Preparation of Aminomethyl Functionalised Silanes via an α-Lithiated Amine: From their Synthesis, Stability and Crystal Structures to Stereochemical Issues

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1. NMR-spectra

1.1. ^{1}H-NMR spectrum of compound (*R*,*R*)-3 and its $ZnBr_2$ complex

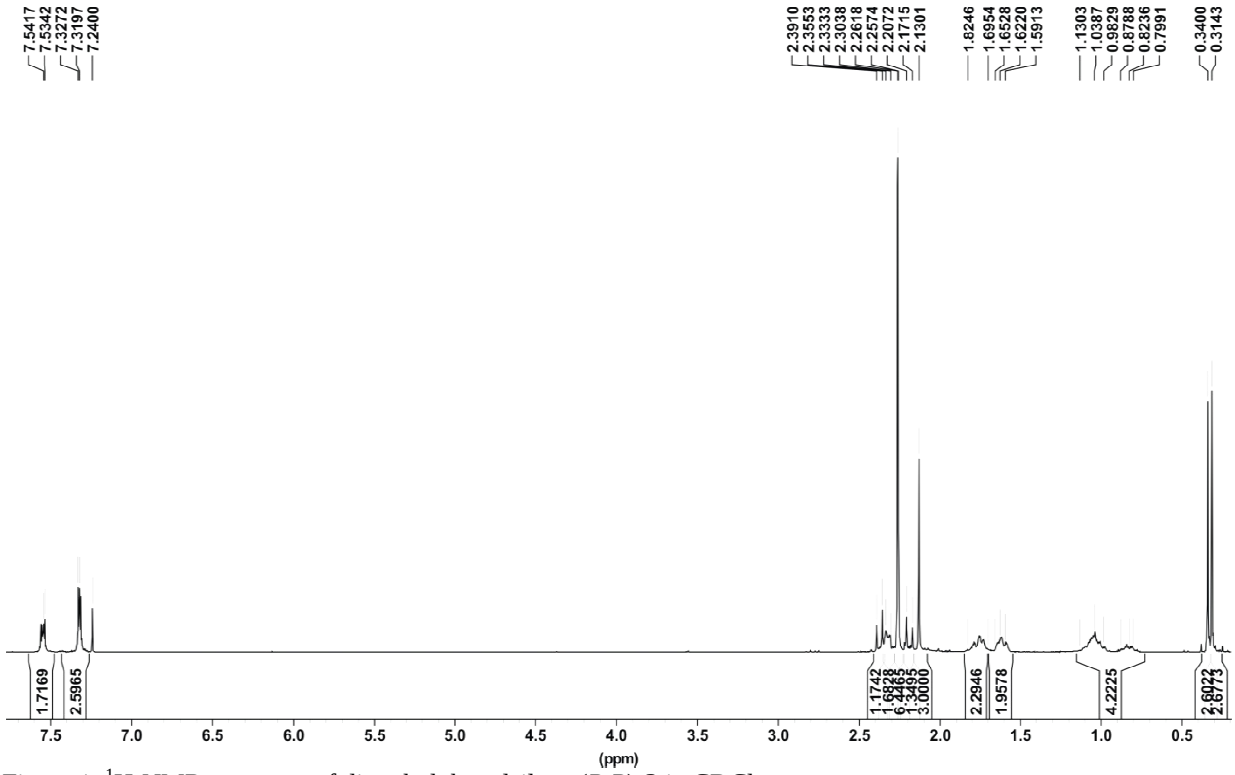

Figure 1. ^{1}H-NMR spectrum of dimethylphenylsilane (*R*,*R*)-**3** in $CDCl_3$.

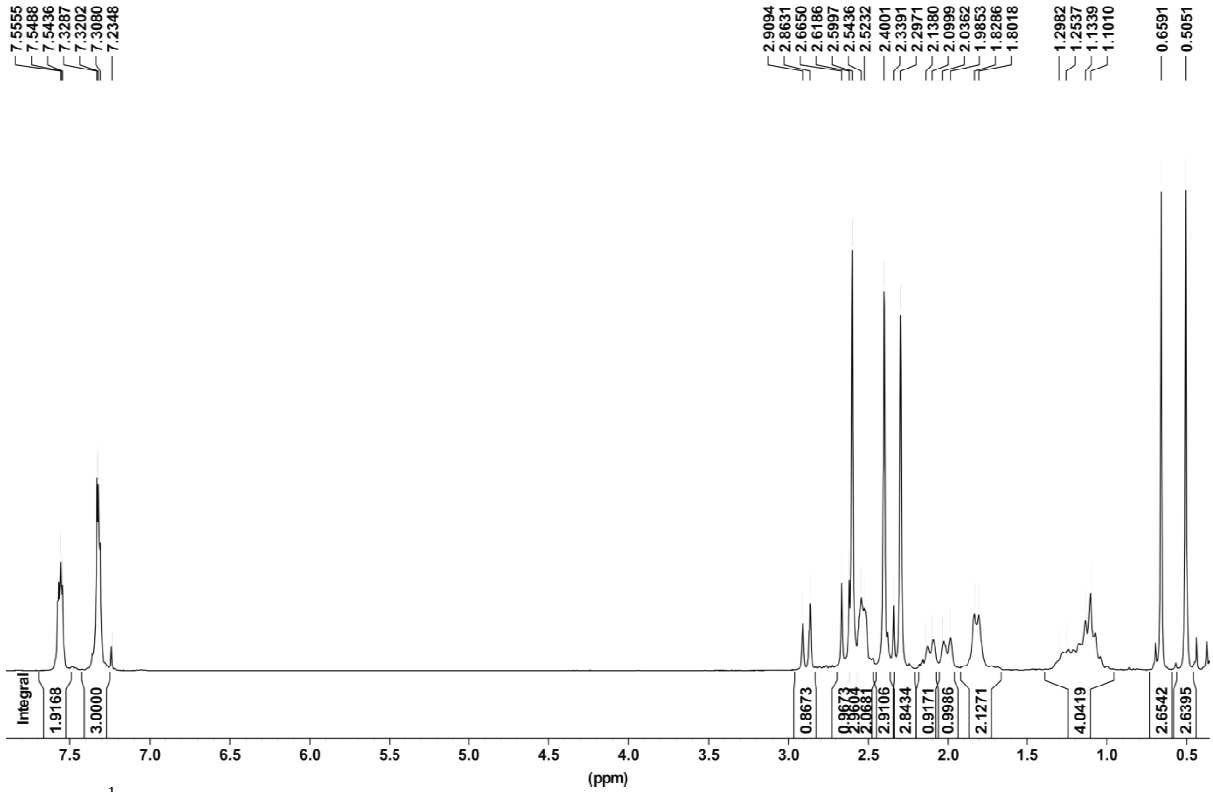

Figure 2. ^{1}H-NMR spectrum of the zinc(II) bromide complex of dimethylphenylsilane (*R*,*R*)-**3** in $CDCl_3$; splitting of the NMe_2 units.

