85(3)	0(3)	-20(4)	-11(3)
C(12)	74(4)	70(4)	45(3)	0(3)	5(3)	-5(3)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)trimethylammoniumiodid.

	x	y	z	U(eq)
H(1)	10036	-1299	344	94
H(1A)	10417	750	113	74
H(2)	10085	2636	-154	90
H(3)	8468	3580	832	95
H(4)	7134	2700	2114	88
H(5)	7395	824	2382	66
H(7)	9252	-745	2276	57
H(8)	6977	-764	1352	50
H(9A)	8027	-741	-419	91
H(9B)	6749	-1557	-281	91
H(9C)	8312	-2005	-274	91
H(10A)	9601	-2757	2025	100
H(10B)	8946	-3304	990	100
H(10C)	8556	-3756	2140	100
H(11A)	6454	-3166	617	96
H(11B)	5462	-2417	1322	96
H(11C)	6032	-3534	1789	96
H(12A)	6953	-2740	3301	94
H(12B)	6465	-1551	2973	94
H(12C)	8058	-1773	3273	94

Kationen (-)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)trimethylammoniumiodid ($C_{12}H_{20}NOI$)

Table 1. Crystal data and structure refinement for (-)-(2-Hydroxy-1-methyl-2-phenylethyl)trimethyl-ammoniumiodid

Diffractometer type	CAD 4	
Empirical formula	C_{12} H_{20} I N O	
Formula weight	321.19	
Temperature	293(2) K	
Wavelength	71.069 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 942.6(2) pm	α= 90°.
	b = 1215.7(3) pm	β= 90°.
	c = 1239.1(3) pm	γ = 90°.
Volume	1.4199(6) nm^3	
Z	4	
Density (calculated)	1.502 g/cm^3	
Absorption coefficient	2.235 mm^{-1}	
F(000)	640	
Crystal size	0.50 x 0.40 x 0.40 mm^3	
Theta range for data collection	2.35 to 29.97°.	
Index ranges	-13<=h<=13, -17<=k<=17, -17<=l<=17	
Reflections collected	4705	
Independent reflections	4124 [R(int) = 0.0210]	
Completeness to theta = 29.97°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4124 / 0 / 137	
Goodness-of-fit on F^2	1.120	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0935	
R indices (all data)	R1 = 0.0624, wR2 = 0.1034	
Absolute structure parameter[99]	-0.06(4)	
Extinction coefficient	0.0287(14)	
Largest diff. peak and hole	0.559 and -0.786 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (-)-(2-Hydroxy-1-methyl-2-phenylethyl)trimethylammoniumiodid.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	6249(1)	-268(1)	6353(1)	62(1)
O(1)	-282(3)	-1111(3)	5953(3)	66(1)
N(1)	2459(3)	-2329(3)	6781(3)	46(1)
C(6)	1053(4)	594(4)	6275(3)	47(1)
C(7)	883(4)	-639(4)	6495(4)	47(1)
C(9)	2286(5)	-1408(5)	4936(4)	62(1)
C(5)	255(5)	1127(5)	5522(4)	62(1)
C(8)	2237(4)	-1244(4)	6159(3)	42(1)
C(11)	2776(6)	-2079(5)	7937(4)	66(1)
C(12)	1219(6)	-3097(4)	6735(4)	67(1)
C(1)	2052(5)	1184(4)	6877(4)	57(1)
C(10)	3742(6)	-2919(4)	6341(4)	66(1)
C(3)	1406(8)	2825(5)	5940(6)	82(2)
C(4)	443(6)	2264(6)	5355(5)	75(2)
C(2)	2218(6)	2302(5)	6705(5)	73(2)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (-)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)trimethylammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	41(1)	48(1)	97(1)	-1(1)	1(1)	-2(1)
O(1)	36(1)	76(2)	86(2)	-27(2)	-6(2)	-3(2)
N(1)	36(2)	52(2)	50(2)	-6(2)	6(1)	-3(2)
C(6)	44(2)	54(2)	42(2)	-1(2)	8(2)	4(2)
C(7)	34(2)	55(2)	52(2)	-11(2)	3(2)	-4(2)
C(9)	58(3)	80(3)	47(2)	-6(2)	10(2)	9(3)
C(5)	55(3)	82(4)	50(3)	0(2)	3(2)	7(3)
C(8)	32(1)	49(2)	46(2)	-3(2)	2(2)	-1(2)
C(11)	76(3)	73(3)	48(3)	-2(2)	-7(2)	7(3)
C(12)	55(2)	64(3)	81(3)	-2(2)	5(3)	-21(3)
C(1)	53(2)	55(3)	64(3)	-10(2)	-4(2)	0(2)
C(10)	52(2)	57(2)	88(3)	-1(2)	22(3)	10(2)
C(3)	82(4)	59(3)	105(4)	15(3)	44(4)	7(3)
C(4)	73(3)	82(4)	71(3)	26(3)	16(3)	18(3)
C(2)	62(3)	62(3)	95(4)	-11(3)	10(3)	-8(3)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (-)-(2-Hydroxy-1-methyl-2-phenylethyl)trimethylammoniumiodid.

	x	y	z	U(eq)
H(1A)	-78	-1206	5316	99
H(7)	747	-743	7272	56
H(9A)	1701	-2023	4742	92
H(9B)	3246	-1546	4716	92
H(9C)	1942	-757	4584	92
H(5)	-413	741	5120	75
H(8)	3034	-763	6346	51
H(11A)	1964	-1740	8265	98
H(11B)	3572	-1588	7978	98
H(11C)	2997	-2749	8310	98
H(12A)	1424	-3744	7151	100
H(12B)	1043	-3302	5999	100
H(12C)	396	-2739	7025	100
H(1)	2603	827	7392	69
H(10A)	4542	-2430	6345	99
H(10B)	3556	-3154	5615	99
H(10C)	3946	-3548	6783	99
H(3)	1521	3576	5826	98
H(4)	-98	2627	4838	90
H(2)	2878	2698	7105	88

Kationen (+)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)ethyldimethylammonium-iodid ($C_{13}H_{22}NOI$)

Table 1. Crystal data and structure refinement for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)ethyldimethyl-ammoniumiodid

Diffractometer type	CAD 4	
Empirical formula	C_{13} H_{22} I N O	
Formula weight	335.22	
Temperature	293(2) K	
Wavelength	71.069 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 693.5(2) pm	α= 90°.
	b = 1232.8(4) pm	β= 108.72(3)°.
	c = 901.4(2) pm	γ = 90°.
Volume	0.7299(4) nm^3	
Z	2	
Density (calculated)	1.525 g/cm^3	
Absorption coefficient	2.177 mm^{-1}	
F(000)	336	
Crystal size	0.30 x 0.30 x 0.15 mm^3	
Theta range for data collection	2.90 to 27.97°.	
Index ranges	-9<=h<=9, -16<=k<=16, -11<=l<=11	
Reflections collected	5364	
Independent reflections	3520 [R(int) = 0.0108]	
Completeness to theta = 27.97°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3520 / 1 / 152	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0189, wR2 = 0.0473	
R indices (all data)	R1 = 0.0275, wR2 = 0.0495	
Absolute structure parameter[99]	-0.015(19)	
Extinction coefficient	0.0037(7)	
Largest diff. peak and hole	0.277 and -0.269 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)ethyldiimethylammoniumiodid. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	1637(1)	2518(1)	1415(1)	56(1)
O(1)	-3874(4)	8200(2)	4660(2)	65(1)
N(1)	-2808(3)	9728(2)	2124(2)	42(1)
C(1)	-965(5)	6406(2)	2824(3)	53(1)
C(2)	-739(8)	5312(4)	2586(5)	64(1)
C(3)	-1956(7)	4568(2)	2969(4)	71(1)
C(4)	-3425(8)	4904(3)	3585(5)	72(1)
C(5)	-3685(5)	6003(2)	3810(3)	59(1)
C(6)	-2460(6)	6768(2)	3441(3)	43(1)
C(7)	-2642(5)	7974(3)	3717(4)	44(1)
C(8)	-3565(4)	8546(2)	2123(2)	40(1)
C(9)	-5877(4)	8461(3)	1528(4)	63(1)
C(10)	-3759(5)	10214(3)	536(3)	64(1)
C(11)	-561(7)	9716(4)	2388(6)	58(1)
C(12)	-3304(7)	10411(3)	3347(4)	54(1)
C(13)	-2674(5)	11585(2)	3376(4)	62(1)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)ethyldimethylammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	66(1)	59(1)	47(1)	4(1)	25(1)	-2(1)
O(1)	94(2)	63(1)	52(1)	11(1)	43(1)	26(1)
N(1)	48(1)	42(1)	38(1)	3(1)	15(1)	3(1)
C(1)	64(2)	45(1)	51(1)	2(1)	22(1)	5(1)
C(2)	88(3)	50(2)	55(2)	-2(2)	25(2)	21(2)
C(3)	111(3)	45(2)	48(2)	-1(1)	12(2)	2(2)
C(4)	94(3)	54(2)	66(2)	9(2)	21(2)	-24(2)
C(5)	70(2)	56(2)	57(2)	6(1)	28(1)	-6(1)
C(6)	56(1)	40(1)	35(1)	5(1)	16(1)	0(1)
C(7)	51(2)	48(1)	34(1)	2(1)	15(1)	5(1)
C(8)	45(1)	41(1)	34(1)	-1(1)	11(1)	0(1)
C(9)	50(2)	64(2)	65(2)	6(1)	6(1)	-4(1)
C(10)	84(2)	58(2)	46(1)	16(1)	17(1)	13(2)
C(11)	46(2)	56(2)	78(3)	2(2)	27(2)	2(2)
C(12)	70(2)	46(2)	52(2)	-4(1)	29(2)	1(1)
C(13)	66(2)	48(2)	74(2)	-8(1)	27(1)	-2(1)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)ethyldimethylammoniumiodid.

	x	y	z	U(eq)
H(1)	-4690	8680	4249	97
H(1A)	-115	6906	2571	63
H(2)	249	5082	2161	77
H(3)	-1789	3833	2812	86
H(4)	-4248	4396	3853	87
H(5)	-4698	6225	4214	71
H(7)	-1277	8268	4232	52
H(8)	-3076	8147	1373	49
H(9A)	-6273	7720	1586	94
H(9B)	-6378	8704	460	94
H(9C)	-6438	8906	2162	94
H(10A)	-3070	10877	458	96
H(10B)	-5169	10364	379	96
H(10C)	-3649	9714	-249	96
H(11A)	-268	9215	1672	87
H(11B)	145	9495	3444	87
H(11C)	-121	10429	2215	87
H(12A)	5200(60)	330(30)	3210(40)	81
H(12B)	7190(60)	90(40)	4200(50)	81
H(13A)	-1246	11625	3508	93
H(13B)	-2942	11950	4230	93
H(13C)	-3434	11926	2407	93

Kationen (-)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)ethyldimethylammonium-iodid ($C_{13}H_{22}NOI$)

Table 1. Crystal data and structure refinement for (-)-(2-Hydroxy-1-methyl-2-phenylethyl)ethyldimethyl-ammoniumiodid

Diffractometer type	CAD 4	
Empirical formula	C_{13} H_{22} I N O	
Formula weight	335.22	
Temperature	293(2) K	
Wavelength	71.069 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 693.20(10) pm	α= 90°.
	b = 1231.7(2) pm	β= 108.73(2)°.
	c = 901.2(2) pm	γ = 90°.
Volume	0.7287(2) nm^3	
Z	2	
Density (calculated)	1.528 g/cm^3	
Absorption coefficient	2.181 mm^{-1}	
F(000)	336	
Crystal size	0.25 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.39 to 29.90°.	
Index ranges	-9<=h<=9, -14<=k<=17, -10<=l<=12	
Reflections collected	3750	
Independent reflections	3411 [R(int) = 0.0120]	
Completeness to theta = 29.90°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3411 / 1 / 146	
Goodness-of-fit on F^2	1.289	
Final R indices [I>2sigma(I)]	R1 = 0.0314, wR2 = 0.0783	
R indices (all data)	R1 = 0.0349, wR2 = 0.0798	
Absolute structure parameter[99]	-0.02(3)	
Extinction coefficient	0.099(4)	
Largest diff. peak and hole	0.532 and -0.576 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (-)-(2-Hydroxy-1-methyl-2-phenylethyl)ethyldimethylammoniumiodid. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	8365(1)	7481(1)	8586(1)	55(1)
O(1)	13871(6)	1799(3)	5338(4)	66(1)
N(1)	12801(4)	271(2)	7869(3)	41(1)
C(1)	10970(7)	3592(3)	7185(5)	53(1)
C(2)	10739(12)	4677(5)	7423(8)	66(2)
C(3)	11949(10)	5436(3)	7030(6)	70(1)
C(4)	13441(11)	5091(5)	6419(8)	74(2)
C(5)	13690(7)	4005(4)	6189(5)	59(1)
C(6)	12470(8)	3229(3)	6566(5)	42(1)
C(7)	12637(7)	2026(3)	6278(5)	42(1)
C(8)	13565(5)	1452(3)	7881(4)	40(1)
C(9)	15882(6)	1541(4)	8471(6)	63(1)
C(10)	13760(8)	-215(4)	9470(5)	64(1)
C(11)	10553(9)	274(5)	7610(8)	56(1)
C(12)	13291(8)	-402(4)	6641(6)	53(1)
C(13)	12670(7)	-1584(3)	6611(6)	63(1)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (-)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)ethyldimethylammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	66(1)	58(1)	47(1)	4(1)	26(1)	-2(1)
O(1)	100(2)	61(2)	53(2)	10(1)	47(2)	24(2)
N(1)	47(1)	42(1)	36(1)	4(1)	15(1)	3(1)
C(1)	64(2)	47(2)	53(2)	3(2)	24(2)	6(2)
C(2)	94(5)	51(3)	55(3)	-5(2)	28(3)	17(3)
C(3)	111(4)	41(2)	48(2)	-1(2)	10(2)	5(2)
C(4)	98(4)	56(3)	63(3)	9(2)	20(3)	-25(3)
C(5)	71(2)	55(2)	58(2)	9(2)	31(2)	-8(2)
C(6)	56(2)	39(2)	33(2)	1(1)	16(2)	-2(2)
C(7)	53(2)	44(2)	30(2)	1(1)	15(2)	6(2)
C(8)	45(2)	40(2)	33(2)	0(1)	12(1)	1(1)
C(9)	49(2)	66(2)	63(3)	4(2)	4(2)	-3(2)
C(10)	83(3)	60(2)	43(2)	15(2)	13(2)	10(2)
C(11)	45(2)	53(3)	75(4)	1(2)	26(2)	-2(2)
C(12)	66(3)	48(2)	50(2)	-7(2)	25(2)	-2(2)
C(13)	67(3)	48(2)	78(3)	-7(2)	30(2)	-1(2)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (-)-(2-Hydroxy-1-methyl-2-phenylethyl)ethyldimethylammoniumiodid.

	x	y	z	U(eq)
H(1)	14566	1260	5677	99
H(1A)	10121	3091	7437	64
H(2)	9755	4902	7855	79
H(3)	11767	6172	7173	84
H(4)	14278	5598	6163	88
H(5)	14694	3785	5773	70
H(7)	11269	1735	5763	50
H(8)	13076	1851	8631	48
H(9A)	16440	1121	7810	94
H(9B)	16393	1272	9525	94
H(9C)	16272	2288	8451	94
H(10A)	12964	-824	9600	96
H(10B)	13811	321	10256	96
H(10C)	15117	-453	9576	96
H(11A)	9843	521	6567	84
H(11B)	10263	751	8354	84
H(11C)	10114	-448	7744	84
H(12A)	14746	-367	6821	64
H(12B)	12612	-86	5621	64
H(13A)	13555	-1948	7515	94
H(13B)	12769	-1923	5679	94
H(13C)	11290	-1629	6619	94

Kationen (+)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)dimethylammoniumiodid ($C_{11}H_{18}NOI$)

Table 1. Crystal data and structure refinement for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)dimethyl-ammoniumiodid

Diffractometer type	CAD 4	
Empirical formula	C_{11} H_{18} I N O	
Formula weight	307.16	
Temperature	293(2) K	
Wavelength	71.069 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 588.7(2) pm	α= 90°.
	b = 772.2(3) pm	β= 101.00°.
	c = 1465.3(6) pm	γ = 90°.
Volume	0.6539(4) nm^3	
Z	2	
Density (calculated)	1.555 g/cm^3	
Absorption coefficient	2.422 mm^{-1}	
F(000)	302	
Crystal size	0.40 x 0.30 x 0.10 mm^3	
Theta range for data collection	2.83 to 24.95°.	
Index ranges	-6<=h<=6, -9<=k<=9, -17<=l<=17	
Reflections collected	2638	
Independent reflections	2261 [R(int) = 0.0289]	
Completeness to theta = 24.95°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2261 / 1 / 128	
Goodness-of-fit on F^2	1.119	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.1068	
R indices (all data)	R1 = 0.0476, wR2 = 0.1143	
Absolute structure parameter[99]	-0.03(5)	
Extinction coefficient	0.002(2)	
Largest diff. peak and hole	1.233 and -0.972 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)dimethylammoniumiodid.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	9925(1)	11951(1)	1475(1)	56(1)
O(1)	3143(9)	8668(8)	2644(4)	56(1)
N(1)	7005(11)	8026(8)	1460(4)	45(1)
C(1)	5301(13)	8308(10)	4547(6)	46(2)
C(2)	6203(16)	8345(11)	5483(6)	57(2)
C(3)	8326(17)	9142(12)	5801(6)	61(2)
C(4)	9468(16)	9929(13)	5187(6)	63(2)
C(5)	8560(13)	9883(11)	4245(5)	51(2)
C(6)	6443(13)	9077(9)	3917(5)	42(2)
C(7)	5546(12)	8997(10)	2874(5)	41(2)
C(8)	6868(13)	7573(9)	2456(5)	37(2)
C(9)	5895(16)	5793(12)	2546(6)	51(2)
C(10)	8636(12)	6950(20)	1085(5)	61(2)
C(11)	4755(17)	8115(15)	787(6)	68(3)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-2-phenyl-ethyl)dimethylammoniumiodid. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	71(1)	39(1)	56(1)	4(1)	12(1)	9(1)
O(1)	45(3)	55(3)	66(3)	-8(3)	5(2)	9(2)
N(1)	56(4)	38(3)	42(3)	-2(2)	9(3)	1(3)
C(1)	45(4)	33(3)	63(5)	-9(3)	17(3)	-4(3)
C(2)	82(6)	40(4)	59(5)	-5(3)	35(4)	-1(4)
C(3)	81(6)	54(5)	48(4)	-9(4)	8(4)	4(4)
C(4)	58(5)	67(6)	63(5)	-11(4)	9(4)	-6(4)
C(5)	47(4)	55(5)	51(4)	-3(4)	11(3)	-6(3)
C(6)	52(4)	31(3)	44(4)	-5(3)	10(3)	2(3)
C(7)	42(4)	33(4)	49(4)	-1(3)	8(3)	8(3)
C(8)	39(4)	34(4)	36(3)	2(2)	5(3)	2(3)
C(9)	59(5)	36(4)	59(5)	2(4)	15(4)	4(4)
C(10)	66(4)	70(5)	50(3)	-15(8)	18(3)	12(8)
C(11)	64(5)	94(7)	40(4)	5(4)	-3(4)	18(5)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-2-phenylethyl)dimethylammoniumiodid.