1.2. ^{1}H-NMR spectrum of compound (*R*,*R*)-4 and its $ZnBr_2$ complex

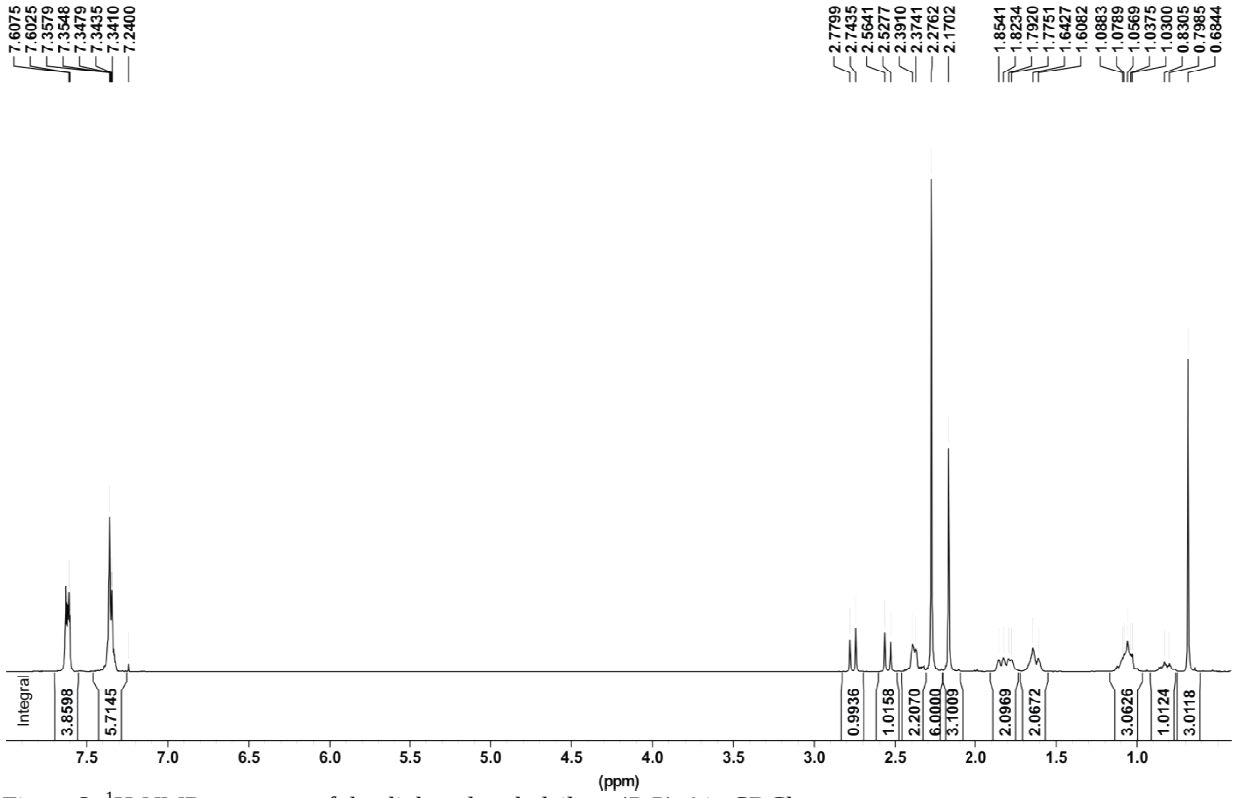

Figure 3. ^{1}H-NMR spectrum of the diphenylmethylsilane (*R*,*R*)-**4** in $CDCl_3$.

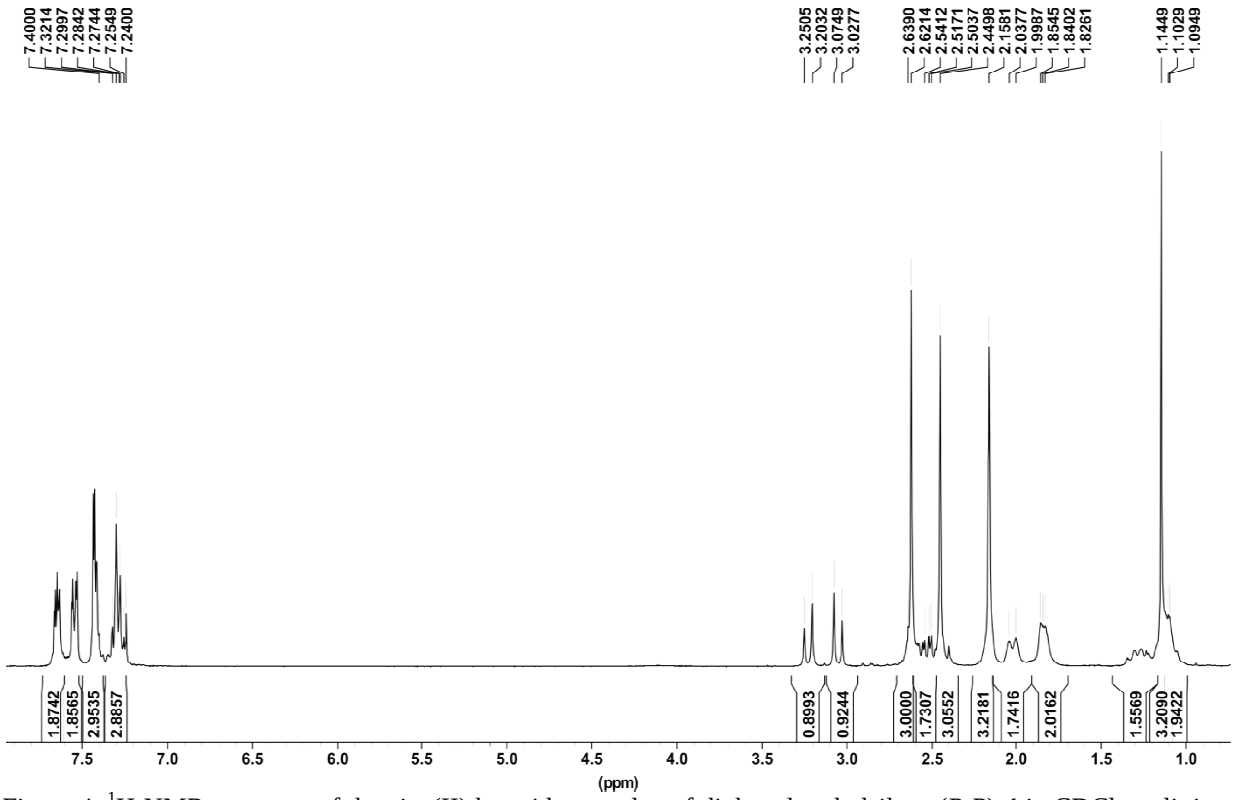

Figure 4. ^{1}H-NMR spectrum of the zinc(II) bromide complex of diphenylmethylsilane (*R*,*R*)-**4** in $CDCl_3$; splitting of the NMe_2 units.

1.3. ^{1}H-NMR spectrum of the transmetallation products compound (*R*,*R*)-7 and (*R*,*R*)-8

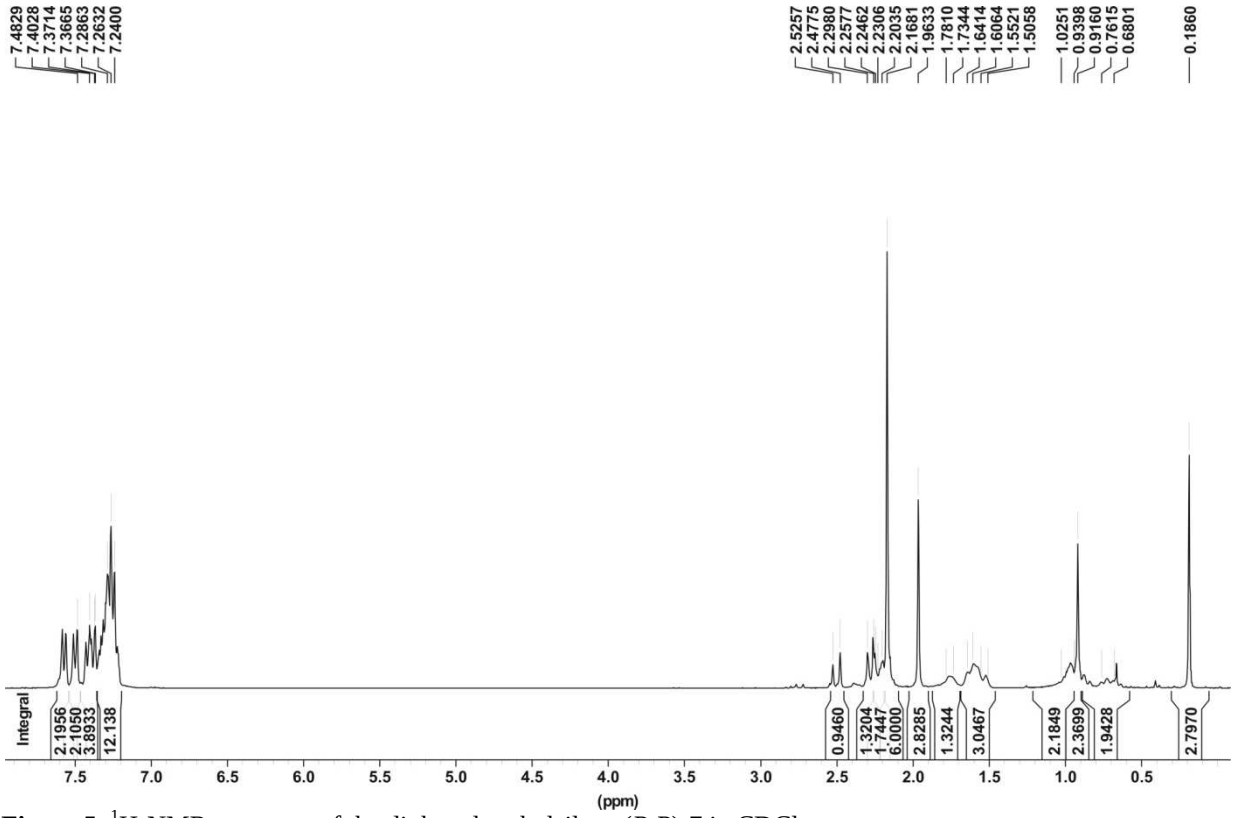

Figure 5. ^{1}H-NMR spectrum of the diphenylmethylsilane (*R*,*R*)-**7** in $CDCl_3$.

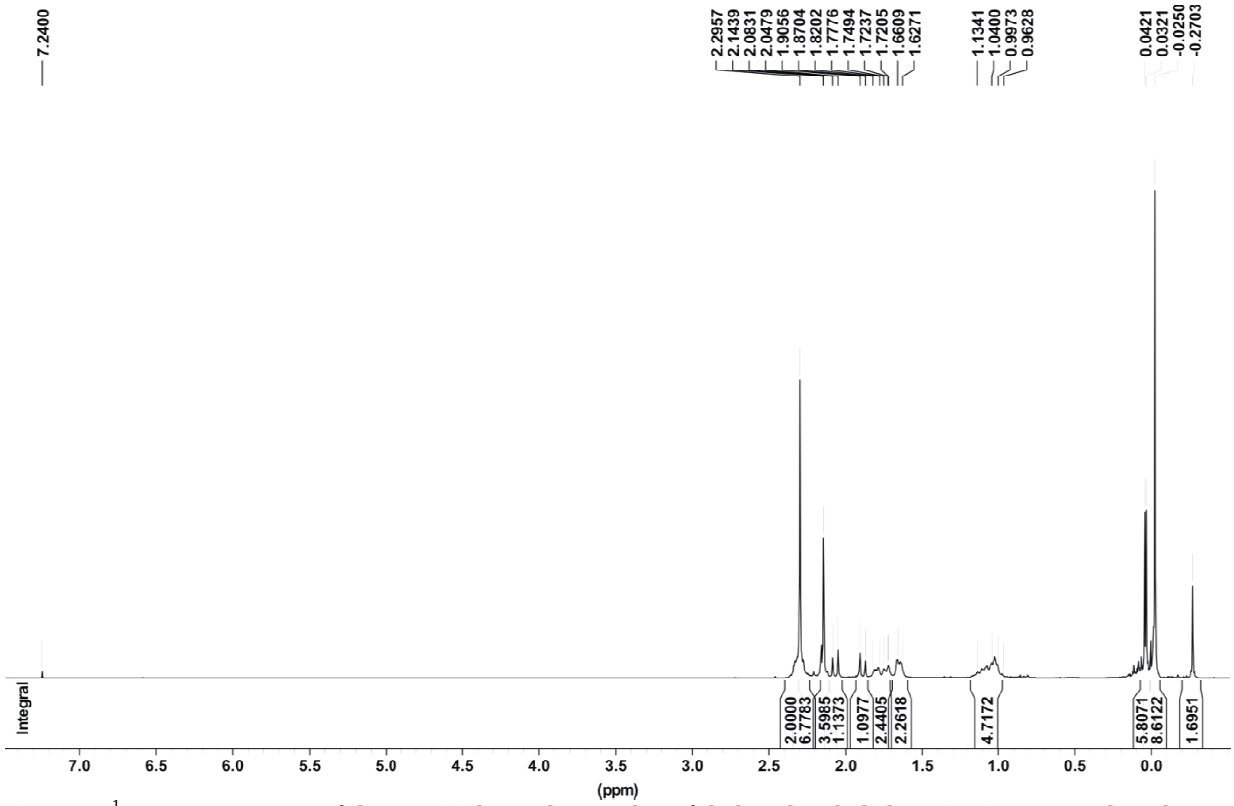

Figure 6. ^{1}H-NMR spectrum of the zinc(II) bromide complex of diphenylmethylsilane (*R*,*R*)-**4** in $CDCl_3$; splitting of the NMe_2 units.

Crystal Structure Determination

2.1 Crystallographic data for compound (*R*,*R*)-5

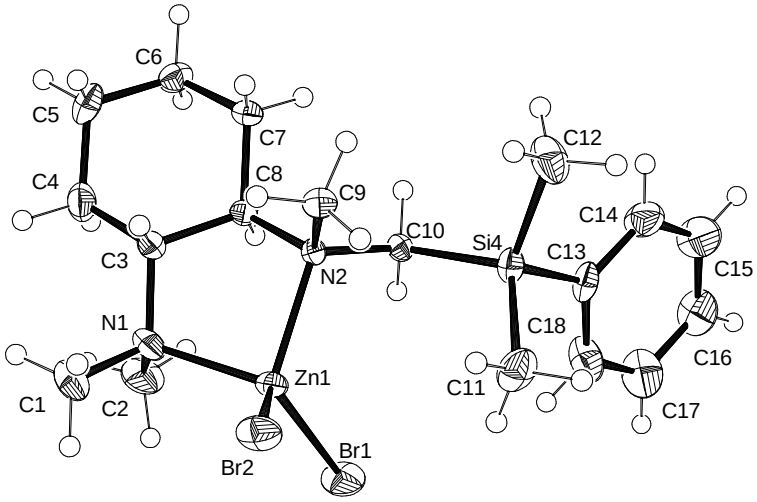

Figure 7. ORTEP plot of (*R*,*R*)-**5** at 50 % probability level.