	x	y	z	U(eq)
H(1)	2534	8946	3081	84
H(1A)	3896	7754	4336	55
H(2)	5399	7840	5902	69
H(3)	8967	9139	6432	74
H(4)	10860	10496	5402	76
H(5)	9366	10394	3828	61
H(7)	5857	10111	2602	50
H(8)	8456	7571	2812	44
H(9A)	5850	5569	3187	76
H(9B)	6858	4947	2327	76
H(9C)	4357	5728	2183	76
H(10A)	10122	6997	1491	92
H(10B)	8770	7368	480	92
H(10C)	8093	5776	1036	92
H(11A)	5045	8254	168	102
H(11B)	3872	9082	939	102
H(11C)	3902	7065	821	102

Umsetzungen chiraler Kationen mit Kupferiodid
Bis-((R)-(1-Phenylethyl)trimethylammonium)heptaiodopentacuprat(I) · 3 CH_3CN ([(R)-$C_{11}H_{18}N]_2[Cu_5I_7 \cdot 2\ CH_3CN] \cdot CH_3CN$)

Table 1. Crystal data and structure refinement for Bis((R)-(1-Phenylethyl)trimethylammonium)-heptaiodopentacuprat(I)·3CH_3CN

Diffractometer type	CAD 4	
Empirical formula	$C_{28}\ H_{45}\ Cu_5\ I_7\ N_5$	
Formula weight	1657.69	
Temperature	293(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 1698.0(3) pm	α= 90°.
	b = 861.20(10) pm	β= 97.590(10)°.
	c = 3123.7(3) pm	γ = 90°.
Volume	4.5278(11) nm^3	
Z	4	
Density (calculated)	2.432 g/cm^3	
Absorption coefficient	7.108 mm^{-1}	
F(000)	3056	
Crystal size	0.15 x 0.03 x 0.03 mm^3	
Theta range for data collection	2.66 to 22.46°.	
Index ranges	0<=h<=18, 0<=k<=9, -33<=l<=33	
Reflections collected	6321	
Independent reflections	6321 [R(int) = 0.0000]	
Completeness to theta = 22.46°	99.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6321 / 1 / 482	
Goodness-of-fit on F^2	0.962	
Final R indices [I>2sigma(I)]	R1 = 0.0636, wR2 = 0.1793	
R indices (all data)	R1 = 0.1177, wR2 = 0.2289	
Absolute structure parameter[99]	0.18(14)	
Extinction coefficient	0.00021(10)	
Largest diff. peak and hole	1.431 and -1.567 e.$Å^{-3}$	
Absorption correction	psi-scan	
Effective transmission (min. / max.)	0.4927 / 0.9901	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis((R)-(1-Phenylethyl)trimethylammonium)-heptaiodopentacuprat(I)·3CH_3CN. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(11)	7101(2)	9072(4)	9083(1)	29(1)
I(12)	7395(2)	3855(4)	9202(1)	26(1)
I(13)	9390(2)	6877(4)	9075(1)	29(1)
I(14)	7522(2)	6289(4)	8000(1)	29(1)
I(15)	5181(2)	6003(5)	8427(1)	34(1)
I(16)	8381(2)	6961(4)	10319(1)	32(1)
I(17)	5812(2)	6232(5)	9857(1)	42(1)
I(21)	7628(2)	12227(4)	5838(1)	31(1)
I(22)	7917(2)	6995(5)	5926(1)	34(1)
I(23)	5581(2)	9181(5)	5955(1)	38(1)
I(24)	7424(2)	9750(4)	7012(1)	32(1)
I(25)	9818(2)	10039(5)	6622(1)	41(1)
I(26)	9209(3)	9682(7)	5166(1)	65(1)
I(27)	6638(3)	9350(6)	4735(1)	62(1)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis((R)-(1-Phenylethyl)trimethylammonium)-heptaiodopentacuprat(I)·3CH_3CN. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(11)	6588(4)	4658(9)	8424(2)	35(2)
Cu(12)	7829(3)	6507(8)	8855(2)	32(2)
Cu(13)	8487(3)	8343(8)	9569(2)	33(2)
Cu(14)	7290(4)	6414(10)	9693(2)	45(2)
Cu(15)	6184(4)	6567(12)	9082(2)	55(2)
Cu(21)	8419(4)	11339(9)	6616(2)	38(2)
Cu(22)	7140(4)	9543(8)	6160(2)	36(2)
Cu(23)	7736(5)	9745(11)	5353(2)	54(2)
Cu(24)	6504(4)	7815(10)	5461(2)	47(2)
Cu(25)	8867(5)	9449(10)	5960(2)	58(2)
N(11)	6330(20)	2570(60)	8176(11)	34(11)
C(111)	6160(30)	1200(70)	8071(14)	36(12)
C(112)	5880(30)	-280(80)	7883(15)	55(15)
N(12)	8940(20)	10540(60)	9713(12)	43(12)
C(121)	9170(30)	11620(70)	9799(15)	37(13)
C(122)	9380(20)	13250(60)	9848(12)	25(11)
N(21)	8680(30)	13490(70)	6870(14)	58(14)
C(211)	8830(20)	14700(60)	7004(12)	25(11)
C(212)	9040(20)	16240(60)	7132(12)	28(11)
N(22)	6020(20)	5860(60)	5308(12)	46(12)
C(221)	5840(30)	4340(60)	5265(14)	31(12)
C(222)	5520(30)	2820(80)	5174(16)	49(16)
N(51)	5850(20)	4420(50)	6776(10)	33(10)
C(511)	5560(30)	3480(60)	6367(14)	50(12)
C(510)	6570(30)	5430(60)	6600(15)	53(13)
C(59)	6000(30)	3410(70)	7144(16)	62(14)
C(57)	5210(20)	5770(50)	6803(11)	29(9)
C(58)	5460(20)	7000(60)	7131(12)	33(10)
C(56)	4370(30)	5160(60)	6841(13)	38(11)
C(55)	4220(30)	4760(60)	7219(13)	43(11)
C(54)	3430(40)	4000(90)	7301(19)	75(18)
C(53)	2870(40)	3840(80)	6922(18)	70(18)
C(52)	3070(30)	4410(70)	6530(16)	60(14)
C(51)	3740(40)	4990(80)	6463(19)	79(18)
N(61)	9150(30)	1780(60)	8266(12)	49(12)
C(611)	9430(30)	1340(70)	8746(15)	54(13)
C(610)	9320(40)	3560(90)	8220(20)	89(19)
C(69)	8250(20)	1430(50)	8174(13)	37(10)
C(67)	9580(30)	1000(60)	7934(15)	53(13)
C(68)	9330(30)	-720(60)	7939(13)	37(11)
C(66)	10450(30)	1380(70)	8018(16)	60(15)
C(65)	11000(30)	550(70)	8349(17)	64(15)
C(64)	11820(30)	820(80)	8352(18)	70(16)
C(63)	12180(30)	1780(80)	8072(17)	66(17)
C(62)	11600(40)	2730(90)	7810(20)	90(20)
C(61)	10800(40)	2330(100)	7680(20)	100(20)
N(71)	7000(20)	11700(60)	10580(12)	46(11)
C(711)	6640(20)	11130(50)	10144(12)	32(10)
C(710)	6370(30)	12650(70)	10753(15)	57(13)
C(79)	7700(20)	12950(50)	10510(12)	32(10)
C(77)	7330(30)	10320(60)	10892(14)	47(12)
C(78)	6650(20)	9120(50)	10907(12)	34(10)
C(76)	7680(20)	10940(50)	11320(12)	31(9)
C(75)	7350(30)	11180(60)	11679(14)	45(12)
C(74)	7590(30)	11720(70)	12120(16)	60(15)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis((R)-(1-Phenylethyl)trimethylammonium)-heptaiodopentacuprat(I)·3CH_3CN. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(73)	8450(30)	11790(60)	12146(14)	41(12)
C(72)	8930(40)	11360(80)	11777(19)	76(17)
C(71)	8510(30)	10910(70)	11387(16)	60(14)
N(91)	5240(40)	1860(110)	9050(20)	120(20)
C(91)	4100(40)	890(80)	8415(18)	74(17)
C(92)	4630(30)	1380(90)	8663(17)	53(15)
N(81)	1890(30)	9670(80)	5607(16)	80(16)
C(811)	1440(40)	11110(100)	5780(20)	100(20)
C(810)	2670(60)	10030(130)	5540(30)	140(30)
C(89)	1610(60)	9100(130)	5150(30)	150(40)
C(87)	2290(40)	8320(100)	5890(20)	100(20)
C(88)	1500(40)	7370(100)	5970(20)	100(20)
C(86)	2690(40)	8990(90)	6380(20)	85(19)
C(85)	2110(40)	9280(90)	6640(20)	90(20)
C(84)	2780(30)	9750(70)	7045(15)	51(14)
C(83)	3480(90)	9700(200)	7250(50)	220(70)
C(82)	3700(40)	9720(100)	6970(20)	83(19)
C(81)	3620(70)	9430(170)	6530(40)	180(50)
C(101)	10440(40)	4610(120)	6400(20)	90(20)
C(102)	9910(30)	4280(80)	5952(15)	53(14)
N(101)	10770(20)	4790(60)	6743(13)	58(11)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Bis((R)-(1-Phenylethyl)-trimethylammonium)heptaiodopentacuprat(I)·3CH_3CN. The anisotropic displacement factor exponent takes the form: $-2\pi^2$[h^2a^*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
I(11)	30(2)	27(2)	28(1)	-5(2)	-2(1)	7(2)
I(12)	26(2)	25(2)	27(1)	2(2)	0(1)	-2(2)
I(13)	25(2)	30(2)	31(1)	1(2)	2(1)	1(2)
I(14)	29(2)	33(2)	26(1)	1(2)	3(1)	-6(2)
I(15)	24(2)	45(2)	31(1)	-2(2)	0(1)	-4(2)
I(16)	35(2)	33(2)	26(1)	0(2)	-1(1)	-3(2)
I(17)	35(2)	59(3)	35(2)	-4(2)	12(1)	-7(2)
I(21)	36(2)	25(2)	31(2)	1(2)	4(1)	-2(2)
I(22)	35(2)	30(2)	38(2)	-1(2)	5(1)	-1(2)
I(23)	33(2)	38(2)	41(2)	-1(2)	-1(1)	-1(2)
I(24)	36(2)	34(2)	27(1)	0(2)	5(1)	1(2)
I(25)	31(2)	36(2)	56(2)	1(2)	8(2)	0(2)
I(26)	80(3)	63(3)	59(2)	2(2)	38(2)	8(3)
I(27)	88(3)	65(3)	30(2)	3(2)	-4(2)	3(3)
Cu(11)	37(4)	37(4)	30(3)	-6(3)	2(2)	-1(3)
Cu(12)	36(3)	27(4)	34(3)	9(3)	4(2)	5(3)
Cu(13)	31(3)	29(4)	39(3)	0(3)	2(3)	0(3)
Cu(14)	32(3)	54(5)	46(3)	-1(4)	-2(3)	-12(4)
Cu(15)	38(4)	91(7)	33(3)	-1(4)	2(3)	-9(4)
Cu(21)	31(3)	33(4)	51(3)	1(3)	13(3)	-5(3)
Cu(22)	50(4)	20(4)	37(3)	-2(3)	5(3)	-6(3)
Cu(23)	72(5)	46(5)	50(3)	-15(4)	22(3)	3(4)
Cu(24)	64(5)	37(4)	38(3)	-2(3)	-3(3)	-2(4)
Cu(25)	77(5)	40(5)	57(4)	-12(4)	7(3)	-27(4)

Umsetzungen chiraler Kationen mit Kupferiodid
Bis-((R/S)-(1-Cyclohexylethyl)trimethylammonium)tetraiododicuprat(I) ($[(R/S)\text{-}C_{11}H_{24}N]_2[Cu_2I_4]$)

Table 1. Crystal data and structure refinement for Bis((R/S)-(1-Cyclohexylethyl)trimethylammonium)-tetraiododicuprat(I)

Diffractometer type	CAD 4	
Empirical formula	$C_{22}\ H_{48}\ Cu_2\ I_4\ N_2$	
Formula weight	487.65	
Temperature	293(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Triclinic	
Space group	P -1 (No.2)	
Unit cell dimensions	a = 931.8(7) pm	α= 62.26(2)°.
	b = 991.7(4) pm	β= 90.04(3)°.
	c = 983.5(2) pm	γ = 77.86(5)°.
Volume	0.7813(7) nm^3	
Z	1	
Density (calculated)	2.073 g/cm^3	
Absorption coefficient	5.325 mm^{-1}	
F(000)	464	
Crystal size	0.20 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.87 to 29.94°.	
Index ranges	-13<=h<=13, -13<=k<=12, -13<=l<=0	
Reflections collected	4760	
Independent reflections	4508 [R(int) = 0.0279]	
Completeness to theta = 29.94°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4508 / 0 / 136	
Goodness-of-fit on F^2	1.123	
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0756	
R indices (all data)	R1 = 0.0366, wR2 = 0.0793	
Largest diff. peak and hole	2.033 and -1.326 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis((R/S)-(1-Cyclohexylethyl)trimethylammonium)-tetraiododicuprat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	-2232(1)	4215(1)	-2333(1)	24(1)
I(2)	1244(1)	701(1)	1408(1)	25(1)
Cu(1)	758(1)	-1436(1)	791(1)	22(1)
N(1)	8063(3)	4098(3)	2857(3)	19(1)
C(1)	5424(4)	2459(4)	1528(4)	25(1)
C(2)	5513(5)	1233(5)	993(5)	30(1)
C(3)	5815(5)	-406(5)	2356(5)	31(1)
C(4)	7222(5)	-750(4)	3369(5)	33(1)
C(5)	7116(5)	473(4)	3934(4)	28(1)
C(6)	6830(4)	2134(4)	2557(4)	20(1)
C(7)	6639(4)	3493(4)	2972(4)	20(1)
C(8)	6047(4)	3122(5)	4504(4)	26(1)
C(9)	8480(5)	4711(4)	1240(4)	26(1)
C(10)	9349(4)	2850(5)	3958(5)	29(1)
C(11)	7791(6)	5451(5)	3204(5)	35(1)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis((R/S)-(1-Cyclohexyl-ethyl)trimethylammonium)-tetraiododicuprat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	31(1)	19(1)	19(1)	-8(1)	-2(1)	1(1)
I(2)	26(1)	22(1)	26(1)	-13(1)	-5(1)	-2(1)
Cu(1)	24(1)	19(1)	20(1)	-9(1)	1(1)	-1(1)
N(1)	28(1)	16(1)	14(1)	-9(1)	3(1)	-3(1)
C(1)	27(2)	23(2)	23(2)	-10(1)	-1(1)	-4(1)
C(2)	35(2)	31(2)	24(2)	-12(2)	2(2)	-13(2)
C(3)	35(2)	25(2)	35(2)	-15(2)	0(2)	-10(2)
C(4)	32(2)	17(2)	44(2)	-12(2)	-5(2)	-3(1)
C(5)	33(2)	21(2)	23(2)	-6(1)	-5(1)	-5(1)
C(6)	22(2)	18(1)	19(1)	-10(1)	2(1)	-4(1)
C(7)	21(2)	20(1)	17(1)	-9(1)	1(1)	0(1)
C(8)	28(2)	30(2)	21(2)	-14(1)	8(1)	-4(1)
C(9)	40(2)	25(2)	16(2)	-11(1)	5(1)	-10(2)
C(10)	26(2)	28(2)	26(2)	-9(2)	-5(1)	-3(1)
C(11)	54(3)	27(2)	35(2)	-22(2)	14(2)	-13(2)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis((R/S)-(1-Cyclohexylethyl)trimethylammonium)-tetraiododicuprat(I).

	x	y	z	U(eq)
H(1A)	4578	2463	2102	31
H(1B)	5280	3488	633	31
H(2A)	4590	1444	394	36
H(2B)	6295	1300	330	36
H(3A)	5914	-1166	1982	37
H(3B)	4988	-504	2966	37
H(4A)	8061	-734	2784	40
H(4B)	7375	-1789	4253	40
H(5A)	6320	406	4580	33
H(5B)	8030	254	4552	33
H(6)	7664	2182	1942	23
H(7)	5892	4369	2181	24
H(8A)	6767	2306	5328	40
H(8B)	5153	2778	4529	40
H(8C)	5844	4045	4631	40
H(9A)	7622	5384	519	40
H(9B)	8868	3848	1046	40
H(9C)	9217	5293	1120	40
H(10A)	10182	3297	3896	43
H(10B)	9603	2023	3686	43
H(10C)	9083	2432	4994	43
H(11A)	8643	5887	3028	52
H(11B)	7609	5088	4263	52
H(11C)	6948	6241	2540	52

Umsetzungen chiraler Kationen mit Kupferiodid
Bis-((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammonium)heptaiodo-pentacuprat(I) ($[(+)\text{-}C_{12}H_{20}NO]_2\,{}^{1}_{\infty}[Cu_5I_7]$)

Table 1. Crystal data and structure refinement for Bis((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammonium)heptaiodopentacuprat(I)