Table S1 Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for compound (*R*,*R*)-**5**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	2882(1)	11830(1)	9213(1)	21(1)
Br(1)	4539(1)	11620(1)	8211(1)	39(1)
Br(2)	1583(1)	13951(1)	8689(1)	32(1)
Si(4)	1605(1)	8589(1)	6902(1)	24(1)
N(1)	3310(2)	11745(4)	11008(3)	29(1)
C(8)	2423(3)	9080(4)	10546(3)	16(1)
C(3)	2516(3)	10469(4)	11409(3)	21(1)
C(7)	1676(3)	7713(4)	10957(3)	22(1)
C(5)	2006(3)	8649(5)	12992(3)	33(1)
C(4)	2850(4)	9920(5)	12658(3)	34(1)
C(6)	2038(3)	7221(4)	12201(3)	26(1)
N(2)	1996(2)	9669(3)	9340(2)	15(1)
C(13)	2549(3)	7242(4)	6091(3)	28(1)
C(10)	2311(3)	8483(4)	8454(3)	17(1)
C(9)	719(3)	9961(4)	9196(3)	20(1)
C(14)	2154(4)	5758(5)	5687(4)	41(1)
C(2)	4568(3)	11361(6)	11297(4)	45(1)
C(1)	3076(4)	13298(5)	11539(4)	47(1)
C(12)	66(3)	7769(5)	6745(4)	41(1)
C(18)	3611(3)	7782(5)	5813(4)	41(1)

C(11)	1601(4)	10627(5)	6241(4)	39(1)
C(17)	4267(3)	6886(6)	5117(4)	49(1)
C(16)	3858(4)	5418(5)	4705(4)	45(1)
C(15)	2816(4)	4862(5)	4993(4)	50(1)

Table S2 Anisotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	20(1)	17(1)	28(1)	-1(1)	8(1)	-2(1)
Br(1)	24(1)	42(1)	54(1)	-3(1)	20(1)	-4(1)
Br(2)	35(1)	18(1)	46(1)	3(1)	13(1)	5(1)
Si(4)	27(1)	26(1)	17(1)	-2(1)	0(1)	3(1)
N(1)	29(2)	22(2)	37(2)	-6(2)	1(1)	-9(2)
C(8)	12(2)	19(2)	19(2)	-2(2)	1(1)	-1(1)
C(3)	20(2)	22(2)	22(2)	-3(2)	2(2)	-4(1)
C(7)	21(2)	21(2)	25(2)	0(2)	5(2)	-1(1)
C(5)	43(2)	42(2)	16(2)	4(2)	7(2)	5(2)
C(4)	45(2)	31(2)	25(2)	-6(2)	1(2)	-1(2)
C(6)	27(2)	28(2)	24(2)	6(2)	3(2)	-1(2)
N(2)	16(1)	14(1)	15(2)	-2(1)	0(1)	0(1)
C(13)	38(2)	29(2)	16(2)	-1(2)	1(2)	11(2)
C(10)	16(2)	17(2)	20(2)	-2(1)	2(1)	0(1)
C(9)	14(2)	20(2)	27(2)	1(2)	4(2)	1(1)
C(14)	53(3)	31(2)	44(3)	-3(2)	23(2)	-2(2)
C(2)	32(2)	59(3)	42(3)	2(2)	-10(2)	-22(2)
C(1)	68(3)	31(2)	42(3)	-12(2)	10(2)	-13(2)
C(12)	28(2)	48(3)	44(3)	-10(2)	-6(2)	2(2)
C(18)	27(2)	50(3)	43(3)	-17(2)	-2(2)	1(2)
C(11)	55(3)	34(2)	28(2)	9(2)	4(2)	10(2)
C(17)	26(2)	67(3)	54(3)	-15(3)	6(2)	6(2)
C(16)	51(3)	42(3)	44(3)	-9(2)	14(2)	16(2)
C(15)	69(3)	30(2)	56(3)	-11(2)	27(3)	1(2)

Table S3 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**5**.

	x	y	z	U(eq)
H(8)	3231	8652	10520	20
H(3)	1718	10950	11378	26
H(7A)	846	8050	10878	27
H(7B)	1737	6777	10447	27
H(5A)	2228	8318	13806	40
H(5B)	1203	9089	12929	40
H(4A)	3655	9483	12739	41
H(4B)	2836	10843	13187	41
H(6A)	1501	6386	12430	32
H(6B)	2840	6772	12272	32
H(10A)	2148	7408	8750	21
H(10B)	3168	8552	8434	21
H(9A)	503	10562	8480	31
H(9B)	504	10575	9858	31
H(9C)	303	8939	9155	31
H(14)	1431	5355	5884	49
H(2A)	5041	12115	10903	68
H(2B)	4717	10274	11042	68
H(2C)	4776	11442	12137	68
H(1A)	3216	13208	12385	70
H(1B)	2260	13605	11313	70
H(1C)	3597	14110	11272	70
H(12A)	-460	8548	7043	61
H(12B)	50	6774	7187	61
H(12C)	-189	7559	5926	61
H(18)	3899	8784	6102	49
H(11A)	1333	10557	5412	59
H(11B)	2395	11068	6349	59
H(11C)	1074	11323	6618	59
H(17)	4996	7279	4925	59
H(16)	4300	4803	4223	54
H(15)	2538	3849	4717	60

2.2 Crystallographic data for compound (*R*,*R*)-6

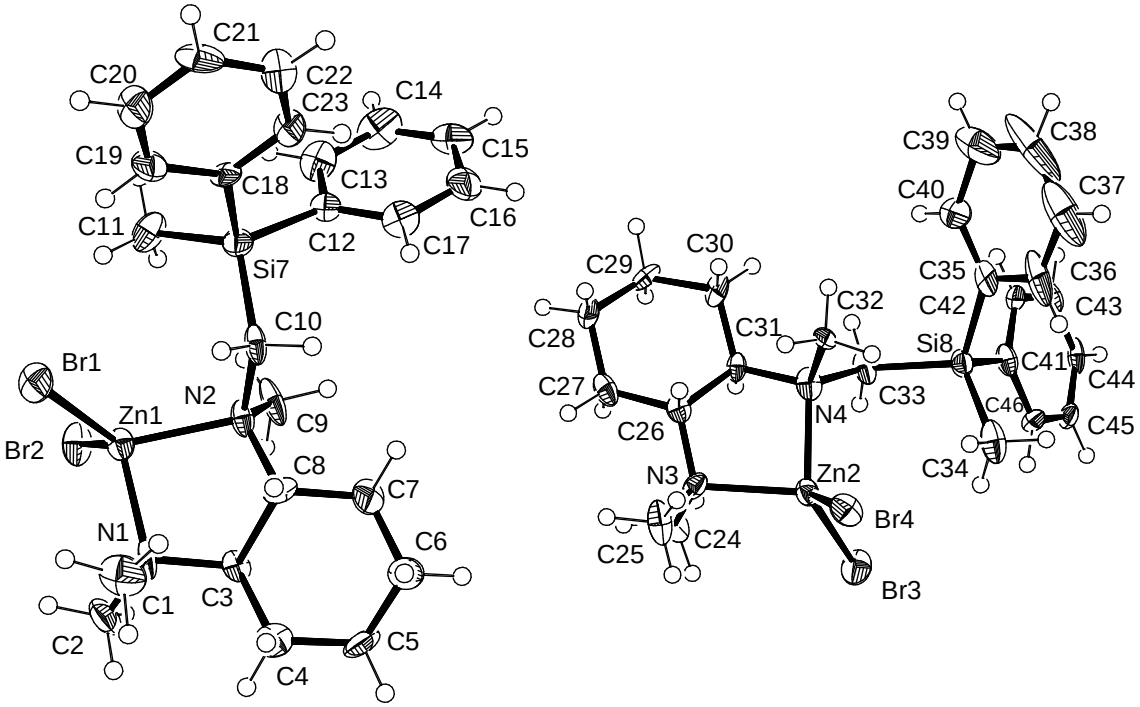

Figure 8 ORTEP plot of (*R*,*R*)-**6** at 50 % probability level.