Diffractometer type	CCD	
Empirical formula	$C_{24}\ H_{40}\ Cu_5\ I_7\ N_2\ O_2$	
Formula weight	1594.58	
Temperature	173(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 1388.42(15) pm	α= 90°.
	b = 1030.76(11) pm	β= 111.060(2)°.
	c = 1470.96(16) pm	γ = 90°.
Volume	1.9645(4) nm^3	
Z	2	
Density (calculated)	2.696 g/cm^3	
Absorption coefficient	8.187 mm^{-1}	
F(000)	1460	
Crystal size	0.20 x 0.04 x 0.03 mm^3	
Theta range for data collection	1.48 to 30.09°.	
Index ranges	-19<=h<=19, -14<=k<=14, -20<=l<=20	
Reflections collected	20579	
Independent reflections	11074 [R(int) = 0.0709]	
Completeness to theta = 30.09°	98.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11074 / 1 / 327	
Goodness-of-fit on F^2	0.923	
Final R indices [I>2sigma(I)]	R1 = 0.0639, wR2 = 0.1374	
R indices (all data)	R1 = 0.1166, wR2 = 0.1594	
Absolute structure parameter[99]	-0.03(6)	
Extinction coefficient	0.00176(16)	
Largest diff. peak and hole	3.117 and -2.916 e.$Å^{-3}$	
Absorption correction	sadabs	
Effective transmission (min. / max.)	0.1351 / 0.3203	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammonium)heptaiodopentacuprat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	6643(1)	4005(1)	2622(1)	24(1)
I(2)	3830(1)	4631(1)	3445(1)	21(1)
I(3)	5021(1)	618(1)	3370(1)	23(1)
I(4)	6345(1)	7049(1)	4494(1)	22(1)
I(5)	6736(1)	3173(1)	5634(1)	22(1)
I(6)	3454(1)	2822(1)	806(1)	27(1)
I(7)	1542(1)	1368(1)	2541(1)	27(1)
Cu(1)	4823(2)	2571(2)	4470(2)	27(1)
Cu(2)	5906(2)	4602(2)	4024(2)	27(1)
Cu(3)	4972(2)	2869(2)	2530(2)	33(1)
Cu(4)	3323(2)	661(2)	3891(2)	30(1)
Cu(5)	3139(2)	2445(3)	2455(2)	37(1)
N(1)	9715(11)	873(15)	6255(11)	28(3)
O(1)	8978(9)	2554(11)	4229(9)	29(3)
C(11)	7820(12)	-640(20)	3426(15)	37(5)
C(12)	7579(15)	-1520(20)	2599(14)	41(5)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammonium)heptaiodopentacuprat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(13)	7967(17)	-1300(20)	1887(15)	42(5)
C(14)	8586(17)	-130(20)	1963(15)	41(5)
C(15)	8827(16)	650(20)	2751(14)	36(4)
C(16)	8449(13)	414(16)	3500(11)	22(4)
C(17)	8739(13)	1220(17)	4417(12)	22(4)
C(18)	9683(12)	652(16)	5199(12)	20(3)
C(19)	10715(15)	1095(18)	5103(13)	33(4)
C(110)	8767(17)	200(20)	6366(15)	45(6)
C(111)	9642(16)	2305(19)	6450(14)	35(4)
C(112)	10631(18)	230(20)	6979(15)	42(5)
N(2)	4061(10)	7323(15)	708(11)	30(4)
O(2)	2639(10)	8901(14)	1416(10)	40(3)
C(21)	1271(13)	5688(19)	1147(13)	29(4)
C(22)	254(14)	5227(18)	855(12)	28(4)
C(23)	-564(14)	6070(20)	567(14)	34(4)
C(24)	-386(14)	7382(18)	601(13)	31(4)
C(25)	621(12)	7859(19)	883(13)	30(4)
C(26)	1463(11)	7035(17)	1138(12)	21(3)
C(27)	2556(12)	7511(18)	1360(12)	24(4)
C(28)	2877(13)	7117(17)	509(14)	28(4)
C(29)	2216(14)	7710(20)	-466(12)	32(4)
C(210)	4310(15)	8720(20)	548(15)	40(5)
C(211)	4345(19)	6460(20)	-6(17)	56(6)
C(212)	4693(18)	6980(20)	1748(16)	49(6)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Bis((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammonium)heptaiodopentacuprat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	9(1)	32(1)	32(1)	-1(1)	10(1)	-2(1)
I(2)	10(1)	22(1)	31(1)	2(1)	8(1)	2(1)
I(3)	16(1)	22(1)	35(1)	-1(1)	13(1)	1(1)
I(4)	16(1)	22(1)	30(1)	0(1)	11(1)	-2(1)
I(5)	11(1)	22(1)	33(1)	0(1)	6(1)	3(1)
I(6)	12(1)	42(1)	26(1)	2(1)	6(1)	0(1)
I(7)	10(1)	35(1)	37(1)	-3(1)	10(1)	-4(1)
Cu(1)	14(1)	28(1)	41(1)	1(1)	12(1)	1(1)
Cu(2)	18(1)	26(1)	40(1)	-2(1)	13(1)	-2(1)
Cu(3)	12(1)	46(2)	39(1)	9(1)	5(1)	-7(1)
Cu(4)	18(1)	28(1)	41(1)	-1(1)	8(1)	-2(1)
Cu(5)	21(1)	54(2)	41(1)	-5(1)	16(1)	-14(1)
N(1)	12(7)	38(9)	37(8)	-1(7)	12(6)	12(7)
O(1)	20(7)	20(6)	47(8)	5(6)	12(6)	3(5)
C(11)	0(7)	57(13)	53(12)	-14(10)	7(8)	-17(8)
C(12)	25(10)	51(13)	33(10)	-8(9)	-7(8)	-22(10)
C(13)	34(12)	48(13)	40(11)	-8(10)	10(9)	11(10)
C(14)	44(13)	46(13)	37(11)	11(10)	20(10)	19(11)
C(17)	16(8)	27(9)	24(8)	-14(7)	9(7)	-3(7)
C(18)	8(7)	24(8)	30(9)	-7(7)	11(6)	-2(7)
C(110)	36(13)	58(15)	45(12)	-7(11)	18(10)	-6(11)
N(2)	5(6)	42(10)	44(9)	20(7)	10(6)	4(6)
O(2)	32(8)	40(8)	60(9)	-10(7)	32(7)	-18(7)
C(21)	18(9)	37(10)	38(10)	4(9)	16(8)	9(8)

Table 3. (continued)
Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammonium)heptaiodopentacuprat(I).

	U11	U22	U33	U23	U13	U12
C(22)	26(10)	32(10)	23(9)	-3(8)	8(7)	-12(8)
C(23)	13(8)	46(12)	43(11)	6(9)	12(8)	3(8)
C(24)	19(9)	38(11)	30(9)	6(8)	1(7)	1(8)
C(25)	10(8)	42(11)	45(10)	0(9)	19(7)	3(8)
C(26)	7(7)	27(9)	37(9)	-5(8)	15(7)	-3(7)
C(27)	11(8)	37(10)	27(9)	-1(8)	9(7)	2(7)
C(28)	13(8)	22(9)	53(11)	9(8)	17(8)	3(7)
C(29)	28(10)	48(12)	23(8)	-6(8)	12(7)	-5(9)
C(210)	27(10)	50(13)	53(12)	21(10)	27(10)	2(10)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis((+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammonium)heptaiodopentacuprat(I).

	x	y	z	U(eq)
H(1)	9117	2994	4741	44
H(11)	7540	-796	3918	45
H(12)	7148	-2246	2556	49
H(13)	7839	-1882	1358	50
H(14)	8824	79	1451	49
H(15)	9266	1370	2799	43
H(17)	8150	1227	4657	27
H(18)	9642	-308	5093	24
H(19A)	11001	1827	5542	50
H(19B)	10586	1362	4430	50
H(19C)	11208	374	5276	50
H(11A)	8781	-731	6222	68
H(11B)	8133	583	5911	68
H(11C)	8788	306	7034	68
H(11D)	9682	2428	7123	52
H(11E)	8984	2648	6002	52
H(11F)	10213	2767	6350	52
H(11G)	10502	70	7582	63
H(11H)	11236	792	7118	63
H(11I)	10759	-598	6714	63
H(2)	2879	9171	1002	59
H(21)	1832	5095	1350	35
H(22)	131	4321	858	33
H(23)	-1251	5751	345	40
H(24)	-951	7969	431	37
H(25)	730	8770	900	36
H(27)	3031	7112	1978	29
H(28)	2760	6160	433	34
H(29A)	1558	8000	-433	49
H(29B)	2085	7054	-980	49
H(29C)	2579	8448	-612	49
H(21A)	4024	9297	914	60
H(21B)	4007	8925	-147	60
H(21C)	5061	8829	774	60
H(21D)	5039	6689	15	85
H(21E)	3847	6599	-667	85
H(21F)	4333	5551	177	85
H(21G)	5371	6664	1787	74
H(21H)	4338	6305	1976	74
H(21I)	4779	7754	2158	74

Umsetzungen chiraler Kationen mit Silberiodid
(R/S)-(1-Phenylethyl)trimethylammoniumdiiodoargentat(I)
([(R/S)-$C_{11}H_{18}N$] $^{1}_{\infty}[AgI_2]$)

Table 1. Crystal data and structure refinement for (R/S)-(1-Phenylethyl)trimethylammoniumdiiodoargentat(I)

Diffractometer type	CAD 4	
Empirical formula	C_{11} H_{18} Ag I_2 N	
Formula weight	525.93	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1/c (No. 14)	
Unit cell dimensions	a = 745.10(10) pm	α= 90°.
	b = 2298.4(5) pm	β= 110.450(10)°.
	c = 955.5(2) pm	γ = 90°.
Volume	1.5332(5) nm^3	
Z	4	
Density (calculated)	2.278 g/cm^3	
Absorption coefficient	5.316 mm^{-1}	
F(000)	976	
Crystal size	0.30 x 0.08 x 0.03 mm^3	
Theta range for data collection	2.44 to 27.94°.	
Index ranges	0<=h<=9, -30<=k<=0, -12<=l<=11	
Reflections collected	3945	
Independent reflections	3679 [R(int) = 0.0328]	
Completeness to theta = 27.94°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3679 / 0 / 191	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0903	
R indices (all data)	R1 = 0.0876, wR2 = 0.1054	
Extinction coefficient	0.0003(2)	
Largest diff. peak and hole	1.044 and -1.013 e.$Å^{-3}$	
Absorption correction	psi-scan	
Effective transmission (min. / max.)	0.7331 / 0.9653	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (R/S)-(1-Phenylethyl)trimethylammoniumdiiodoargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	4043(1)	4551(1)	2895(1)	43(1)
I(2)	602(1)	4201(1)	6368(1)	50(1)
Ag(1)	2432(1)	5003(1)	5013(1)	58(1)
N(1)	2529(8)	6145(2)	9718(6)	48(1)
C(1)	5235(11)	7148(3)	8617(9)	54(2)
C(2)	6234(13)	7661(4)	8939(11)	69(2)
C(3)	5574(12)	8131(3)	9463(9)	59(2)
C(4)	3853(12)	8101(3)	9665(9)	58(2)
C(5)	2790(10)	7597(3)	9317(8)	49(2)
C(6)	3472(8)	7107(3)	8822(6)	36(1)
C(7)	2327(9)	6549(3)	8373(7)	42(1)
C(8)	268(12)	6663(4)	7436(11)	64(2)
C(9)	4589(12)	6071(4)	10665(10)	62(2)
C(10)	1765(15)	5553(4)	9128(11)	72(3)
C(11)	1502(19)	6373(6)	10690(12)	91(3)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (R/S)-(1-Phenylethyl)trimethyl-ammoniumdiiodoargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	37(1)	44(1)	47(1)	-2(1)	15(1)	-1(1)
I(2)	39(1)	51(1)	64(1)	8(1)	23(1)	2(1)
Ag(1)	46(1)	64(1)	65(1)	-1(1)	21(1)	-1(1)
N(1)	43(3)	51(3)	46(3)	5(3)	11(2)	-8(3)
C(1)	54(4)	42(4)	73(5)	-10(4)	32(4)	0(3)
C(2)	53(5)	61(5)	102(7)	-2(5)	37(5)	-12(4)
C(3)	53(4)	45(4)	68(5)	1(4)	7(4)	-11(4)
C(4)	69(5)	32(4)	68(5)	-18(3)	18(4)	-3(3)
C(5)	38(3)	52(4)	57(4)	-10(3)	16(3)	0(3)
C(6)	37(3)	39(3)	31(3)	-3(3)	9(2)	0(3)
C(7)	42(3)	40(3)	41(3)	-2(3)	13(3)	-7(3)
C(8)	48(4)	66(6)	61(5)	-1(4)	-3(4)	-8(4)
C(9)	51(4)	65(5)	53(5)	6(4)	-3(4)	-7(4)
C(10)	78(6)	54(5)	71(6)	7(4)	9(5)	-32(5)
C(11)	104(8)	125(10)	67(6)	0(6)	59(6)	2(8)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (R/S)-(1-Phenylethyl)trimethylammoniumdiiodoargentat(I).

	x	y	z	U(eq)
H(1)	5730(110)	6830(40)	8270(90)	64
H(2)	7400(130)	7690(40)	8790(100)	83
H(3)	6290(120)	8470(40)	9680(90)	71
H(4)	3400(110)	8420(40)	10040(90)	69
H(5)	1590(110)	7580(30)	9420(80)	59
H(7)	2880(100)	6340(30)	7730(80)	50
H(8A)	-390(150)	6300(40)	7150(110)	96
H(8B)	210(140)	6870(50)	6550(120)	96
H(8C)	-330(140)	6890(50)	8000(110)	96
H(9A)	5000(140)	6400(40)	11320(100)	93
H(9B)	5350(150)	6050(40)	10040(110)	93
H(9C)	4740(140)	5720(50)	11250(110)	93
H(10A)	430(160)	5580(50)	8530(120)	108
H(10B)	1920(150)	5290(50)	9950(120)	108
H(10C)	2460(150)	5400(50)	8530(130)	108
H(11A)	100(200)	6360(60)	10160(140)	136
H(11B)	1890(180)	6770(60)	10970(130)	136
H(11C)	1810(180)	6140(50)	11570(140)	136

Umsetzungen chiraler Kationen mit Silberiodid
Bis-((R)-(1-Phenylethyl)trimethylammonium)octaiodohexaargentat(I) ($[(R)\text{-}C_{11}H_{18}N]_2\ {}^{3}_{\infty}[Ag_6I_8]$)

Table 1. Crystal data and structure refinement for Bis-((R)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I)

Diffractometer type	CAD 4	
Empirical formula	$C_{22}\ H_{36}\ Ag_6\ I_8\ N_2$	
Formula weight	1990.95	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 1185.5(2) pm	α= 90°.
	b = 1496.4(2) pm	β= 90°.
	c = 2312.0(2) pm	γ = 90°.
Volume	4.1014(10) nm^3	
Z	4	
Density (calculated)	3.224 g/cm^3	
Absorption coefficient	8.847 mm^{-1}	
F(000)	3552	
Crystal size	0.23 x 0.13 x 0.13 mm^3	
Theta range for data collection	2.36 to 24.99°.	
Index ranges	-14<=h<=14, -17<=k<=17, -27<=l<=27	
Reflections collected	8064	
Independent reflections	7216 [R(int) = 0.0382]	
Completeness to theta = 24.99°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7216 / 0 / 334	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0858	
R indices (all data)	R1 = 0.0528, wR2 = 0.0916	
Absolute structure parameter[99]	-0.01(4)	
Extinction coefficient	0.00014(4)	
Largest diff. peak and hole	1.523 and -1.299 e.$Å^{-3}$	
Absorption correction	psi-scan	
Effective transmission (min. / max.)	0.7278 / 0.9609	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis-((R)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	1362(1)	7127(1)	847(1)	51(1)
I(2)	-2246(1)	8351(1)	923(1)	48(1)
I(3)	-1357(1)	5824(1)	-207(1)	51(1)
I(4)	44(1)	7948(1)	2655(1)	58(1)
I(5)	610(1)	10301(1)	1213(1)	58(1)
I(6)	-4888(1)	6130(1)	654(1)	51(1)
I(7)	-1641(1)	5551(1)	1809(1)	61(1)
I(8)	-2296(1)	10332(1)	2449(1)	66(1)
Ag(1)	-565(1)	7216(1)	1546(1)	63(1)
Ag(2)	-2546(1)	6436(1)	818(1)	68(1)
Ag(3)	-600(1)	7527(1)	124(1)	75(1)
Ag(4)	-884(1)	9170(1)	1834(1)	68(1)
Ag(5)	1246(1)	8928(1)	464(1)	70(1)
Ag(6)	137(1)	6014(1)	2575(1)	81(1)
N(1)	4081(9)	8341(8)	2138(4)	50(3)
C(11)	6205(12)	7692(11)	2962(7)	63(4)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis-((R)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(12)	6861(13)	7022(13)	3203(8)	77(5)
C(13)	6340(16)	6348(12)	3493(7)	75(4)
C(14)	5186(18)	6321(11)	3563(7)	80(5)
C(15)	4542(13)	7005(12)	3322(6)	66(4)
C(16)	5030(11)	7683(10)	3016(5)	52(3)
C(17)	4265(11)	8424(9)	2791(6)	52(3)
C(18)	4661(13)	9357(11)	2969(7)	68(4)
C(19)	3682(18)	7405(12)	1999(8)	84(5)
C(110)	3142(14)	8980(12)	1971(7)	72(4)
C(111)	5091(17)	8504(13)	1788(8)	89(5)
N(2)	1512(14)	4080(8)	475(6)	78(4)
C(21)	3133(13)	3089(12)	-504(7)	70(4)
C(22)	3253(19)	2545(16)	-940(9)	97(7)
C(23)	2820(20)	1746(17)	-960(9)	96(7)
C(24)	2200(20)	1396(12)	-499(12)	106(8)
C(25)	2092(15)	1957(11)	-7(8)	81(5)
C(26)	2541(12)	2792(8)	-5(6)	51(3)
C(27)	2473(13)	3388(9)	512(5)	58(4)
C(28)	3600(20)	3790(14)	674(9)	110(8)
C(29)	462(19)	3629(15)	278(13)	131(10)
C(210)	1789(16)	4797(11)	27(7)	77(5)
C(211)	1360(40)	4510(18)	1049(10)	210(20)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Bis-((R)-(1-Phenylethyl)trimethyl-ammonium)octaiodohexaargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	47(1)	47(1)	60(1)	-1(1)	-1(1)	-1(1)
I(2)	48(1)	47(1)	50(1)	-1(1)	-2(1)	4(1)
I(3)	52(1)	52(1)	49(1)	-4(1)	-6(1)	3(1)
I(4)	85(1)	43(1)	48(1)	-4(1)	-13(1)	3(1)
I(5)	64(1)	52(1)	59(1)	-10(1)	16(1)	-10(1)
I(6)	48(1)	54(1)	52(1)	5(1)	-2(1)	-5(1)
I(7)	74(1)	54(1)	55(1)	13(1)	-17(1)	-23(1)
I(8)	47(1)	53(1)	100(1)	-17(1)	10(1)	-1(1)
Ag(1)	74(1)	60(1)	57(1)	-2(1)	1(1)	-12(1)
Ag(2)	66(1)	72(1)	68(1)	-1(1)	-9(1)	-7(1)
Ag(3)	81(1)	69(1)	76(1)	2(1)	1(1)	-16(1)
Ag(4)	79(1)	53(1)	74(1)	-2(1)	8(1)	3(1)
Ag(5)	79(1)	59(1)	73(1)	-10(1)	-3(1)	1(1)
Ag(6)	71(1)	70(1)	103(1)	-4(1)	-25(1)	18(1)
N(1)	47(6)	60(7)	43(6)	-6(5)	1(4)	1(5)
C(11)	47(8)	71(10)	70(9)	-9(7)	-5(7)	-4(7)
C(12)	55(9)	88(12)	88(12)	-32(10)	-14(8)	17(9)
C(13)	78(11)	70(11)	77(10)	5(8)	-7(9)	9(9)
C(14)	112(15)	69(10)	59(9)	7(8)	-7(9)	19(10)
C(15)	62(9)	78(10)	59(8)	3(8)	3(7)	11(8)
C(16)	41(7)	75(9)	39(6)	-9(6)	1(5)	10(6)
C(17)	49(7)	56(8)	51(7)	-5(6)	-4(6)	-1(6)
C(18)	61(9)	72(10)	71(9)	-20(8)	-15(7)	-2(8)
C(19)	100(13)	74(11)	79(11)	-15(9)	-27(10)	-1(10)
N(2)	120(12)	44(7)	72(8)	15(6)	41(8)	10(8)