Table S4 Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for compound (*R*,*R*)-**6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Br(1)	7677(1)	-2552(1)	8130(1)	38(1)
Br(2)	4449(1)	-2630(1)	8183(1)	38(1)
Br(3)	-1731(1)	8948(1)	5379(1)	39(1)
Br(4)	1576(1)	8755(1)	5464(1)	32(1)
C(1)	6266(6)	-2204(7)	6312(4)	49(3)
C(2)	4439(6)	-2870(6)	6345(4)	41(2)
C(3)	4741(5)	-685(6)	6350(4)	21(2)
C(4)	4509(6)	-467(7)	5561(4)	36(2)
C(5)	3975(7)	770(7)	5345(4)	44(2)
C(6)	4718(7)	1763(7)	5734(4)	49(2)
C(7)	4962(6)	1571(7)	6549(4)	36(2)
C(8)	5485(6)	339(6)	6789(4)	26(2)
C(9)	4799(5)	572(6)	7859(5)	41(3)
C(10)	6853(5)	701(6)	7994(4)	28(2)
C(11)	6938(5)	-387(6)	9494(4)	36(2)
C(12)	6624(5)	2347(7)	9230(4)	25(2)
C(13)	6296(6)	2451(8)	9844(5)	41(2)
C(14)	5972(6)	3540(10)	10072(5)	49(3)

C(15)	5992(6)	4587(8)	9692(5)	42(3)
C(16)	6308(6)	4519(7)	9081(5)	40(2)
C(17)	6607(5)	3397(7)	8847(4)	34(2)
C(18)	8841(5)	1125(7)	9262(4)	23(2)
C(19)	9554(6)	126(7)	9394(4)	36(2)
C(20)	10738(6)	258(8)	9656(4)	40(2)
C(21)	11200(6)	1386(8)	9778(4)	39(2)
C(22)	10517(6)	2387(8)	9613(4)	36(2)
C(23)	9334(5)	2257(7)	9371(4)	31(2)
C(24)	-951(5)	6222(6)	6350(4)	43(2)
C(25)	854(6)	5885(6)	6102(4)	43(3)
C(26)	845(6)	6849(6)	7228(4)	22(2)
C(27)	752(6)	5807(6)	7724(4)	30(2)
C(28)	1371(6)	5951(6)	8494(4)	31(2)
C(29)	1001(6)	7116(6)	8768(4)	30(2)
C(30)	1175(5)	8168(6)	8325(4)	29(2)
C(31)	549(5)	8055(6)	7536(4)	20(2)
C(32)	1893(5)	9465(6)	7244(4)	21(2)
C(33)	-22(5)	10170(5)	7176(4)	26(2)
C(34)	182(6)	11656(6)	5893(4)	42(2)
C(35)	1556(6)	12417(7)	7377(5)	30(2)
C(36)	2236(6)	13077(6)	7051(6)	55(3)
C(37)	3195(9)	13696(10)	7435(7)	83(4)
C(38)	3464(8)	13634(10)	8181(9)	106(6)
C(39)	2857(8)	12956(8)	8551(6)	72(3)
C(40)	1879(6)	12337(7)	8125(4)	38(2)
C(41)	-1004(6)	12673(6)	6932(5)	27(2)
C(42)	-948(5)	13262(6)	7575(4)	25(2)
C(43)	-1801(6)	14031(6)	7636(4)	31(2)
C(44)	-2738(6)	14198(6)	7043(4)	27(2)
C(45)	-2838(5)	13638(7)	6418(4)	27(2)
C(46)	-1973(6)	12853(6)	6348(4)	26(2)
N(1)	5272(4)	-1910(5)	6602(3)	24(2)
N(2)	5732(4)	113(5)	7572(3)	25(2)
N(3)	242(5)	6693(5)	6471(3)	23(2)
N(4)	669(4)	9086(5)	7067(3)	25(2)
Si(7)	7256(2)	911(2)	8985(1)	26(1)
Si(8)	211(2)	11706(2)	6828(1)	25(1)
Zn(1)	5825(1)	-1792(1)	7699(1)	25(1)
Zn(2)	139(1)	8433(1)	6027(1)	23(1)

Table S5 Anisotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	22(1)	38(1)	52(1)	0(1)	6(1)	11(1)
Br(2)	29(1)	30(1)	60(1)	10(1)	21(1)	1(1)
Br(3)	23(1)	40(1)	48(1)	11(1)	2(1)	-2(1)
Br(4)	29(1)	32(1)	38(1)	-5(1)	16(1)	-7(1)
C(1)	41(5)	60(6)	52(6)	-14(5)	21(5)	7(4)
C(2)	58(6)	20(5)	46(6)	-8(4)	17(5)	-10(4)
C(3)	11(4)	21(4)	34(6)	0(4)	10(4)	-10(3)
C(4)	23(4)	42(5)	39(6)	2(5)	2(4)	-18(4)
C(5)	52(6)	46(6)	21(5)	16(5)	-11(4)	-21(5)
C(6)	64(6)	37(5)	36(6)	1(5)	-4(5)	-15(5)
C(7)	27(5)	28(5)	48(7)	3(5)	1(5)	-13(4)
C(8)	19(4)	37(5)	19(5)	3(4)	2(4)	-3(4)
C(9)	19(4)	14(4)	92(8)	-7(5)	20(5)	2(4)
C(10)	14(4)	14(4)	56(6)	6(4)	11(4)	2(3)
C(11)	34(5)	45(5)	35(6)	17(5)	17(4)	4(4)
C(12)	23(4)	29(4)	24(5)	-2(5)	9(4)	0(4)
C(13)	29(5)	47(5)	50(7)	8(6)	17(5)	4(5)
C(14)	43(5)	74(7)	40(6)	3(6)	26(5)	17(6)
C(15)	29(5)	54(6)	41(7)	-21(6)	5(5)	17(5)
C(16)	29(5)	34(5)	50(7)	-5(5)	0(5)	-6(4)
C(17)	26(4)	44(5)	37(5)	-1(5)	18(4)	3(5)
C(18)	11(4)	30(5)	22(5)	-3(4)	-2(4)	6(4)
C(19)	28(5)	31(5)	43(6)	-6(5)	-2(4)	-7(4)
C(20)	26(5)	36(5)	58(7)	-2(5)	10(5)	12(4)
C(21)	12(4)	59(6)	41(6)	-21(5)	1(4)	-3(5)
C(22)	32(5)	35(5)	48(6)	4(5)	24(4)	0(5)
C(23)	21(4)	30(5)	43(6)	0(5)	9(4)	11(4)
C(24)	34(5)	28(5)	61(7)	5(5)	4(5)	-30(4)
C(25)	51(6)	21(4)	66(7)	8(5)	31(5)	6(4)
C(26)	19(4)	21(4)	28(6)	0(4)	10(4)	-3(4)
C(27)	29(5)	18(4)	46(6)	-5(5)	13(4)	3(4)
C(28)	38(5)	22(4)	31(6)	11(4)	8(5)	0(4)
C(29)	30(4)	41(5)	16(5)	12(4)	1(4)	5(4)
C(30)	33(4)	25(5)	33(5)	8(4)	17(4)	22(4)
C(31)	16(4)	16(4)	30(5)	6(4)	9(4)	5(3)
C(32)	21(4)	17(4)	23(5)	-2(4)	0(4)	-6(4)