Table 3. (continued)

Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis-((R)-(1-Phenylethyl)trimethyl-ammonium)octaiodohexaargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^*2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(21)	64(9)	82(11)	63(9)	11(8)	5(7)	7(8)
C(22)	111(16)	96(16)	82(13)	1(11)	24(11)	52(13)
C(23)	103(15)	103(17)	82(13)	-26(12)	-14(12)	49(13)
C(24)	115(17)	47(10)	160(20)	-18(12)	-54(16)	32(10)
C(25)	90(12)	41(8)	113(14)	12(9)	-34(10)	3(8)
C(26)	59(8)	37(7)	58(8)	-1(6)	-13(6)	-5(6)
C(27)	90(10)	50(8)	36(6)	6(6)	-1(6)	-5(7)
C(28)	151(19)	84(13)	96(14)	18(11)	-75(14)	-41(13)
C(29)	88(14)	86(15)	220(30)	47(17)	66(17)	11(12)
C(210)	100(13)	61(10)	71(10)	20(8)	17(9)	8(9)
C(211)	460(60)	95(18)	88(16)	-21(13)	120(30)	40(30)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis-((R)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I).

	x	y	z	U(eq)
H(11)	6552	8155	2761	75
H(12)	7642	7034	3168	93
H(13)	6775	5890	3649	90
H(14)	4846	5858	3766	96
H(15)	3763	6999	3370	80
H(17)	3527	8334	2973	62
H(18A)	4149	9796	2819	102
H(18B)	5402	9463	2816	102
H(18C)	4682	9398	3383	102
H(19A)	3018	7273	2221	126
H(19B)	4265	6985	2094	126
H(19C)	3511	7364	1594	126
H(11A)	2487	8861	2202	109
H(11B)	2959	8900	1570	109
H(11C)	3386	9584	2034	109
H(11D)	5676	8097	1902	133
H(11E)	5343	9107	1846	133
H(11F)	4915	8414	1387	133
H(21)	3430	3663	-520	84
H(22)	3671	2740	-1256	116
H(23)	2937	1398	-1288	115
H(24)	1869	832	-514	128
H(25)	1711	1750	318	98
H(27)	2271	2996	835	70
H(28A)	3515	4163	1008	166
H(28B)	3881	4141	357	166
H(28C)	4129	3320	758	166
H(29A)	591	3353	-91	197
H(29B)	-132	4061	244	197
H(29C)	250	3181	555	197
H(21A)	2462	5108	141	116
H(21B)	1174	5213	3	116
H(21C)	1904	4522	-343	116
H(21D)	2051	4807	1157	319
H(21E)	1185	4062	1332	319
H(21F)	763	4938	1029	319

Umsetzungen chiraler Kationen mit Silberiodid
Bis-((S)-(1-Phenylethyl)trimethylammonium)octaiodohexaargentat(I)
([(S)-$C_{11}H_{18}N]_2\ {}^3_\infty[Ag_6I_8]$)

Table 1. Crystal data and structure refinement for Bis-((S)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I)

Diffractometer type	CCD	
Empirical formula	$C_{22}\ H_{36}\ Ag_6\ I_8\ N_2$	
Formula weight	1990.95	
Temperature	293(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 1182.07(6) pm	α= 90°.
	b = 1490.12(8) pm	β= 90°.
	c = 2309.17(11) pm	γ = 90°.
Volume	4.0674(4) nm^3	
Z	4	
Density (calculated)	3.251 g/cm^3	
Absorption coefficient	8.921 mm^{-1}	
F(000)	3552	
Crystal size	0.30 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.63 to 20.81°.	
Index ranges	-11<=h<=11, -14<=k<=14, -23<=l<=23	
Reflections collected	21974	
Independent reflections	4247 [R(int) = 0.0614]	
Completeness to theta = 20.81°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4247 / 0 / 344	
Goodness-of-fit on F^2	0.889	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0737	
R indices (all data)	R1 = 0.0401, wR2 = 0.0777	
Absolute structure parameter[99]	0.01(5)	
Extinction coefficient	0.00010(3)	
Largest diff. peak and hole	0.893 and -0.749 e.$Å^{-3}$	
Absorption correction	sadabs	
Effective transmission (min. / max.)	0.5578 / 0.8411	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis-((S)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	8642(1)	2876(1)	9159(1)	35(1)
I(2)	12250(1)	1646(1)	9080(1)	34(1)
I(3)	11366(1)	4193(1)	10206(1)	35(1)
I(4)	9942(1)	2056(1)	7346(1)	41(1)
I(5)	9405(1)	-310(1)	8786(1)	39(1)
I(6)	14901(1)	3874(1)	9340(1)	36(1)
I(7)	11658(1)	4455(1)	8184(1)	44(1)
I(8)	12311(1)	-318(1)	7546(1)	47(1)
Ag(1)	10567(1)	2795(1)	8457(1)	42(1)
Ag(2)	12549(1)	3567(1)	9181(1)	47(1)
Ag(3)	10610(1)	2475(1)	9875(1)	49(1)
Ag(4)	10894(1)	842(1)	8169(1)	45(1)
Ag(5)	8769(1)	1062(1)	9544(1)	47(1)
Ag(6)	9856(1)	3996(1)	7425(1)	53(1)
N(1)	5962(10)	1668(9)	7870(6)	32(4)
C(11)	5453(15)	3005(13)	6676(7)	38(5)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis-((S)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(12)	4800(19)	3674(12)	6426(8)	50(5)
C(13)	3630(20)	3639(14)	6499(9)	54(6)
C(14)	3149(13)	2989(12)	6778(8)	37(5)
C(15)	3800(16)	2326(12)	7028(8)	39(5)
C(16)	4940(13)	2319(11)	6989(6)	24(4)
C(17)	5720(13)	1582(12)	7214(7)	29(4)
C(18)	5350(14)	657(16)	7035(8)	53(6)
C(19)	4909(15)	1450(16)	8232(8)	62(6)
C(110)	6867(16)	1013(13)	8045(7)	44(5)
C(111)	6287(19)	2589(13)	7998(7)	52(6)
N(2)	8432(15)	5906(9)	9523(6)	50(4)
C(21)	6872(16)	6900(13)	10483(10)	57(6)
C(22)	6760(20)	7400(30)	10972(10)	79(10)
C(23)	7207(19)	8220(20)	10971(12)	76(9)
C(24)	7794(18)	8585(12)	10533(13)	76(8)
C(25)	7880(17)	8049(14)	10029(9)	54(6)
C(26)	7459(15)	7188(11)	9999(8)	37(5)
C(27)	7511(13)	6624(10)	9482(6)	25(4)
C(28)	6420(30)	6238(14)	9324(11)	94(10)
C(29)	8222(18)	5203(12)	9958(8)	49(6)
C(210)	9550(20)	6365(17)	9738(13)	97(13)
C(211)	8610(50)	5480(20)	8967(13)	210(30)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Bis-((S)-(1-Phenylethyl)trimethyl-ammonium)octaiodohexaargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	30(1)	35(1)	40(1)	-2(1)	-1(1)	1(1)
I(2)	32(1)	34(1)	34(1)	0(1)	-2(1)	1(1)
I(3)	35(1)	36(1)	33(1)	-1(1)	-6(1)	1(1)
I(4)	62(1)	30(1)	31(1)	-2(1)	-10(1)	1(1)
I(5)	42(1)	35(1)	40(1)	-5(1)	10(1)	-6(1)
I(6)	34(1)	40(1)	34(1)	4(1)	-1(1)	-4(1)
I(7)	54(1)	38(1)	38(1)	8(1)	-13(1)	-17(1)
I(8)	33(1)	39(1)	71(1)	-14(1)	8(1)	-2(1)
Ag(1)	48(1)	40(1)	38(1)	-1(1)	0(1)	-8(1)
Ag(2)	45(1)	50(1)	45(1)	-1(1)	-6(1)	-5(1)
Ag(3)	52(1)	47(1)	48(1)	1(1)	1(1)	-10(1)
Ag(4)	52(1)	38(1)	46(1)	-1(1)	5(1)	2(1)
Ag(5)	51(1)	41(1)	49(1)	-7(1)	-3(1)	1(1)
Ag(6)	46(1)	49(1)	64(1)	0(1)	-14(1)	10(1)
N(1)	13(7)	39(9)	45(9)	-1(7)	-5(6)	-5(7)
C(11)	36(11)	56(13)	23(11)	-20(10)	-6(9)	13(11)
C(12)	71(16)	39(12)	39(12)	-10(10)	7(11)	-11(12)
C(13)	64(16)	35(13)	62(15)	11(11)	-2(13)	5(13)
C(14)	17(9)	40(11)	54(13)	-27(11)	-7(9)	2(9)
C(15)	34(12)	46(12)	38(12)	-8(10)	-9(10)	-8(10)
C(16)	23(10)	41(10)	8(9)	5(8)	3(8)	10(9)
C(17)	20(9)	47(11)	20(10)	2(8)	11(7)	5(8)
C(18)	19(10)	91(19)	49(12)	-19(12)	-13(9)	11(11)
C(19)	18(10)	121(18)	49(12)	-1(13)	28(10)	10(12)
C(110)	59(13)	58(12)	16(10)	13(9)	-1(9)	-4(11)
C(111)	71(16)	52(12)	33(10)	0(9)	-18(11)	3(12)

Table 3. (continued)

Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis-((S)-(1-Phenylethyl)trimethyl-ammonium)octaiodohexaargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^*2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
N(2)	89(12)	28(9)	34(10)	-8(8)	12(9)	-14(9)
C(21)	60(13)	51(13)	60(16)	-14(11)	22(12)	12(10)
C(22)	41(18)	150(30)	48(16)	-3(18)	-6(13)	-10(20)
C(23)	42(14)	110(20)	80(20)	-31(19)	-21(14)	5(14)
C(24)	62(14)	18(11)	150(20)	-33(14)	-35(16)	11(10)
C(25)	64(15)	42(14)	56(16)	19(12)	-28(12)	16(12)
C(26)	44(12)	31(12)	37(12)	0(9)	20(9)	8(10)
C(27)	39(10)	24(9)	12(9)	3(7)	-9(8)	5(8)
C(28)	150(20)	39(13)	100(20)	17(13)	-70(20)	-18(15)
C(29)	74(16)	28(11)	45(13)	17(9)	37(12)	2(11)
C(210)	100(20)	61(18)	130(30)	40(19)	90(20)	58(19)
C(211)	460(70)	90(30)	80(30)	20(20)	120(40)	110(40)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Bis-((S)-(1-Phenylethyl)trimethylammonium)-octaiodohexaargentat(I).

	x	y	z	U(eq)
H(11)	6236	3015	6634	46
H(12)	5134	4134	6215	59
H(13)	3184	4094	6344	65
H(14)	2365	2969	6810	44
H(15)	3441	1868	7230	47
H(17)	6448	1681	7022	35
H(18A)	5851	220	7200	80
H(18B)	5368	610	6621	80
H(18C)	4594	550	7170	80
H(19A)	4325	1878	8148	94
H(19B)	5096	1477	8636	94
H(19C)	4646	858	8137	94
H(11A)	6985	1049	8456	66
H(11B)	7558	1156	7847	66
H(11C)	6635	415	7944	66
H(11D)	5712	2990	7860	78
H(11E)	6992	2723	7810	78
H(11F)	6371	2660	8409	78
H(21)	6536	6336	10473	68
H(22)	6390	7177	11296	95
H(23)	7103	8564	11301	91
H(24)	8120	9151	10559	91
H(25)	8235	8287	9704	65
H(27)	7729	7020	9162	30
H(28A)	6522	5807	9020	140
H(28B)	5922	6706	9192	140
H(28C)	6092	5949	9655	140
H(29A)	7994	5477	10316	74
H(29B)	8902	4864	10019	74
H(29C)	7633	4812	9824	74
H(21A)	9392	6716	10078	146
H(21B)	9841	6747	9439	146
H(21C)	10098	5912	9830	146
H(21D)	7987	5096	8879	314
H(21E)	9298	5134	8980	314
H(21F)	8681	5934	8673	314

Umsetzungen chiraler Kationen mit Silberiodid
(R)-(1-Cyclohexylethyl)trimethylammoniumtriiododiargentat(I)
([(R)-$C_{11}H_{24}N$] $_{\infty}^{1}$[Ag_2I_3])

Table 1. Crystal data and structure refinement for (R)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I)

Diffractometer type	CAD 4	
Empirical formula	C_{11} H_{24} Ag_2 I_3 N	
Formula weight	766.75	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 742.00(10) pm	α= 90°.
	b = 2446.0(3) pm	β= 90°.
	c = 1041.0(2) pm	γ = 90°.
Volume	1.8893(5) nm^3	
Z	4	
Density (calculated)	2.696 g/cm^3	
Absorption coefficient	6.959 mm^{-1}	
F(000)	1400	
Crystal size	0.40 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.66 to 24.95°.	
Index ranges	0<=h<=8, 0<=k<=29, -12<=l<=12	
Reflections collected	3643	
Independent reflections	3298 [R(int) = 0.0149]	
Completeness to theta = 24.95°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3298 / 0 / 227	
Goodness-of-fit on F^2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0287, wR2 = 0.0685	
R indices (all data)	R1 = 0.0416, wR2 = 0.0727	
Absolute structure parameter[99]	0.03(5)	
Extinction coefficient	0.00122(9)	
Largest diff. peak and hole	1.071 and -1.117 e.$Å^{-3}$	
Absorption correction	psi-scan	
Effective transmission (min. / max.)	0.7759 / 0.9839	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (R)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	3568(1)	7790(1)	8575(1)	43(1)
I(2)	3588(1)	8278(1)	12691(1)	51(1)
I(3)	-1366(1)	8855(1)	9857(1)	53(1)
Ag(1)	1149(1)	8086(1)	10670(1)	66(1)
Ag(2)	6018(1)	8113(1)	10639(1)	69(1)
N(1)	6508(11)	11490(3)	10563(6)	46(2)
C(1)	4853(15)	10025(4)	10543(10)	59(3)
C(2)	3341(17)	9698(4)	9918(12)	69(3)
C(3)	3760(20)	9590(5)	8518(12)	82(4)
C(4)	4120(20)	10115(5)	7835(13)	86(4)
C(5)	5684(19)	10422(5)	8440(10)	69(3)
C(6)	5271(12)	10551(4)	9840(9)	47(2)
C(7)	6752(13)	10864(4)	10568(8)	48(2)
C(8)	8627(16)	10701(5)	10124(14)	74(3)
C(9)	6417(17)	11737(4)	9259(9)	57(2)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (R)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(10)	4819(16)	11638(5)	11265(13)	65(3)
C(11)	8052(15)	11749(6)	11278(12)	68(3)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for (R)-(1-Cyclohexylethyl)trimethyl-ammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	33(1)	53(1)	43(1)	0(1)	0(1)	-1(1)
I(2)	36(1)	67(1)	50(1)	-7(1)	-2(1)	0(1)
I(3)	42(1)	50(1)	66(1)	-3(1)	-4(1)	2(1)
Ag(1)	49(1)	83(1)	66(1)	-4(1)	-6(1)	8(1)
Ag(2)	52(1)	88(1)	68(1)	-4(1)	4(1)	-8(1)
N(1)	43(4)	47(3)	48(3)	0(3)	0(4)	-1(4)
C(1)	60(6)	67(6)	49(6)	2(5)	12(5)	-1(5)
C(2)	66(7)	54(6)	88(7)	-13(5)	4(7)	-26(6)
C(3)	90(9)	63(6)	93(8)	-15(6)	-36(8)	9(7)
C(4)	122(12)	72(8)	63(7)	-13(6)	-10(8)	-6(7)
C(5)	96(9)	72(7)	39(5)	-1(5)	-3(5)	-6(6)
C(6)	44(5)	54(5)	44(5)	3(4)	-6(4)	10(4)
C(7)	54(6)	56(5)	35(4)	10(4)	-10(4)	1(4)
C(8)	43(5)	65(6)	116(9)	9(6)	9(7)	17(6)
C(9)	51(5)	66(6)	55(5)	16(4)	6(6)	10(6)
C(10)	59(7)	65(7)	71(7)	-10(6)	10(6)	5(5)
C(11)	57(7)	77(8)	70(7)	-5(7)	-17(5)	-20(6)

Table 4. Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for (R)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).