C(33)	9(4)	18(4)	50(6)	2(4)	8(4)	-1(3)
C(34)	41(5)	22(4)	68(7)	7(5)	25(5)	6(4)
C(35)	30(4)	12(4)	50(6)	0(5)	13(4)	17(4)
C(36)	31(5)	14(4)	125(9)	6(6)	33(6)	11(4)
C(37)	46(7)	30(6)	187(13)	-22(10)	55(9)	0(6)
C(38)	26(6)	34(7)	262(18)	-62(12)	47(10)	-5(5)
C(39)	44(6)	39(6)	105(10)	-31(7)	-21(6)	21(5)
C(40)	29(5)	29(5)	46(6)	-4(6)	-7(4)	18(5)
C(41)	28(4)	19(5)	40(6)	3(4)	16(4)	-7(4)
C(42)	31(4)	19(4)	22(5)	7(4)	5(4)	-4(4)
C(43)	25(4)	22(5)	49(6)	-3(5)	16(4)	-10(4)
C(44)	16(4)	15(4)	55(6)	13(5)	17(4)	5(4)
C(45)	26(4)	21(4)	27(5)	11(4)	-4(4)	0(4)
C(46)	32(5)	27(5)	16(5)	5(4)	3(4)	-3(4)
N(1)	12(3)	9(3)	55(5)	3(3)	13(3)	2(3)
N(2)	19(3)	16(3)	43(5)	3(4)	14(3)	3(3)
N(3)	25(4)	26(4)	20(4)	5(3)	6(3)	10(3)
N(4)	12(3)	25(4)	42(4)	4(3)	14(3)	-3(3)
Si(7)	21(1)	28(1)	27(2)	0(1)	4(1)	-1(1)
Si(8)	27(1)	17(1)	31(2)	2(1)	6(1)	2(1)
Zn(1)	18(1)	23(1)	34(1)	1(1)	8(1)	1(1)
Zn(2)	21(1)	19(1)	29(1)	1(1)	6(1)	-2(1)

Table S6 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**6**.

	x	y	z	U(eq)
H(1A)	6671	-2913	6562	74
H(1B)	6781	-1509	6388	74
H(1C)	5986	-2379	5799	74
H(2A)	4294	-2966	5828	61
H(2B)	3733	-2656	6451	61
H(2C)	4729	-3633	6585	61
H(3)	3998	-658	6458	26
H(4A)	5225	-520	5431	43
H(4B)	3994	-1105	5294	43
H(5A)	3238	808	5451	52
H(5B)	3836	883	4824	52
H(6A)	5437	1765	5605	59
H(6B)	4342	2555	5596	59

H(7A)	4247	1646	6680	44
H(7B)	5482	2213	6805	44
H(8)	6224	314	6676	31
H(9A)	4755	1457	7816	62
H(9B)	4958	343	8363	62
H(9C)	4079	215	7585	62
H(10A)	6874	1514	7783	33
H(10B)	7465	222	7889	33
H(11A)	6120	-444	9416	55
H(11B)	7314	-270	10005	55
H(11C)	7213	-1136	9332	55
H(13)	6292	1746	10122	49
H(14)	5733	3568	10493	59
H(15)	5790	5342	9853	51
H(16)	6326	5232	8812	48
H(17)	6803	3363	8411	41
H(19)	9238	-663	9306	43
H(20)	11211	-438	9747	48
H(21)	11993	1480	9977	47
H(22)	10844	3173	9662	43
H(23)	8869	2959	9282	37
H(24A)	-923	5388	6527	65
H(24B)	-1348	6237	5837	65
H(24C)	-1353	6735	6606	65
H(25A)	946	5083	6327	64
H(25B)	1600	6229	6136	64
H(25C)	422	5809	5597	64
H(26)	1664	6907	7255	26
H(27A)	-59	5684	7684	36
H(27B)	1027	5060	7549	36
H(28A)	2195	5974	8556	37
H(28B)	1209	5255	8768	37
H(29A)	1444	7242	9273	36
H(29B)	193	7059	8748	36
H(30A)	923	8918	8512	35
H(30B)	1993	8251	8378	35
H(31)	-273	8007	7505	24
H(32A)	2131	9814	7725	32
H(32B)	1981	10070	6896	32
H(32C)	2361	8756	7224	32
H(33A)	94	10254	7697	31

H(33B)	-828	9962	6961	31
H(34A)	243	12481	5722	63
H(34B)	-530	11292	5611	63
H(34C)	818	11169	5842	63
H(36)	2032	13105	6544	66
H(37)	3648	14140	7203	100
H(38)	4099	14082	8453	127
H(39)	3083	12909	9058	86
H(40)	1440	11862	8352	46
H(42)	-313	13131	7978	30
H(43)	-1749	14437	8073	37
H(44)	-3324	14727	7083	32
H(45)	-3489	13770	6025	33
H(46)	-2044	12447	5908	31

2.3 Crystallographic data for compound (*R*,*R*)-9

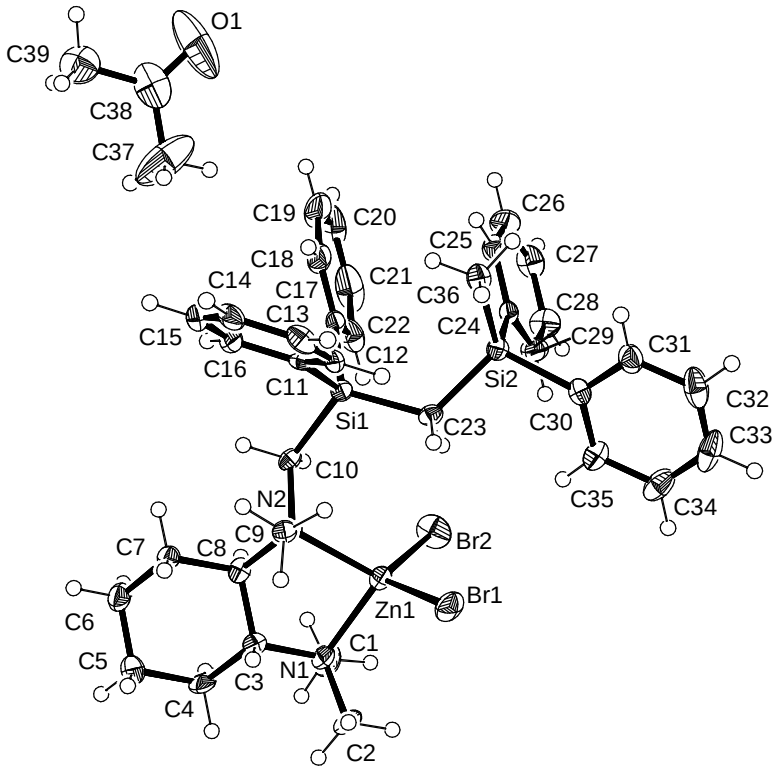

Figure 9 ORTEP plot of (*R*,*R*)-**9** at 50 % probability level.

Table S7 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**9**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Br(1)	9651(1)	7105(1)	-55(1)	36(1)
Br(2)	10155(1)	4716(1)	-272(1)	45(1)
C(1)	12324(3)	5226(2)	778(1)	48(1)
C(2)	12282(3)	6686(2)	719(2)	52(1)
C(3)	11388(2)	6019(2)	1677(1)	25(1)
C(4)	12359(2)	5815(2)	2138(1)	37(1)
C(5)	12059(2)	5896(2)	2882(1)	37(1)
C(6)	11110(2)	5358(2)	3040(1)	32(1)
C(7)	10135(2)	5587(2)	2607(1)	24(1)
C(8)	10402(2)	5504(2)	1853(1)	20(1)
C(9)	8884(2)	6455(2)	1594(1)	21(1)
C(10)	8661(2)	4992(2)	1400(1)	20(1)
C(11)	6353(2)	5706(2)	1539(1)	21(1)
C(12)	5832(2)	6406(2)	1319(1)	22(1)
C(13)	5168(2)	6865(2)	1735(1)	30(1)