	x	y	z	U(eq)
H(1A)	4520(140)	10110(40)	11420(100)	70
H(1B)	5930(140)	9800(40)	10570(90)	70
H(2A)	3190(150)	9350(50)	10370(100)	83
H(2B)	2220(160)	9900(50)	9990(120)	83
H(3A)	4800(170)	9350(50)	8450(120)	98
H(3B)	2740(180)	9410(50)	8120(120)	98
H(4A)	3050(190)	10340(50)	7860(140)	103
H(4B)	4390(170)	10040(50)	6940(130)	103
H(5A)	5890(150)	10760(40)	7970(100)	83
H(5B)	6770(170)	10200(50)	8390(110)	83
H(6)	4180(120)	10780(30)	9860(90)	57
H(7)	6660(130)	10750(40)	11470(80)	58
H(8A)	9510(190)	10840(60)	10720(140)	112
H(8B)	8850(190)	10850(50)	9290(130)	112
H(8C)	8700(200)	10310(50)	10080(130)	112
H(9A)	5290(180)	11640(50)	8860(130)	86
H(9B)	7390(170)	11600(50)	8750(120)	86
H(9C)	6500(160)	12130(50)	9330(100)	86

Table 4. (continued)

Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for (R)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).

	x	y	z	U(eq)
H(10A)	4910(170)	11520(50)	12140(130)	97
H(10B)	3810(170)	11460(50)	10870(110)	97
H(10C)	4650(170)	12030(50)	11240(120)	97
H(11A)	8000(180)	11640(50)	12170(130)	102
H(11B)	7970(170)	12140(50)	11210(120)	102
H(11C)	9170(180)	11630(50)	10910(130)	102

Umsetzungen chiraler Kationen mit Silberiodid
(S)-(1-Cyclohexylethyl)trimethylammoniumtriiododiargentat(I)
([(S)-$C_{11}H_{24}N$] $^{1}_{\infty}[Ag_2I_3]$)

Table 1. Crystal data and structure refinement for (S)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I)

Diffractometer type	CAD 4	
Empirical formula	$C_{11}H_{24}Ag_2I_3N$	
Formula weight	766.75	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	$P\,2_12_12_1$ (No. 19)	
Unit cell dimensions	a = 742.0(10) pm	α= 90°.
	b = 2446(3) pm	β= 90°.
	c = 1041(2) pm	γ = 90°.
Volume	1.89(1) nm^3	
Z	4	
Density (calculated)	2.696 g/cm^3	
Absorption coefficient	6.959 mm^{-1}	
F(000)	1400	
Crystal size	0.30 x 0.20 x 0.18 mm^3	
Theta range for data collection	1.66 to 24.94°.	
Index ranges	0<=h<=8, 0<=k<=28, -12<=l<=12	
Reflections collected	3832	
Independent reflections	3290 [R(int) = 0.0196]	
Completeness to theta = 24.94°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3290 / 0 / 227	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0320, wR2 = 0.0705	
R indices (all data)	R1 = 0.0567, wR2 = 0.0765	
Absolute structure parameter[99]	0.01(6)	
Extinction coefficient	0.00084(8)	
Largest diff. peak and hole	0.890 and -1.040 e.$Å^{-3}$	
Absorption correction	psi-scan	
Effective transmission (min. / max.)	0.5970 / 0.9856	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	3568(1)	7791(1)	6425(1)	43(1)
I(2)	3591(1)	8278(1)	2310(1)	52(1)
I(3)	-1365(1)	8855(1)	5144(1)	53(1)
Ag(1)	1151(1)	8087(1)	4330(1)	66(1)
Ag(2)	6017(1)	8114(1)	4361(1)	70(1)
N(1)	8523(13)	8510(3)	9438(7)	46(2)
C(1)	10141(18)	9979(5)	9434(12)	56(3)
C(2)	11668(18)	10293(5)	10094(14)	67(3)
C(3)	11210(30)	10415(5)	11479(15)	84(4)
C(4)	10900(20)	9889(6)	12176(16)	90(5)
C(5)	9320(20)	9586(6)	11565(11)	67(4)
C(6)	9723(14)	9450(4)	10159(10)	44(2)
C(7)	8249(15)	9133(4)	9431(10)	49(3)
C(8)	6346(19)	9302(5)	9871(15)	67(3)
C(9)	10212(17)	8360(6)	8725(12)	55(3)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(10)	8550(20)	8270(5)	10749(11)	59(3)
C(11)	6939(16)	8249(6)	8748(14)	65(4)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-Cyclohexylethyl)trimethyl-ammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	34(1)	52(1)	42(1)	1(1)	0(1)	0(1)
I(2)	38(1)	67(1)	51(1)	6(1)	2(1)	-1(1)
I(3)	43(1)	50(1)	66(1)	3(1)	3(1)	4(1)
Ag(1)	50(1)	84(1)	65(1)	4(1)	6(1)	9(1)
Ag(2)	53(1)	88(1)	68(1)	5(1)	-4(1)	-9(1)
N(1)	40(4)	54(5)	45(4)	1(3)	0(5)	-5(5)
C(1)	71(8)	43(6)	53(7)	0(5)	10(6)	-5(6)
C(2)	58(8)	43(6)	100(9)	-1(6)	6(8)	-1(6)
C(3)	89(11)	57(8)	104(11)	-26(7)	-30(10)	21(8)
C(4)	110(14)	86(11)	74(9)	-28(9)	-31(9)	15(9)
C(5)	95(10)	68(9)	36(6)	0(6)	3(6)	2(7)
C(6)	48(6)	45(6)	40(5)	0(5)	-6(5)	7(5)
C(7)	48(7)	55(6)	45(5)	11(5)	-2(5)	3(5)
C(8)	43(6)	52(7)	106(10)	3(7)	7(8)	14(7)
C(9)	57(7)	55(7)	53(7)	-13(6)	8(6)	6(6)
C(10)	56(7)	63(7)	58(6)	21(6)	9(7)	-9(8)
C(11)	45(7)	68(8)	83(9)	-21(8)	-11(6)	-8(6)

Table 4. Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).

	x	y	z	U(eq)
H(1A)	10490(150)	9890(50)	8560(110)	67
H(1B)	9070(150)	10210(40)	9400(100)	67
H(2A)	12770(170)	10080(50)	10060(120)	80
H(2B)	11880(170)	10630(50)	9640(110)	80
H(3A)	12200(200)	10610(60)	11880(140)	100
H(3B)	10140(190)	10640(60)	11520(130)	100
H(4A)	10600(200)	9960(60)	13070(150)	108
H(4B)	12000(200)	9670(60)	12140(160)	108
H(5A)	8250(180)	9810(50)	11610(120)	80
H(5B)	9100(160)	9250(50)	12040(110)	80
H(6)	10820(130)	9230(40)	10140(90)	53
H(7)	8350(150)	9250(40)	8530(90)	59
H(8A)	5500(200)	9180(60)	9250(150)	101
H(8B)	6300(200)	9690(60)	9960(130)	101
H(8C)	6100(200)	9130(60)	10680(130)	101
H(9A)	10240(170)	8550(50)	7910(120)	82
H(9B)	10230(170)	7970(50)	8580(120)	82
H(9C)	11240(180)	8460(50)	9220(110)	82

Table 4. (continued)

Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-Cyclohexylethyl)trimethylammonium-triiododiargentat(I).

	x	y	z	U(eq)
H(10A)	7400(200)	8340(50)	11160(140)	89
H(10B)	9500(190)	8430(50)	11240(140)	89
H(10C)	8730(180)	7880(50)	10690(110)	89
H(11A)	5800(200)	8350(60)	9180(140)	98
H(11B)	7080(190)	7860(60)	8750(130)	98
H(11C)	6900(190)	8380(50)	7880(140)	98

Umsetzungen chiraler Kationen mit Silberiodid
(+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammoniumtriiododiargentat(I) ([(+)-$C_{12}H_{20}NO$] $^{1}_{\infty}$[Ag_2I_3])

Table 1. Crystal data and structure refinement for (+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammoniumtriiododiargentat(I)

Diffractometer type	CAD 4	
Empirical formula	C_{12} H_{20} Ag_2 I_3 N O	
Formula weight	790.73	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Triclinic	
Space group	P 1 (No. 1)	
Unit cell dimensions	a = 724.5(4) pm	α= 72.88(2)°.
	b = 993.8(3) pm	β= 82.47(4)°.
	c = 1580.1(6) pm	γ = 87.87(3)°.
Volume	1.0779(8) nm^3	
Z	2	
Density (calculated)	2.436 g/cm^3	
Absorption coefficient	6.107 mm^{-1}	
F(000)	720	
Crystal size	0.10 x 0.30 x 0.10 mm^3	
Theta range for data collection	1.36 to 25.00°.	
Index ranges	-8<=h<=8, -11<=k<=11, -18<=l<=18	
Reflections collected	7594	
Independent reflections	7594 [R(int) = 0.0000]	
Completeness to theta = 25.00°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7594 / 3 / 344	
Goodness-of-fit on F^2	1.143	
Final R indices [I>2sigma(I)]	R1 = 0.0578, wR2 = 0.1631	
R indices (all data)	R1 = 0.0606, wR2 = 0.1665	
Absolute structure parameter[99]	0.03(5)	
Extinction coefficient	0.0310(12)	
Largest diff. peak and hole	3.869 and -1.470 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammoniumtriiododiargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	9293(1)	770(1)	2048(1)	55(1)
I(2)	14120(1)	-2654(1)	3216(1)	48(1)
I(3)	14846(1)	-440(1)	335(1)	64(1)
I(4)	8667(1)	-1740(1)	4926(1)	52(1)
I(5)	9614(1)	-3596(1)	1822(1)	62(1)
I(6)	3876(1)	1415(1)	3818(1)	71(1)
Ag(1)	11959(2)	-1346(2)	1706(1)	79(1)
Ag(2)	6505(2)	-626(1)	3540(1)	69(1)
Ag(3)	7065(2)	-1378(2)	1708(1)	77(1)
Ag(4)	11481(2)	-555(1)	3540(1)	69(1)
N(1)	8723(14)	3652(12)	4682(9)	53(3)
O(1)	6592(15)	4036(12)	6490(9)	74(3)
C(11)	8410(20)	2643(17)	7946(11)	70(4)
C(12)	9260(30)	2015(19)	8684(13)	80(5)
C(13)	11190(30)	1770(20)	8635(18)	93(6)
C(14)	12300(30)	2300(30)	7789(16)	98(7)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (+)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammoniumtriiododiargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(15)	11470(20)	2920(20)	7034(14)	84(5)
C(16)	9410(20)	3070(15)	7139(11)	59(3)
C(17)	8520(20)	3795(15)	6304(10)	60(3)
C(18)	8672(17)	2804(13)	5713(10)	52(3)
C(19)	7270(20)	1715(18)	6003(14)	77(5)
C(110)	8820(30)	2660(20)	4167(13)	74(4)
C(111)	10448(19)	4548(17)	4403(11)	65(4)
C(112)	7080(20)	4609(19)	4483(14)	75(5)
N(2)	14990(20)	-5429(17)	10581(9)	68(3)
O(2)	14478(16)	-5173(13)	8737(7)	73(3)
C(21)	10920(20)	-4119(16)	-1761(9)	58(3)
C(22)	9360(30)	-3490(20)	-2082(13)	84(5)
C(23)	8680(30)	-2330(20)	-1963(16)	90(6)
C(24)	19660(30)	-1600(20)	-1420(20)	105(8)
C(25)	11220(20)	-2300(18)	8908(12)	68(4)
C(26)	11868(16)	-3497(14)	8766(8)	47(3)
C(27)	13700(18)	-4186(16)	9134(9)	57(3)
C(28)	13246(19)	-4927(16)	10117(10)	59(3)
C(29)	11830(30)	-6060(30)	10362(15)	106(8)
C(210)	14610(30)	-5410(60)	11529(14)	200(20)
C(211)	16700(30)	-4230(30)	10058(19)	118(9)
C(212)	15820(40)	-6790(30)	10470(30)	147(14)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for (+)-(2-Hydroxy-1-methyl-1-phenyl-ethyl)trimethylammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	44(1)	50(1)	67(1)	-12(1)	-13(1)	-1(1)
I(2)	36(1)	56(1)	56(1)	-20(1)	-11(1)	2(1)
I(3)	58(1)	70(1)	64(1)	-17(1)	-14(1)	1(1)
I(4)	40(1)	57(1)	62(1)	-19(1)	-9(1)	3(1)
I(5)	45(1)	81(1)	71(1)	-38(1)	-14(1)	2(1)
I(6)	38(1)	71(1)	115(1)	-43(1)	-16(1)	3(1)
Ag(1)	64(1)	90(1)	86(1)	-31(1)	-12(1)	1(1)
Ag(2)	59(1)	76(1)	78(1)	-27(1)	-18(1)	5(1)
Ag(3)	64(1)	88(1)	86(1)	-31(1)	-21(1)	3(1)
Ag(4)	53(1)	74(1)	83(1)	-29(1)	-4(1)	-2(1)
N(1)	30(5)	55(6)	79(8)	-29(6)	-2(5)	5(4)
O(1)	53(6)	75(7)	100(8)	-38(6)	-13(6)	28(5)
C(11)	78(10)	71(9)	70(10)	-34(8)	-6(8)	-13(8)
C(12)	83(11)	67(10)	86(12)	-15(8)	-10(9)	4(8)
C(13)	88(13)	86(12)	116(17)	-39(12)	-29(12)	2(10)
C(14)	87(13)	132(18)	104(15)	-66(14)	-57(13)	39(13)
C(15)	61(9)	99(13)	95(13)	-40(11)	-5(9)	19(9)
C(16)	58(8)	54(7)	77(9)	-30(6)	-25(7)	9(6)
C(17)	61(8)	54(7)	67(8)	-26(6)	0(7)	24(6)
C(18)	42(6)	43(6)	76(8)	-23(6)	-14(6)	9(5)
C(19)	68(10)	65(9)	107(13)	-41(9)	-5(9)	-18(8)
C(110)	71(9)	89(11)	85(10)	-56(9)	-14(8)	-20(8)
C(111)	40(6)	74(9)	79(10)	-24(8)	6(6)	-10(6)
C(112)	46(7)	76(10)	120(14)	-47(10)	-30(8)	17(7)

Table 3. (continued)

Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (+)-(2-Hydroxy-1-methyl-1-phenyl-ethyl)trimethylammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^*2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
N(2)	64(8)	89(9)	53(7)	-16(6)	-30(6)	19(7)
O(2)	66(6)	93(8)	54(5)	-17(5)	-4(5)	34(6)
C(21)	56(8)	78(9)	42(6)	-20(6)	-7(5)	-8(7)
C(22)	94(13)	80(11)	88(12)	-24(9)	-46(11)	-16(10)
C(23)	95(13)	81(11)	112(15)	-37(11)	-67(12)	27(10)
C(24)	87(13)	68(11)	160(20)	-24(12)	-53(14)	37(10)
C(25)	56(8)	74(9)	85(11)	-35(8)	-19(7)	4(7)
C(26)	35(5)	61(7)	38(5)	-6(5)	-3(4)	0(5)
C(27)	47(7)	68(8)	50(7)	-7(6)	-14(5)	1(6)
C(28)	46(7)	71(8)	55(7)	-10(6)	-11(6)	0(6)
C(29)	59(10)	122(16)	97(14)	31(12)	-7(9)	-23(10)
C(210)	60(12)	440(70)	53(11)	-20(20)	-11(9)	70(20)
C(211)	87(13)	140(20)	140(20)	-30(16)	-70(14)	-33(13)
C(212)	150(20)	120(20)	220(40)	-100(20)	-90(20)	100(20)

Umsetzungen chiraler Kationen mit Silberiodid
(-)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethylammoniumtriiododiargentat(I)
([(-)-$C_{12}H_{20}NO$] $^{1}_{\infty}[Ag_2I_3]$ · ½ C_3H_6O)

Table 1. Crystal data and structure refinement for (-)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammoniumtriiododiargentat(I)

Diffractometer type	CAD 4	
Empirical formula	$C_{13.50}\ H_{26}\ Ag_2\ I_3\ N\ O_{1.50}$	
Formula weight	822.79	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Triclinic	
Space group	P 1 (No. 1)	
Unit cell dimensions	a = 724.1(2) pm	α= 73.01(2)°.
	b = 996.3(3) pm	β= 82.53(2)°.
	c = 1584.6(4) pm	γ = 87.86(2)°.
Volume	1.0840(5) nm^3	
Z	2	
Density (calculated)	2.521 g/cm^3	
Absorption coefficient	6.079 mm^{-1}	
F(000)	758	
Crystal size	0.20 x 0.20 x 0.08 mm^3	
Theta range for data collection	2.71 to 25.01°.	
Index ranges	-8<=h<=8, -11<=k<=11, -18<=l<=18	
Reflections collected	7971	
Independent reflections	7601 [R(int) = 0.0184]	
Completeness to theta = 25.01°	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7601 / 3 / 380	
Goodness-of-fit on F^2	2.312	
Final R indices [I>2sigma(I)]	R1 = 0.1023, wR2 = 0.2340	
R indices (all data)	R1 = 0.1388, wR2 = 0.3070	
Absolute structure parameter[99]	-0.04(10)	
Extinction coefficient	0.0011(7)	
Largest diff. peak and hole	2.948 and -4.623 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (-)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammoniumtriiododiargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	9615(3)	2338(2)	9496(2)	58(1)
I(2)	14786(2)	5766(2)	8325(1)	49(1)
I(3)	4070(3)	3557(3)	11204(2)	66(1)
I(4)	10247(3)	4857(2)	6611(1)	54(1)
I(5)	15034(3)	1704(3)	7725(2)	75(1)
I(6)	9289(3)	6701(2)	9730(2)	64(1)
Ag(1)	12402(4)	3739(3)	7992(2)	74(1)
Ag(2)	6951(5)	4452(4)	9831(2)	83(1)
Ag(3)	7432(4)	3660(3)	8002(2)	72(1)
Ag(4)	11848(5)	4489(3)	9829(2)	79(1)
N(1)	14020(40)	8540(30)	980(20)	73(10)
O(1)	14400(40)	8250(30)	2830(17)	76(7)
C(11)	17930(50)	7240(40)	3270(20)	72(10)
C(12)	19510(50)	6690(40)	3570(30)	82(12)
C(13)	20100(120)	5350(50)	3420(60)	190(40)
C(14)	19380(60)	4930(40)	2900(30)	75(11)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (-)-(2-Hydroxy-1-methyl-1-phenylethyl)trimethyl-ammoniumtriiododiargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(15)	17700(60)	5380(40)	2660(30)	78(10)
C(16)	17000(40)	6630(30)	2790(20)	60(8)
C(17)	15270(40)	7280(30)	2410(20)	55(7)
C(18)	15590(40)	8010(30)	1430(20)	54(7)
C(19)	17070(60)	9250(50)	1200(40)	160(30)
C(110)	14450(90)	8460(70)	50(40)	150(30)
C(111)	12230(80)	7400(60)	1330(40)	124(19)
C(112)	13270(80)	9900(50)	1100(50)	150(30)
N(2)	10240(40)	9460(30)	6860(20)	73(10)
O(2)	12350(30)	9060(30)	5050(20)	84(8)
C(21)	10470(40)	10420(30)	3600(30)	63(9)
C(22)	9690(50)	11140(40)	2800(30)	84(12)
C(23)	7750(70)	11330(40)	2830(40)	108(17)
C(24)	6560(70)	10910(50)	3700(40)	120(20)
C(25)	7620(60)	10220(50)	4520(40)	103(16)
C(26)	9460(40)	9980(30)	4433(19)	51(7)
C(27)	10320(40)	9390(30)	5200(30)	69(10)
C(28)	10150(30)	10200(30)	5900(18)	41(6)
C(29)	11640(50)	11410(30)	5630(30)	87(14)
C(210)	10120(40)	10430(30)	7427(19)	52(7)
C(211)	11890(50)	8470(50)	7050(40)	91(13)
C(212)	8460(40)	8460(40)	7180(20)	65(9)
O(3)	13600(30)	6530(30)	4580(17)	75(7)
C(31)	14690(50)	5770(40)	5040(20)	71(10)
C(32)	15360(70)	6350(70)	5610(30)	130(20)
C(33)	15430(90)	4510(50)	4950(30)	121(19)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for (-)-(2-Hydroxy-1-methyl-1-phenyl-ethyl)trimethylammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	53(1)	42(1)	77(2)	-12(1)	-16(1)	-4(1)
I(2)	43(1)	49(1)	60(1)	-20(1)	-12(1)	-3(1)
I(3)	68(2)	59(1)	72(2)	-16(1)	-15(1)	-4(1)
I(4)	49(1)	47(1)	69(1)	-19(1)	-13(1)	-3(1)
I(5)	47(1)	62(1)	129(2)	-43(2)	-23(1)	1(1)
I(6)	51(1)	74(1)	82(2)	-40(1)	-17(1)	-5(1)
Ag(1)	68(2)	71(2)	91(2)	-30(2)	-21(2)	0(2)
Ag(2)	73(2)	81(2)	99(2)	-33(2)	-10(2)	-8(2)
Ag(3)	63(2)	66(2)	89(2)	-28(2)	-4(2)	-7(1)
Ag(4)	73(2)	78(2)	96(2)	-34(2)	-20(2)	-4(2)
N(1)	70(20)	45(15)	90(20)	-4(14)	10(16)	31(14)
O(1)	79(17)	67(15)	89(17)	-35(13)	-16(13)	35(13)
C(11)	80(20)	70(20)	80(20)	-37(19)	-12(18)	-30(19)
C(12)	60(20)	49(19)	130(40)	-30(20)	-20(20)	-3(16)
C(13)	250(80)	60(30)	240(90)	-70(40)	120(70)	-60(40)
C(14)	100(30)	43(18)	90(30)	-15(18)	-70(20)	20(18)
C(15)	90(30)	50(18)	110(30)	-40(20)	-40(20)	16(17)
C(16)	54(17)	36(14)	80(20)	0(14)	-17(16)	-2(12)
C(17)	52(17)	55(17)	56(17)	-14(14)	0(13)	-4(13)
C(18)	58(18)	53(16)	59(17)	-15(14)	-35(14)	8(13)

Table 3. (continued)

Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for (-)-(2-Hydroxy-1-methyl-1-phenyl-ethyl)trimethylammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^*2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(19)	60(20)	110(30)	210(60)	130(40)	-70(30)	-20(20)
C(110)	200(60)	170(50)	120(40)	-40(40)	-160(40)	80(50)
C(111)	110(40)	120(40)	140(50)	-30(30)	-30(30)	-60(30)
C(112)	120(40)	50(20)	280(80)	-40(40)	-40(50)	50(30)
N(2)	55(17)	70(19)	120(30)	-66(19)	13(16)	-22(14)
O(2)	56(14)	83(17)	130(20)	-53(17)	-29(14)	14(12)
C(21)	46(16)	40(15)	110(30)	-31(17)	-25(18)	-11(13)
C(22)	70(20)	50(20)	130(40)	-50(20)	-10(20)	14(18)
C(23)	100(30)	50(20)	160(50)	0(30)	-10(30)	20(20)
C(24)	130(40)	90(30)	200(60)	-60(30)	-150(40)	30(30)
C(25)	90(30)	90(30)	140(40)	-70(30)	30(30)	-30(20)
C(26)	60(20)	43(14)	50(16)	-13(12)	-17(15)	-3(13)
C(27)	34(15)	38(16)	140(30)	-38(18)	9(17)	-5(12)
C(28)	31(13)	40(14)	50(15)	-10(12)	-9(11)	-2(10)
C(29)	70(20)	46(17)	150(40)	0(20)	-50(20)	-40(17)
C(210)	43(15)	68(18)	56(17)	-28(14)	-20(12)	-21(13)
C(211)	70(20)	90(30)	140(40)	-70(30)	-20(20)	10(20)
C(212)	54(18)	65(19)	59(19)	14(15)	-22(15)	-3(15)
O(3)	56(13)	87(17)	76(16)	-6(13)	-26(12)	-9(12)
C(31)	70(20)	70(20)	60(20)	-12(17)	20(18)	-13(18)
C(32)	90(30)	200(60)	100(30)	-10(40)	-80(30)	-10(30)
C(33)	190(50)	80(30)	70(30)	20(20)	-50(30)	50(30)

Umsetzungen chiraler Kationen mit Silberiodid
(S)-(1-(1-Naphthyl)ethyl)dimethylammoniumtriiododiargentat(I)
([(S)-$C_{14}H_{18}N$] $^{1}_{\infty}[Ag_2I_3]$)

Table 1. Crystal data and structure refinement for (S)-(1-(1-Naphthyl)ethyl)dimethylammonium-triiododiargentat(I)

Diffractometer type	CCD	
Empirical formula	$C_{14}H_{18}Ag_2I_3N$	
Formula weight	796.73	
Temperature	213(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 976.36(7) pm	α= 90°.
	b = 730.48(5) pm	β= 91.254(2)°.
	c = 1361.70(10) pm	γ = 90°.
Volume	0.97095(12) nm^3	
Z	2	
Density (calculated)	2.725 g/cm^3	
Absorption coefficient	6.777 mm^{-1}	
F(000)	724	
Crystal size	0.30 x 0.05 x 0.05 mm^3	
Theta range for data collection	1.50 to 30.03°.	
Index ranges	-13<=h<=13, -10<=k<=10, -18<=l<=18	
Reflections collected	11203	
Independent reflections	5456 [R(int) = 0.0922]	
Completeness to theta = 30.03°	98.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5456 / 1 / 182	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.0923	
R indices (all data)	R1 = 0.0608, wR2 = 0.1116	
Absolute structure parameter[99]	0.03(5)	
Extinction coefficient	0.0061(4)	
Largest diff. peak and hole	1.835 and -1.370 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-(1-Naphthyl)ethyl)dimethylammoniumtriiododiargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	6673(1)	2984(2)	4628(1)	30(1)
I(2)	5546(1)	-1957(2)	2601(1)	31(1)
I(3)	2377(1)	3016(2)	3406(1)	33(1)
Ag(1)	4492(1)	585(1)	3918(1)	44(1)
Ag(2)	5490(1)	439(1)	6116(1)	45(1)
N(1)	10854(6)	3389(9)	6885(6)	37(2)
C(1)	10784(8)	3907(11)	8683(7)	31(2)
C(2)	10643(10)	2427(13)	9304(10)	55(3)
C(3)	11417(11)	2282(18)	10176(10)	79(5)
C(4)	12341(10)	3594(19)	10434(8)	71(5)
C(5)	12530(9)	5134(15)	9825(8)	45(2)
C(6)	11754(8)	5305(10)	8933(6)	30(2)
C(7)	12011(9)	6855(11)	8335(8)	42(2)
C(8)	12956(9)	8100(20)	8618(10)	75(4)
C(9)	13661(9)	7970(30)	9529(12)	86(5)
C(10)	13466(11)	6600(20)	10109(11)	70(4)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-(1-Naphthyl)ethyl)dimethylammoniumtriiododiargentat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(11)	9956(7)	4046(9)	7737(6)	28(2)
C(12)	8571(6)	3130(20)	7719(6)	37(2)
C(13)	10487(10)	4290(20)	5930(8)	61(3)
C(14)	10899(11)	1343(15)	6797(11)	74(5)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-(1-Naphthyl)ethyl)dimethyl-ammoniumtriiododiargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
I(1)	28(1)	25(1)	37(1)	1(1)	0(1)	-1(1)
I(2)	24(1)	31(1)	37(1)	-1(1)	0(1)	-1(1)
I(3)	33(1)	25(1)	41(1)	0(1)	-4(1)	2(1)
Ag(1)	42(1)	36(1)	54(1)	-6(1)	-7(1)	4(1)
Ag(2)	44(1)	37(1)	55(1)	-4(1)	-2(1)	6(1)
N(1)	21(3)	40(6)	50(4)	-19(3)	2(3)	-2(3)
C(1)	22(4)	36(4)	36(5)	-1(4)	2(3)	-3(3)
C(2)	37(5)	53(6)	74(8)	29(5)	-12(5)	-11(4)
C(3)	41(6)	114(10)	83(9)	65(8)	-9(6)	-6(6)
C(4)	37(5)	139(15)	36(6)	31(6)	0(4)	5(6)
C(5)	27(4)	75(6)	34(5)	-15(5)	2(4)	5(4)
C(6)	24(3)	34(4)	30(4)	-5(3)	3(3)	2(3)
C(7)	37(4)	26(4)	60(7)	-3(4)	-11(4)	-4(3)
C(8)	47(5)	41(5)	135(11)	18(11)	-21(6)	-19(8)
C(9)	41(5)	50(6)	165(15)	-53(12)	-24(7)	-2(9)
C(10)	38(5)	89(9)	81(9)	-54(7)	-29(6)	7(6)
C(11)	22(3)	21(3)	43(5)	-8(3)	4(3)	1(3)
C(12)	20(3)	38(4)	52(4)	-6(7)	-1(3)	4(6)
C(13)	42(6)	98(9)	41(7)	-18(6)	-1(5)	-10(5)
C(14)	41(6)	46(6)	136(14)	-56(7)	3(7)	-1(5)

Table 4. Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-(1-Naphthyl)ethyl)dimethylammonium-triiododiargentat(I).

	x	y	z	U(eq)
H(1)	11734	3755	7042	44
H(2)	10013	1499	9137	66
H(3)	11298	1264	10588	95
H(4)	12857	3477	11022	85
H(7)	11520	7011	7740	50
H(8)	13150	9084	8198	89
H(9)	14283	8890	9719	103
H(10)	13934	6545	10719	84
H(11)	9786	5367	7625	34
H(12A)	8127	3327	7083	56
H(12B)	8012	3654	8229	56
H(12C)	8684	1831	7834	56
H(13A)	10477	5604	6016	91

Table 4. (continued)

Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for (S)-(1-(1-Naphthyl)ethyl)dimethylammonium-triiododiargentat(I).

	x	y	z	U(eq)
H(13B)	9588	3875	5708	91
H(13C)	11159	3962	5445	91
H(14A)	11146	813	7430	111
H(14B)	11574	999	6319	111
H(14C)	10005	893	6586	111

Nebenprodukte bei Umsetzungen chiraler Kationen mit Silberiodid
Disilbertriiodoargentat(I) ($Ag_2\ {}^{1}_{\infty}[AgI_3] \cdot x\ CH_3CN$)

Table 1. Crystal data and structure refinement for Disilbertriiodoargentat(I)

Diffractometer type	CAD 4	
Empirical formula	$Ag_3 I_3$	
Formula weight	704.31	
Temperature	293(2) K	
Wavelength	71.070 pm (Mo Kα)	
Crystal system	Orthorhombic	
Space group	P $na2_1$ (No. 33)	
Unit cell dimensions	a = 1457.6(2) pm	α= 90°.
	b = 1527.20(10) pm	β= 90°.
	c = 495.1(2) pm	γ = 90°.
Volume	1.1021(5) nm^3	
Z	4	
Density (calculated)	4.245 g/cm^3	
Absorption coefficient	13.600 mm^{-1}	
F(000)	1200	
Crystal size	0.25 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.67 to 28.00°.	
Index ranges	-14<=h<=19, -20<=k<=20, -6<=l<=6	
Reflections collected	7697	
Independent reflections	2663 [R(int) = 0.0350]	
Completeness to theta = 28.00°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2663 / 0 / 57	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.1448	
R indices (all data)	R1 = 0.0554, wR2 = 0.1521	
Absolute structure parameter[99]	0.0(17)	
Extinction coefficient	0.0015(3)	
Largest diff. peak and hole	2.876 and -1.747 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Disilbertriiodoargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	9737(1)	7867(1)	7470(4)	40(1)
Ag(1)	9260(1)	9804(1)	12519(5)	34(1)
I(2)	11917(1)	6373(1)	2519(5)	45(1)
Ag(2)	7361(1)	6761(1)	7497(5)	34(1)
I(3)	8833(1)	5486(1)	2499(5)	43(1)
Ag(3)	10057(1)	6917(1)	2455(6)	53(1)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Disilbertriiodoargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^*2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	43(1)	42(1)	35(1)	0(1)	1(1)	-3(1)
Ag(1)	37(1)	37(1)	28(1)	0(1)	0(1)	1(1)
I(2)	40(1)	45(1)	50(1)	3(1)	4(1)	1(1)
Ag(2)	29(1)	32(1)	41(1)	2(1)	1(1)	4(1)
I(3)	41(1)	37(1)	51(1)	-2(1)	-6(1)	-2(1)
Ag(3)	51(1)	50(1)	60(1)	10(2)	-1(2)	-2(1)

Nebenprodukte bei Umsetzungen chiraler Kationen mit Silberiodid
Silberdiiodoargentat(I) ($Ag\ {}^{1}_{\infty}[AgI_2] \cdot ½\ CH_3CN$)

Table 1. Crystal data and structure refinement for Silberdiiodoargentat(I)

Diffractometer type	CAD 4	
Empirical formula	$C_2\ H_3\ Ag_4\ I_4\ N$	
Formula weight	980.13	
Temperature	293(2) K	
Wavelength	71.069 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1 (No. 4)	
Unit cell dimensions	a = 470.30(10) pm	α= 90°.
	b = 2024.2(3) pm	β= 105.380(10)°.
	c = 886.0(2) pm	γ = 90°.
Volume	0.8132(3) nm^3	
Z	2	
Density (calculated)	4.003 g/cm^3	
Absorption coefficient	12.297 mm^{-1}	
F(000)	844	
Crystal size	0.34 x 0.07 x 0.04 mm^3	
Theta range for data collection	2.01 to 24.96°.	
Index ranges	0<=h<=5, 0<=k<=24, -10<=l<=10	
Reflections collected	1659	
Independent reflections	1475 [R(int) = 0.0335]	
Completeness to theta = 24.96°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1475 / 1 / 86	
Goodness-of-fit on F^2	1.105	
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.1531	
R indices (all data)	R1 = 0.0603, wR2 = 0.1598	
Absolute structure parameter[99]	0.0(3)	
Extinction coefficient	0.0179(14)	
Largest diff. peak and hole	1.915 and -1.572 e.$Å^{-3}$	
Absorption correction	none	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Silberdiiodoargentat(I). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
I(1)	5905(8)	4773(1)	6803(5)	51(1)
I(2)	4112(8)	7329(1)	13212(5)	51(1)
I(3)	6764(8)	6864(2)	8523(5)	53(1)
Ag(4)	40(12)	6042(3)	15009(10)	49(1)
I(5)	3236(7)	5232(2)	11470(5)	49(1)
Ag(1)	1908(3)	3555(3)	8816(2)	37(1)
Ag(2)	2706(13)	6626(3)	10437(7)	75(2)
Ag(3)	7289(12)	5501(2)	9604(7)	72(2)
N(1)	1860(50)	8454(19)	18740(30)	61(7)
C(1)	1250(50)	8610(30)	17510(30)	43(5)
C(2)	10350(100)	8440(40)	15650(60)	105(18)

Table 3. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Silberdiiodoargentat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
I(1)	50(2)	54(2)	52(2)	5(2)	19(2)	2(1)
I(2)	54(2)	44(1)	53(2)	6(2)	9(2)	1(1)
I(3)	52(2)	52(2)	57(2)	-1(2)	19(2)	-2(2)
Ag(4)	34(1)	47(1)	69(1)	23(1)	18(1)	7(1)
I(5)	44(2)	50(2)	53(2)	-2(2)	12(2)	2(1)
Ag(1)	34(1)	38(1)	40(1)	0(2)	11(1)	-2(2)
Ag(2)	82(4)	87(3)	54(2)	-9(3)	14(2)	-1(2)
Ag(3)	73(4)	63(3)	80(3)	3(3)	23(3)	0(2)

Zwischenprodukte bei der Sandmeyer-Reaktion von Paratoluidin
Tris-(4-Methylphenyldiazonium)octabromopentacuprat(I) ($[C_7H_7N_2]_3\ {}^1_\infty[Cu_5Br_8]$)

Table 1. Crystal data and structure refinement for Tris-(4-Methylphenyldiazonium)octabromopentacuprat(I)