C(14)	5001(2)	6625(2)	2401(1)	31(1)
C(15)	5512(2)	5931(2)	2635(1)	33(1)
C(16)	6178(2)	5486(2)	2220(1)	26(1)
C(17)	6765(3)	4012(2)	956(1)	26(1)
C(18)	5744(3)	3805(2)	1183(1)	42(1)
C(19)	5360(4)	3015(2)	1138(2)	69(1)
C(20)	6006(4)	2421(2)	857(2)	73(2)
C(21)	7040(4)	2610(2)	621(2)	66(1)
C(22)	7405(3)	3400(2)	671(1)	40(1)
C(23)	7342(2)	5525(2)	115(1)	21(1)
C(24)	6285(2)	4229(2)	-800(1)	22(1)
C(25)	5467(3)	3676(2)	-656(1)	29(1)
C(26)	5491(3)	2882(2)	-897(1)	39(1)
C(27)	6350(3)	2624(2)	-1297(1)	38(1)
C(28)	7164(3)	3161(2)	-1448(2)	35(1)
C(29)	7138(3)	3955(2)	-1201(1)	31(1)
C(30)	6476(2)	5984(2)	-1268(1)	22(1)
C(31)	5616(3)	6313(2)	-1641(1)	30(1)
C(32)	5789(3)	6731(2)	-2245(2)	41(1)
C(33)	6833(4)	6837(2)	-2480(2)	43(1)
C(34)	7705(3)	6544(2)	-2111(2)	38(1)
C(35)	7531(3)	6121(2)	-1516(1)	29(1)
C(36)	4847(2)	5521(1)	-158(1)	28(1)
N(1)	11664(2)	5953(2)	937(1)	29(1)
N(2)	9444(2)	5688(1)	1394(1)	16(1)
Si(1)	7270(1)	5091(1)	982(1)	20(1)
Si(2)	6230(1)	5319(1)	-508(1)	21(1)
Zn(1)	10169(1)	5866(1)	444(1)	23(1)
C(38)	2987(4)	3577(2)	3051(2)	54(1)
C(39)	2743(3)	3514(2)	3780(2)	57(1)
O(1)	2357(3)	3355(2)	2636(2)	119(1)
C(37)	4049(4)	3957(3)	2887(2)	101(2)

Table S8 Anisotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	41(1)	28(1)	38(1)	15(1)	1(1)	-2(1)
Br(2)	46(1)	41(1)	47(1)	-22(1)	4(1)	7(1)
C(1)	31(2)	75(3)	38(2)	0(2)	10(2)	13(2)

C(2)	40(2)	77(3)	40(2)	26(2)	-1(2)	-28(2)
C(3)	24(2)	27(2)	24(2)	1(1)	2(1)	-4(2)
C(4)	16(2)	58(2)	35(2)	16(2)	0(2)	-12(2)
C(5)	35(2)	47(2)	29(2)	12(2)	-13(2)	-5(2)
C(6)	31(2)	42(2)	24(2)	9(2)	-1(2)	2(2)
C(7)	22(2)	28(2)	23(1)	4(1)	-1(1)	-1(2)
C(8)	21(2)	16(2)	22(2)	3(1)	2(1)	9(2)
C(9)	23(2)	16(2)	24(2)	0(1)	0(1)	-1(2)
C(10)	22(2)	16(2)	22(2)	4(1)	5(1)	1(2)
C(11)	17(2)	23(2)	23(2)	1(1)	-5(1)	-10(2)
C(12)	21(2)	29(2)	15(2)	-3(1)	0(1)	-5(2)
C(13)	30(2)	27(2)	34(2)	-8(1)	-8(2)	0(2)
C(14)	22(2)	47(2)	24(2)	-17(1)	1(1)	-3(2)
C(15)	29(2)	53(2)	18(2)	-1(2)	-2(1)	-9(2)
C(16)	22(2)	34(2)	23(2)	5(1)	-2(1)	0(2)
C(17)	39(2)	20(2)	20(2)	6(1)	-9(1)	-13(2)
C(18)	62(3)	38(2)	25(2)	7(2)	-5(2)	-26(2)
C(19)	109(4)	66(3)	33(2)	9(2)	-7(2)	-62(3)
C(20)	147(5)	37(3)	37(2)	10(2)	-33(3)	-54(3)
C(21)	127(4)	25(2)	46(2)	2(2)	-32(3)	-4(3)
C(22)	61(3)	24(2)	36(2)	-1(2)	-17(2)	-4(2)
C(23)	23(2)	15(1)	24(2)	0(1)	2(1)	-3(1)
C(24)	22(2)	29(2)	16(2)	3(1)	-3(1)	1(2)
C(25)	33(2)	31(2)	24(2)	-1(1)	2(1)	-2(2)
C(26)	46(2)	29(2)	41(2)	-3(2)	-1(2)	-14(2)
C(27)	53(3)	25(2)	34(2)	-10(2)	-6(2)	3(2)
C(28)	35(2)	32(2)	40(2)	-9(2)	6(2)	8(2)
C(29)	25(2)	34(2)	34(2)	-1(2)	2(2)	-3(2)
C(30)	29(2)	20(2)	17(2)	-10(1)	0(1)	2(2)
C(31)	38(2)	29(2)	23(2)	-3(2)	-5(2)	-3(2)
C(32)	67(3)	27(2)	30(2)	1(2)	-17(2)	9(2)
C(33)	88(3)	18(2)	21(2)	0(2)	9(2)	0(2)
C(34)	52(3)	32(2)	31(2)	-4(2)	19(2)	-5(2)
C(35)	33(2)	28(2)	26(2)	4(2)	7(2)	4(2)
C(36)	31(2)	30(2)	23(1)	-2(1)	-1(1)	0(2)
N(1)	23(2)	41(2)	22(1)	4(1)	6(1)	-5(1)
N(2)	17(1)	15(1)	17(1)	2(1)	2(1)	-1(1)
Si(1)	22(1)	19(1)	20(1)	2(1)	-1(1)	-3(1)
Si(2)	21(1)	23(1)	19(1)	-1(1)	1(1)	-1(1)
Zn(1)	25(1)	23(1)	21(1)	1(1)	2(1)	-1(1)
C(38)	63(3)	40(2)	58(3)	-15(2)	-12(2)	31(2)

C(39)	46(3)	59(3)	64(3)	-2(2)	6(2)	13(2)
O(1)	143(3)	124(3)	89(2)	-66(2)	-66(2)	51(3)
C(37)	91(4)	74(3)	138(4)	58(3)	62(3)	33(3)

Table S9 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for compound (*R*,*R*)-**9**.

	x	y	z	U(eq)
H(1A)	12411	5181	286	72
H(1B)	11957	4740	951	72
H(1C)	13040	5277	991	72
H(2A)	11845	7174	804	78
H(2B)	12445	6646	235	78
H(2C)	12963	6720	975	78
H(3)	11187	6598	1766	30
H(4A)	12603	5253	2047	44
H(4B)	12969	6187	2034	44
H(5A)	12688	5739	3167	45
H(5B)	11872	6468	2985	45
H(6A)	10918	5411	3524	38
H(6B)	11309	4784	2953	38
H(7A)	9921	6156	2706	29
H(7B)	9513	5230	2721	29
H(8)	10609	4923	1773	24
H(9A)	8351	6603	1246	31
H(9B)	9422	6892	1639	31
H(9C)	8512	6375	2027	31
H(10A)	8535	4844	1879	24
H(10B)	9032	4523	1186	24
H(12)	5936	6577	864	26
H(13)	4827	7342	1566	37
H(14)	4542	6933	2691	37
H(15)	5401	5760	3089	40
H(16)	6530	5017	2395	32
H(18)	5292	4213	1374	50
H(19)	4654	2884	1301	83
H(20)	5743	1879	825	88
H(21)	7489	2200	428	79
H(22)	8109	3532	507	48
H(23A)	8030	5333	-90	25