Diffractometer type	CCD	
Empirical formula	$C_{21}\ H_{21}\ Br_8\ Cu_5\ N_6$	
Formula weight	1314.42	
Temperature	163(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Monoclinic	
Space group	P 2_1/n (No. 14)	
Unit cell dimensions	a = 1564.43(15) pm	α= 90°.
	b = 1294.11(13) pm	β= 102.472(2)°.
	c = 1688.87(16) pm	γ = 90°.
Volume	3.3385(6) nm^3	
Z	4	
Density (calculated)	2.615 g/cm^3	
Absorption coefficient	12.733 mm^{-1}	
F(000)	2456	
Crystal size	0.40 x 0.03 x 0.03 mm^3	
Theta range for data collection	1.61 to 20.82°.	
Index ranges	-15<=h<=15, -12<=k<=12, -16<=l<=16	
Reflections collected	17643	
Independent reflections	3502 [R(int) = 0.0427]	
Completeness to theta = 20.82°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3502 / 0 / 362	
Goodness-of-fit on F^2	1.078	
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0882	
R indices (all data)	R1 = 0.0415, wR2 = 0.0918	
Extinction coefficient	0.00011(5)	
Largest diff. peak and hole	2.539 and -1.635 e.$Å^{-3}$	
Absorption correction	sadabs	
Effective transmission (min. / max.)	0.1507 / 0.2366	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Tris-(4-Methylphenyldiazonium)octabromopentacuprat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Br(1)	-30(1)	1946(1)	1716(1)	21(1)
Br(2)	-4600(1)	3764(1)	-720(1)	23(1)
Br(3)	-2605(1)	2751(1)	-1853(1)	30(1)
Br(4)	-2453(1)	1900(1)	391(1)	23(1)
Br(5)	-1605(1)	4688(1)	1586(1)	28(1)
Br(6)	-1961(1)	2091(1)	2866(1)	28(1)
Br(7)	-4718(1)	986(1)	-1289(1)	25(1)
Br(8)	1065(1)	4674(1)	1675(1)	30(1)
Cu(9)	-1733(1)	2800(1)	1610(1)	32(1)
Cu(10)	-3415(1)	2643(1)	-785(1)	34(1)
Cu(11)	-346(1)	2270(1)	3091(1)	34(1)
Cu(12)	-245(1)	3826(1)	1896(1)	54(1)
Cu(13)	-3759(1)	1571(1)	-2197(1)	62(1)
N(11)	6634(5)	5969(7)	302(5)	22(2)
N(12)	6451(5)	5284(7)	608(5)	29(2)
C(11)	6890(6)	6855(7)	-74(5)	20(2)
C(12)	6507(6)	7795(8)	34(5)	24(2)
C(13)	6793(6)	8656(7)	-327(5)	24(2)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Tris-(4-Methylphenyldiazonium)octabromopentacuprat(I).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(14)	7442(6)	8566(8)	-777(5)	24(2)
C(15)	7792(6)	7591(8)	-873(6)	24(2)
C(16)	7529(6)	6726(8)	-530(5)	24(2)
C(17)	7728(6)	9497(8)	-1174(6)	35(3)
N(31)	799(6)	6701(7)	334(5)	27(2)
N(32)	1271(7)	6173(7)	181(5)	41(2)
C(31)	206(6)	7385(7)	585(5)	23(2)
C(32)	356(6)	8430(8)	551(6)	28(2)
C(33)	-219(6)	9080(7)	820(6)	28(2)
C(34)	-915(6)	8682(7)	1136(6)	24(2)
C(35)	-1034(6)	7624(7)	1146(6)	23(2)
C(36)	-479(6)	6950(7)	869(5)	22(2)
C(37)	-1514(6)	9408(8)	1430(6)	33(3)
N(41)	6106(5)	1111(7)	1575(5)	25(2)
N(42)	6513(6)	479(7)	1453(6)	37(2)
C(41)	5560(6)	1921(7)	1721(5)	23(2)
C(42)	5760(6)	2917(8)	1512(6)	29(3)
C(47)	3927(6)	4348(7)	2188(6)	28(2)
C(46)	4851(6)	1665(7)	2051(5)	21(2)
C(45)	4330(5)	2473(7)	2188(5)	19(2)
C(44)	4501(6)	3477(7)	2014(5)	20(2)
C(43)	5210(6)	3689(7)	1667(6)	26(2)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Tris-(4-Methylphenyldiazonium)-octabromopentacuprat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Br(1)	20(1)	22(1)	22(1)	-2(1)	6(1)	1(1)
Br(2)	21(1)	22(1)	26(1)	-4(1)	4(1)	4(1)
Br(3)	19(1)	50(1)	21(1)	-2(1)	8(1)	-8(1)
Br(4)	22(1)	28(1)	19(1)	3(1)	4(1)	-1(1)
Br(5)	27(1)	21(1)	34(1)	2(1)	2(1)	6(1)
Br(6)	20(1)	44(1)	19(1)	5(1)	6(1)	-3(1)
Br(7)	25(1)	19(1)	31(1)	-1(1)	6(1)	0(1)
Br(8)	32(1)	25(1)	40(1)	9(1)	21(1)	5(1)
Cu(9)	40(1)	34(1)	24(1)	1(1)	7(1)	-10(1)
Cu(10)	28(1)	47(1)	29(1)	7(1)	12(1)	15(1)
Cu(11)	28(1)	47(1)	27(1)	2(1)	6(1)	2(1)
Cu(12)	24(1)	42(1)	94(1)	23(1)	5(1)	1(1)
Cu(13)	39(1)	64(1)	80(1)	-37(1)	7(1)	-12(1)
N(11)	13(4)	31(6)	21(5)	-10(4)	2(4)	3(4)
N(12)	23(5)	30(6)	35(6)	-3(5)	8(4)	-4(4)
C(11)	22(6)	29(6)	10(5)	0(4)	2(4)	-4(5)
C(12)	24(6)	38(7)	11(5)	-7(5)	5(4)	10(5)
C(13)	28(6)	32(6)	11(5)	-2(5)	-2(5)	7(5)
C(14)	25(6)	43(7)	4(5)	-6(4)	1(4)	4(5)
C(15)	14(5)	36(7)	23(6)	-9(5)	8(5)	0(5)
C(16)	20(5)	33(6)	17(5)	3(5)	2(5)	1(5)
C(17)	35(6)	36(7)	35(7)	6(5)	8(5)	1(5)
N(31)	30(5)	33(6)	21(5)	1(4)	10(4)	-12(5)
N(32)	62(7)	37(6)	30(6)	2(5)	23(5)	-2(5)

Table 3. (continued)

Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Tris-(4-Methylphenyldiazonium)-octabromopentacuprat(I). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^* 2U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(31)	24(6)	25(6)	22(6)	-1(5)	9(5)	-1(5)
C(32)	29(6)	30(7)	24(6)	6(5)	8(5)	-6(5)
C(33)	37(6)	22(6)	22(6)	-2(5)	3(5)	0(5)
C(34)	21(6)	24(6)	22(6)	4(4)	-5(5)	3(5)
C(35)	17(5)	28(7)	23(6)	6(5)	0(5)	-4(5)
C(36)	31(6)	18(6)	19(6)	0(4)	9(5)	-3(5)
C(37)	28(6)	33(6)	37(6)	7(5)	7(5)	4(5)
N(41)	24(5)	26(5)	30(5)	3(4)	15(4)	-3(4)
N(42)	35(6)	28(6)	58(7)	-2(5)	30(5)	-5(5)
C(41)	22(6)	24(6)	22(6)	-4(4)	3(5)	8(5)
C(42)	18(6)	36(7)	37(7)	8(5)	11(5)	3(5)
C(47)	29(6)	27(6)	27(6)	0(5)	4(5)	2(5)
C(46)	22(6)	21(6)	24(6)	-6(4)	10(5)	-10(5)
C(45)	12(5)	32(7)	13(5)	-10(4)	7(4)	-4(5)
C(44)	19(5)	22(6)	16(5)	7(4)	-1(4)	-3(4)
C(43)	30(6)	23(6)	25(6)	9(4)	7(5)	4(5)

Table 4. Calculated hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($pm^2 x\ 10^{-1}$) for Tris-(4-Methylphenyldiazonium)octabromopentacuprat(I).

	x	y	z	U(eq)
H(12)	6068	7848	342	29
H(13)	6544	9313	-268	29
H(15)	8226	7529	-1186	29
H(16)	7769	6066	-598	29
H(17A)	8180	9299	-1467	53
H(17B)	7966	10013	-761	53
H(17C)	7225	9791	-1557	53
H(32)	836	8692	352	33
H(33)	-146	9807	791	33
H(35)	-1510	7353	1349	28
H(36)	-562	6223	873	27
H(37A)	-1320	10120	1377	49
H(37B)	-1508	9262	2000	49
H(37C)	-2110	9321	1106	49
H(42)	6246	3058	1276	35
H(47A)	4144	5005	2020	42
H(47B)	3939	4370	2770	42
H(47C)	3325	4236	1887	42
H(46)	4731	971	2175	26
H(45)	3835	2330	2411	22
H(43)	5318	4382	1532	31

Zwischenprodukte bei der Sandmeyer-Reaktion von Paratoluidin
Bis-(4-Methylphenyldiazonium)tetrabromocuprat(II) ($[C_7H_7N_2]_2$ $[CuBr_4]$)

Table 1. Crystal data and structure refinement for Bis-(4-Methylphenyldiazonium)tetrabromocuprat(II)

Diffractometer type	CAD 4	
Empirical formula	C_{14} H_{14} Br_4 Cu N_4	
Formula weight	621.47	
Temperature	173(2) K	
Wavelength	71.073 pm (Mo Kα)	
Crystal system	Triclinic	
Space group	P –1 (No. 2)	
Unit cell dimensions	a = 736.7(2) pm	α= 87.97(2)°.
	b = 1095.0(2) pm	β= 79.57(4)°.
	c = 1269.4(2) pm	γ = 74.73(4)°.
Volume	0.9715(4) nm^3	
Z	2	
Density (calculated)	2.125 g/cm^3	
Absorption coefficient	9.353 mm^{-1}	
F(000)	590	
Crystal size	0.30 x 0.05 x 0.04 mm^3	
Theta range for data collection	3.04 to 24.97°.	
Index ranges	-8<=h<=6, -12<=k<=12, -15<=l<=0	
Reflections collected	3448	
Independent reflections	3298 [R(int) = 0.0193]	
Completeness to theta = 24.97°	96.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3298 / 0 / 209	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0599, wR2 = 0.1527	
R indices (all data)	R1 = 0.0706, wR2 = 0.1602	
Extinction coefficient	0.0010(10)	
Largest diff. peak and hole	2.743 and -2.009 e.$Å^{-3}$	
Absorption correction	psi-scan	
Effective transmission (min. / max.)	0.5586 / 0.9801	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis-(4-Methylphenyldiazonium)tetrabromocuprat(II).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	1815(1)	2505(1)	2192(1)	16(1)
Br(1)	2425(1)	3988(1)	827(1)	25(1)
Br(2)	1712(2)	796(1)	1104(1)	29(1)
Br(3)	-881(1)	2501(1)	3512(1)	23(1)
Br(4)	3992(1)	2629(1)	3317(1)	22(1)
N(11)	7142(13)	3722(8)	1205(6)	36(2)
N(12)	6398(10)	4547(7)	1700(6)	22(2)
C(11)	5483(11)	5633(7)	2326(6)	19(2)
C(12)	5630(12)	5616(7)	3393(6)	20(2)
C(13)	4810(12)	6747(8)	3961(6)	20(2)
C(14)	3889(12)	7834(8)	3468(7)	22(2)
C(15)	3726(12)	7770(8)	2386(7)	24(2)
C(16)	4529(13)	6689(8)	1790(6)	25(2)
C(17)	3061(14)	9054(8)	4083(7)	31(2)
N(21)	-3348(14)	1099(7)	990(6)	39(2)
N(22)	-2787(11)	270(7)	1494(6)	26(2)
C(21)	-2101(12)	-775(7)	2100(6)	19(2)
C(22)	-2095(12)	-582(7)	3162(7)	21(2)

Table 2. (continued)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for Bis-(4-Methylphenyldiazonium)tetrabromocuprat(II).
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(23)	-1442(13)	-1626(8)	3747(6)	24(2)
C(24)	-719(12)	-2829(7)	3275(6)	21(2)
C(25)	-760(13)	-2968(7)	2183(7)	25(2)
C(26)	-1466(14)	-1950(8)	1584(6)	27(2)
C(27)	22(13)	-3952(9)	3921(7)	30(2)

Table 3. Anisotropic displacement parameters (pm^2x 10^{-1}) for Bis-(4-Methylphenyldiazonium)-tetrabromocuprat(II). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Cu(1)	15(1)	18(1)	14(1)	3(1)	-1(1)	-1(1)
Br(1)	32(1)	21(1)	18(1)	7(1)	1(1)	-2(1)
Br(2)	51(1)	20(1)	18(1)	1(1)	-9(1)	-8(1)
Br(3)	16(1)	26(1)	25(1)	3(1)	2(1)	-2(1)
Br(4)	18(1)	29(1)	19(1)	1(1)	-6(1)	-4(1)
N(11)	48(5)	34(5)	26(4)	-5(4)	-7(4)	-9(4)
N(12)	20(4)	20(4)	27(4)	1(3)	-6(3)	-5(3)
C(11)	15(4)	14(4)	23(4)	-3(3)	2(3)	2(3)
C(12)	18(4)	19(4)	23(4)	5(3)	-2(3)	-7(3)
C(13)	22(4)	25(4)	14(4)	2(3)	3(3)	-8(3)
C(14)	16(4)	20(4)	28(4)	-5(3)	2(3)	-7(3)
C(15)	23(5)	18(4)	23(4)	5(3)	0(4)	5(3)
C(16)	26(5)	33(5)	16(4)	9(3)	-6(3)	-6(4)
C(17)	39(6)	21(4)	26(5)	-3(4)	7(4)	-4(4)
N(21)	61(6)	20(4)	25(4)	1(3)	3(4)	4(4)
N(22)	25(4)	22(4)	25(4)	-6(3)	9(3)	-4(3)
C(21)	18(4)	10(4)	25(4)	4(3)	3(3)	-2(3)
C(22)	22(5)	15(4)	23(4)	-5(3)	2(3)	-3(3)
C(23)	30(5)	24(4)	15(4)	-2(3)	-2(3)	-4(4)
C(24)	22(5)	17(4)	20(4)	3(3)	-2(3)	0(3)
C(25)	30(5)	13(4)	26(4)	1(3)	4(4)	-2(3)
C(26)	35(5)	25(5)	15(4)	0(3)	-2(4)	0(4)
C(27)	27(5)	30(5)	29(5)	7(4)	-7(4)	-1(4)

Table 4. Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for Bis-(4-Methylphenyldiazonium)tetrabromocuprat(II).

	x	y	z	U(eq)
H(12)	6245	4887	3716	24
H(13)	4876	6780	4684	24
H(15)	3053	8484	2069	29
H(16)	4451	6651	1069	30
H(17A)	2086	8950	4666	46
H(17B)	2514	9703	3618	46
H(17C)	4051	9291	4359	46
H(22)	-2517	224	3470	25
H(23)	-1480	-1533	4477	29

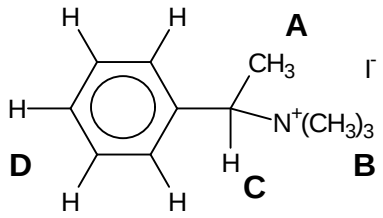
Table 4. (continued)

Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1}) for Bis-(4-Methylphenyldiazonium)tetrabromocuprat(II).

	x	y	z	U(eq)
H(25)	-299	-3766	1862	30
H(26)	-1519	-2039	865	32
H(27A)	1124	-3856	4180	45
H(27B)	371	-4703	3483	45
H(27C)	-952	-4020	4518	45

9.2 Anhang B Kernresonanz-Spektren

(1-Phenylethyl)trimethylammoniumiodid **5**



Im Spektrum des Rohproduktes ist gut zu erkennen, daß es sich nicht um die reine Substanz **5** handeln kann.

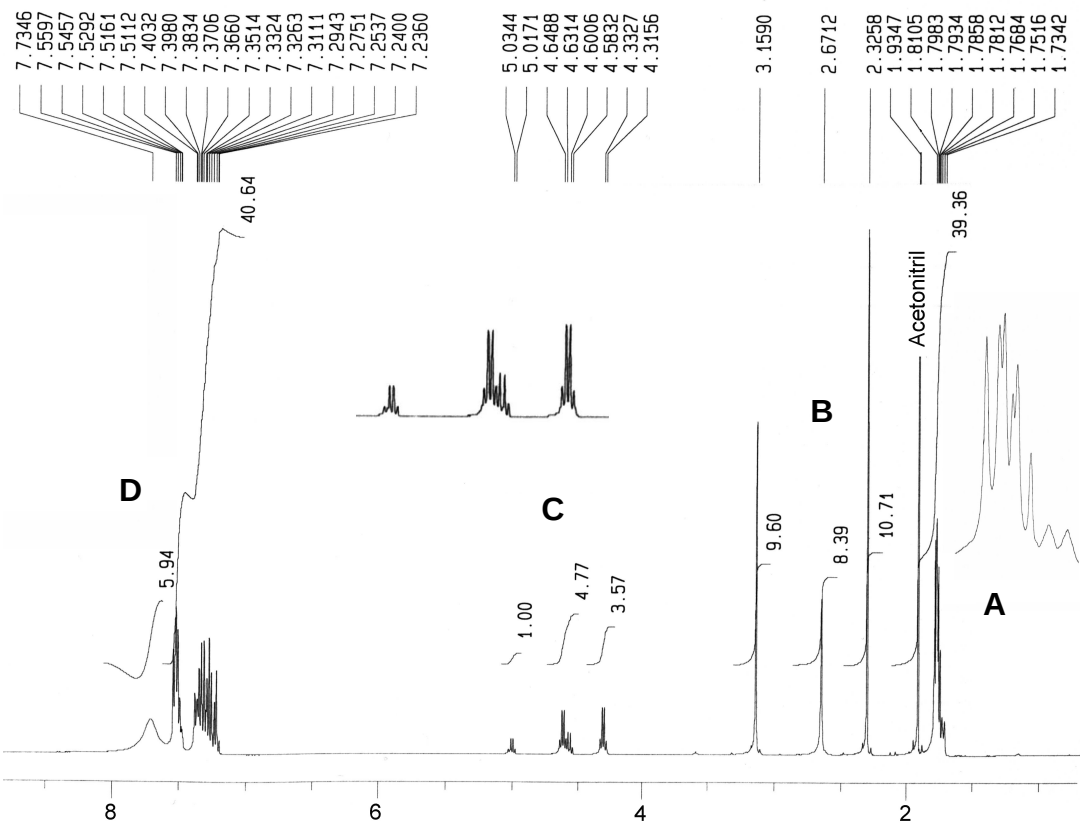


Abb. 60 ^{1}H-Kernresonanzspektrum des Rohproduktgemisches von **5** in $CDCl_3$

Statt des für die A-Wasserstoffatome erwarteten Dubletts und des für das C-Wasserstoffatom erwartete Quartett findet man jeweils vier teilweise überlagerte Dubletts (A) bzw. Quartetts (C). Anstelle des Singuletts für die B-Wasserstoffatome erscheinen drei Singuletts. Diese Erscheinungen sind auf das Vorliegen von vier verschiedenen Verbindungen zurückzuführen: das dreifach methylierte, das zweifach

methylierte und das einfach methylierte Ammoniumiodid und das Hydroiodid des Amins. Nach der Reinigung des Rohproduktes findet man das für **5** erwartete NMR-Spektrum mit einem Dublett (A), einem Singulett (B), einem Quartett (C) und einem Multiplett (D).

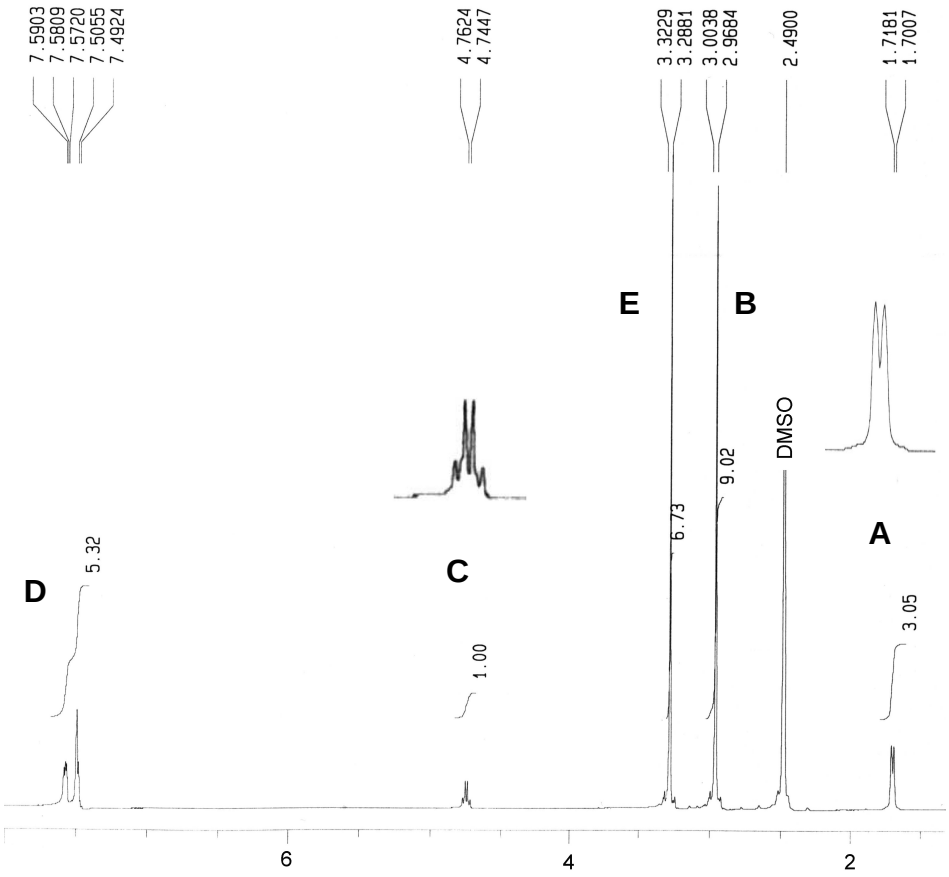
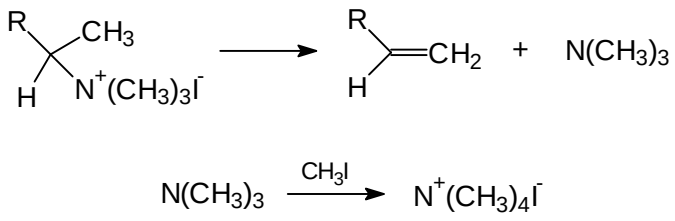


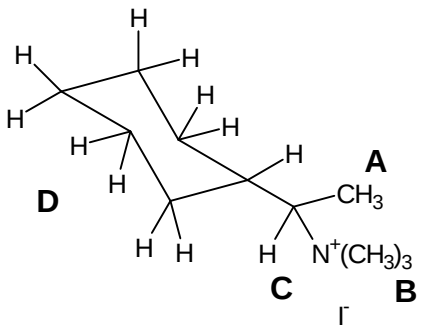
Abb. 61 ^{1}H-Kernresonanzspektrum von (1-Phenyl-ethyl)trimethylammoniumiodid in DMSO (D_6)

Allerdings ist noch ein weiteres Singulett vorhanden (E). Es handelt sich hierbei um die Resonanz von Wasserstoffatomen des durch die Hofmann-Umlagerung entstehenden Nebenproduktes Tetramethylammoniumiodid (s. Reaktionsschema 7).



Reaktionsschema 7 Nebenprodukte aus der Hofmann-Umlagerung

(1-Cyclohexylethyl)trimethylammoniumiodid **6**



Das NMR-Spektrum des Rohproduktes der Umsetzung zu Verbindung **6** zeigt ebenfalls die Verunreinigung durch zweifach und einfach methyliertes Ammoniumiodid und das Hydroiodid des Amins.

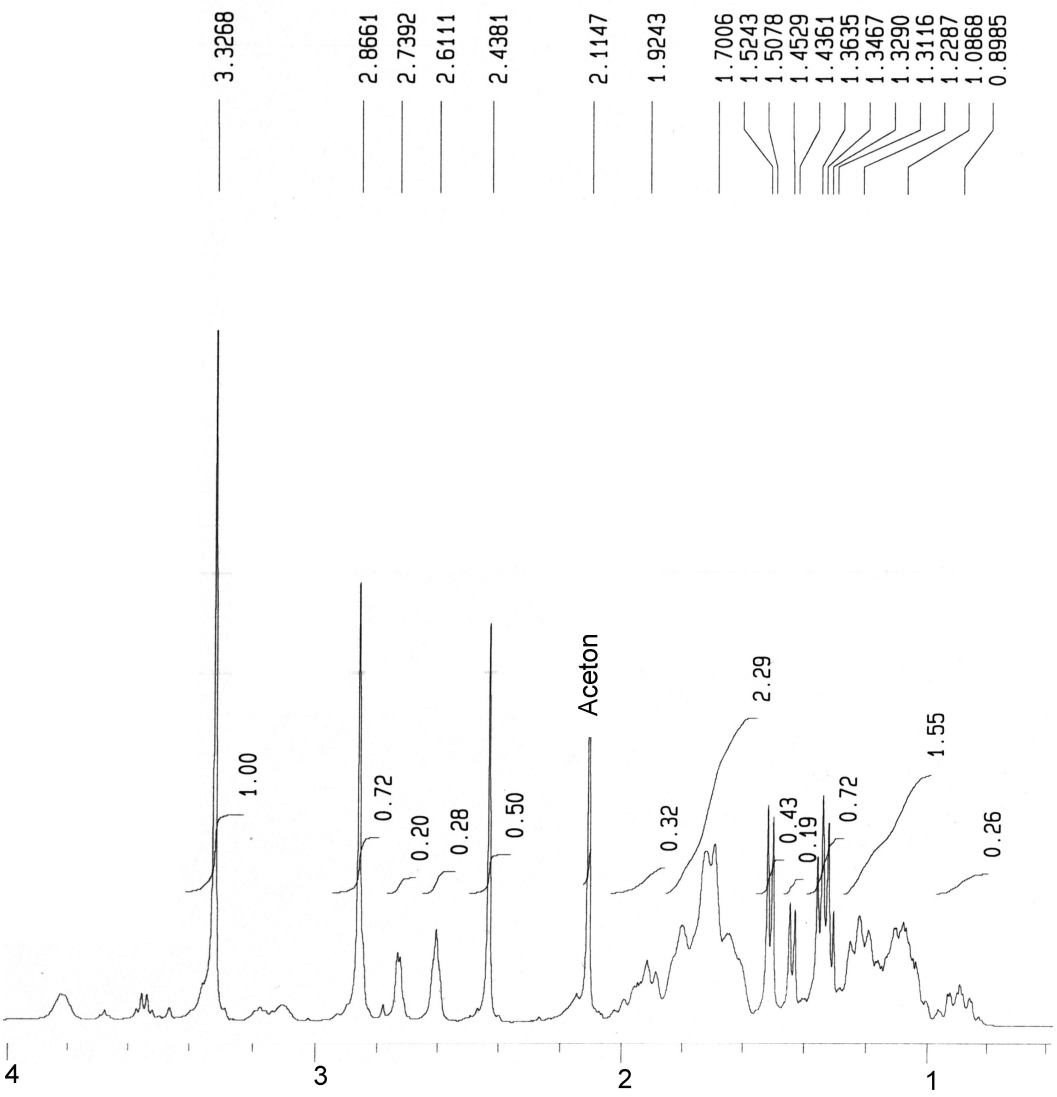


Abb. 62 ^{1}H-Kernresonanzspektrum des Produktgemisches von **6** in DMSO (D_6)

Nach der Aufarbeitung weist das NMR-Spektrum nur noch die erwarteten Peaks auf: ein Dublett (A), ein Singulett (B), ein Quartett (C) und vier Multipletts (D) für die Wasserstoffatome am Cyclohexylring. Das Singulett des Nebenproduktes Tetramethylammoniumiodid aus der Hofmann-Umlagerung ist nicht vorhanden.

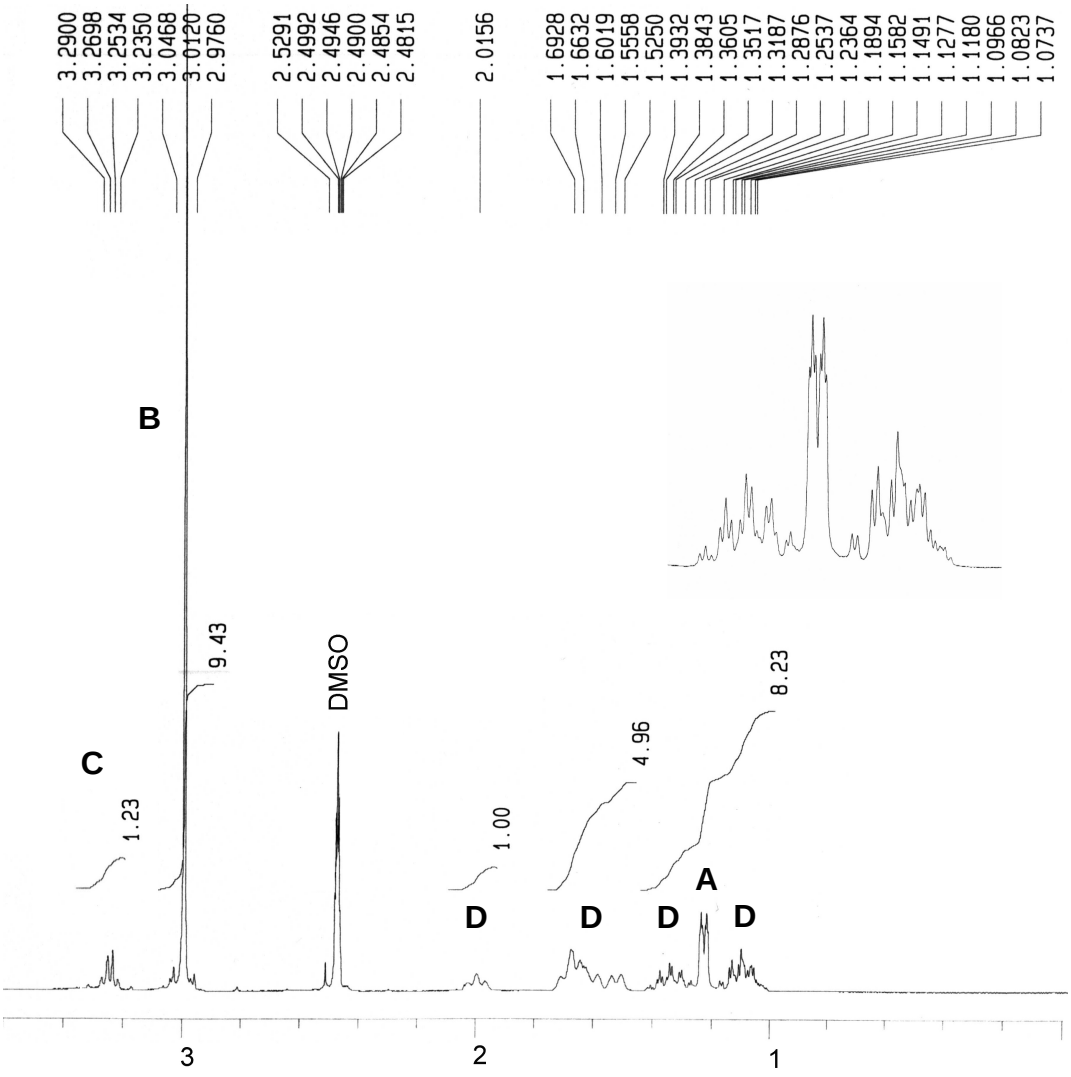
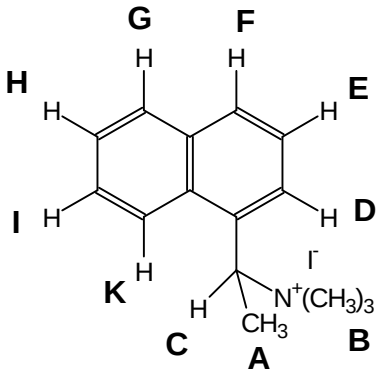


Abb. 63 ^{1}H-Kernresonanzspektrum von (1-Cyclohexyl-ethyl)trimethylammoniumiodid in DMSO (D_6)

(1-(1-Naphthyl)ethyl)trimethylammoniumiodid **8**



Das NMR-Spektrum der Verbindung **8** nach der Reinigung des Rohproduktes zeigt für die A-Wasserstoffatome das erwartete Dublett, für die B-Wasserstoffatome ein Singulett, für das C-Wasserstoffatom ein Quartett und für die Wasserstoffatome des Naphthylliganden vier Dubletts (D, F, G und K) und ein Multiplett (E, H und I).

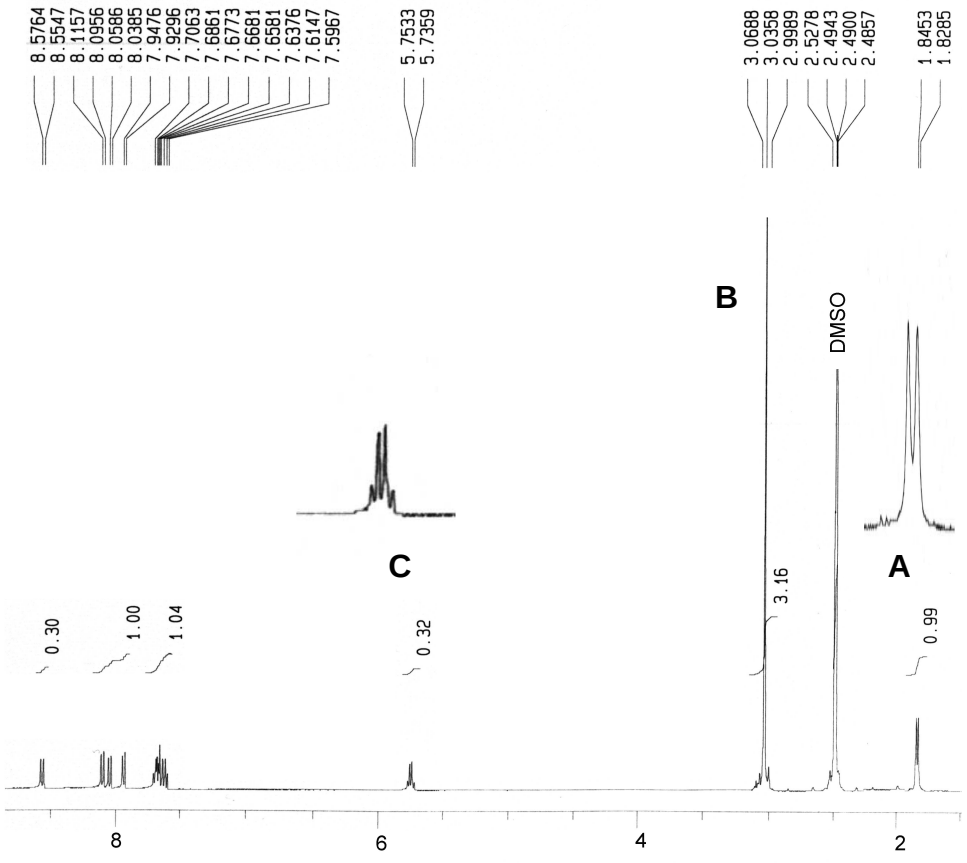


Abb. 64 ^{1}H-Kernresonanzspektrum von (1-(1-Naphthyl)-ethyl)trimethylammoniumiodid in DMSO (D_6)

Auch hier ist kein Nebenprodukt aus der Hofmann-Umlagerung vorhanden.

9.3 Anhang C Verwendete Chemikalien

(R)-1-Phenylethylamin, Art.-Nr. 807031, Fa. MERCK-Schuchardt
(S)-1-Phenylethylamin, Art.-Nr. 807047, Fa. MERCK-Schuchardt
(R)-1-Cyclohexylethylamin, Art.-Nr. 29285, Fa. Fluka Chemika
(S)-1-Cyclohexylethylamin, Art.-Nr. 29287, Fa. Fluka Chemika
(+)-2-Dimethylamino-1-phenylpropanol, Art.-Nr. 66892, Fa. Fluka Chemika
(-)-2-Dimethylamino-1-phenylpropanol, Art.-Nr. 66893, Fa. Fluka Chemika
(R)-1-(1-Naphthyl)ethylamin, Art.-Nr. 9451, Fa. Lancaster
(S)-1-(1-Naphthyl)ethylamin, Art.-Nr. 9461, Fa. Lancaster
Methyliodid, Art.-Nr. 806064, Fa. MERCK-Schuchardt
Natriumcarbonat, Art.-Nr. 6392, Fa. MERCK

Kupferiodid, Art.-Nr. 2748, Fa. MERCK
Silberiodid, Art.-Nr. 10217, Fa. Riedel-de-Haen

Aceton z. S., Fa. MERCK
Acetonitril p. A., Fa. MERCK
Diethylether z. S., Fa. MERCK
Dimethylsulfoxid z. S., Fa. MERCK
Methylenchlorid z. S., Fa. MERCK
Toluol z. S., Fa. MERCK

p-Toluidin, Art.-Nr. 808315, Fa. MERCK-Schuchardt
Kupfer(II)sulfat, Art.-Nr. 12852, Fa. Riedel-de-Haen
Natriumbromid, Art.-Nr. 6520, Fa. MERCK
Natriumsulfit, Art.-Nr. 14451, Fa. Lancaster
Natriumnitrit, Art.-Nr. 822285, Fa. MERCK-Schuchardt
Bromwasserstoffsäure 47%, Fa. MERCK