H(23B)	7403	6122	163	25
H(25)	4871	3844	-384	35
H(26)	4919	2516	-787	46
H(27)	6373	2083	-1465	45
H(28)	7755	2992	-1724	42
H(29)	7715	4316	-1309	37
H(31)	4894	6251	-1478	36
H(32)	5189	6941	-2493	50
H(33)	6955	7112	-2895	51
H(34)	8426	6634	-2267	46
H(35)	8137	5918	-1270	35
H(36A)	4296	5323	-477	42
H(36B)	4753	6107	-90	42
H(36C)	4765	5239	275	42
H(39A)	2013	3287	3841	85
H(39B)	2778	4055	3986	85
H(39C)	3278	3157	3997	85
H(37A)	4241	3836	2417	152
H(37B)	4611	3738	3188	152
H(37C)	3998	4547	2949	152

2.4 Crystallographic data for compound (*R*,*R*)-10

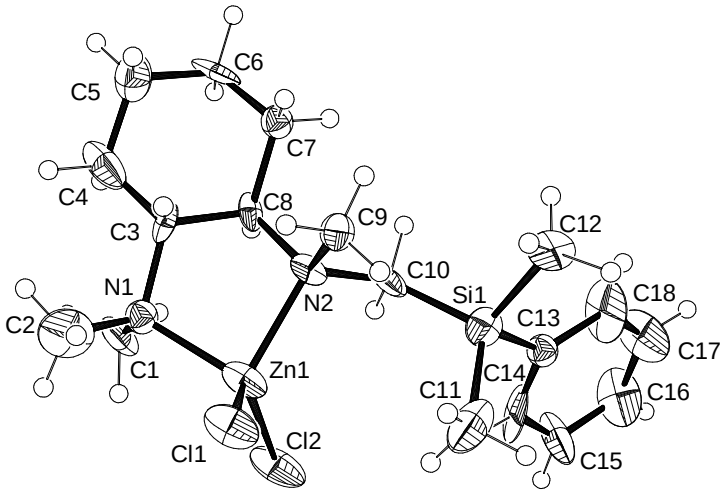

Figure 10 ORTEP plot of (*R*,*R*)-**10** at 50 % probability level. Selected bond lengths (Å) and angles (degree):

Table S10 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**10**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	4655(11)	9903(16)	11170(10)	58(5)
C(2)	3206(12)	11809(18)	11478(13)	66(5)
C(3)	2577(12)	8955(18)	11379(12)	33(4)
C(4)	2913(12)	8472(17)	12634(14)	58(5)
C(5)	2078(12)	7172(18)	13000(11)	53(4)
C(6)	2078(10)	5754(15)	12213(12)	46(4)
C(7)	1655(11)	6231(16)	11006(9)	39(4)
C(8)	2409(9)	7616(15)	10570(10)	26(3)
C(9)	700(10)	8430(14)	9242(10)	32(3)
C(10)	2211(10)	6996(16)	8438(10)	46(4)
C(11)	1571(13)	9148(19)	6301(11)	69(5)
C(12)	23(9)	6278(17)	6799(10)	46(4)
C(13)	2452(14)	5690(20)	6093(10)	65(6)
C(14)	3563(15)	6250(20)	5863(12)	68(5)
C(15)	4276(11)	5340(20)	5118(12)	65(4)
C(16)	3822(13)	3890(20)	4707(14)	71(5)
C(17)	2770(16)	3331(18)	4978(16)	72(5)
C(18)	2119(18)	4190(20)	5678(14)	101(8)
Cl(1)	1653(3)	12412(4)	8790(3)	48(1)
Cl(2)	4470(3)	10122(5)	8194(3)	59(1)
N(1)	3332(7)	10346(16)	10886(9)	43(3)
N(2)	2050(7)	8180(12)	9376(9)	25(3)
Si(1)	1591(3)	7068(5)	6952(3)	38(1)
Zn(1)	2898(1)	10368(2)	9181(1)	39(1)

Table S11 Anisotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	60(10)	45(12)	70(10)	-16(8)	12(8)	-32(8)
C(2)	58(12)	71(13)	65(12)	24(11)	-17(9)	3(10)
C(3)	43(9)	42(10)	12(8)	-6(8)	-5(7)	7(8)
C(4)	42(10)	37(10)	100(15)	-29(10)	21(9)	-10(8)
C(5)	66(11)	51(11)	40(10)	-5(10)	-8(8)	4(10)
C(6)	33(8)	25(11)	83(11)	8(9)	21(7)	-16(6)
C(7)	59(9)	59(9)	5(8)	29(7)	28(6)	30(7)
C(8)	10(7)	36(9)	32(9)	-16(8)	-3(6)	0(6)
C(9)	33(8)	32(8)	31(9)	-3(7)	4(6)	2(7)
C(10)	41(9)	42(10)	59(10)	-20(9)	25(7)	-29(8)

C(11)	62(11)	109(14)	35(9)	2(10)	1(8)	3(10)
C(12)	3(7)	80(12)	54(10)	17(8)	-4(6)	-1(7)
C(13)	77(11)	105(17)	19(9)	-47(10)	38(8)	-79(12)
C(14)	104(15)	71(12)	27(11)	-38(9)	-3(9)	11(11)
C(15)	49(9)	63(10)	86(12)	-43(14)	9(8)	-21(12)
C(16)	42(11)	84(14)	90(14)	-41(12)	16(10)	17(11)
C(17)	78(14)	29(9)	112(16)	-30(11)	26(11)	8(9)
C(18)	150(20)	84(15)	74(14)	-70(13)	36(13)	-15(14)
Cl(1)	39(2)	26(2)	81(3)	5(2)	11(2)	9(2)
Cl(2)	29(2)	41(3)	111(3)	-1(3)	28(2)	-7(2)
N(1)	33(6)	0(5)	101(9)	-21(8)	41(6)	-5(7)
N(2)	3(5)	30(7)	42(8)	7(6)	-6(5)	-1(5)
Si(1)	34(2)	44(3)	36(3)	-1(2)	2(2)	4(2)
Zn(1)	25(1)	24(1)	68(1)	0(1)	12(1)	0(1)

Table S12 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for compound (*R*,*R*)-**10**.

	x	y	z	U(eq)
H(1A)	5143	10581	10708	87
H(1B)	4778	8753	10992	87
H(1C)	4878	10097	11990	87
H(2A)	2451	12317	11211	99
H(2B)	3855	12545	11333	99
H(2C)	3223	11589	12306	99
H(3)	1772	9442	11390	40
H(4A)	3733	8055	12717	70
H(4B)	2873	9438	13136	70
H(5A)	2326	6820	13797	64
H(5B)	1269	7623	12988	64
H(6A)	1559	4893	12482	55
H(6B)	2888	5307	12226	55
H(7A)	821	6587	10982	47
H(7B)	1693	5276	10494	47
H(8)	3213	7134	10532	31
H(9A)	455	8780	8454	48
H(9B)	482	9265	9785	48
H(9C)	306	7404	9402	48
H(10A)	1960	5933	8734	55
H(10B)	3075	6917	8399	55

H(11A)	981	9820	6644	103
H(11B)	1369	9067	5469	103
H(11C)	2352	9648	6449	103
H(12A)	-24	5275	7247	69
H(12B)	-213	6051	5986	69
H(12C)	-506	7098	7083	69
H(14)	3856	7239	6199	81
H(15)	5020	5731	4924	79
H(16)	4265	3262	4214	85
H(17)	2483	2320	4672	86
H(18)	1402	3728	5891	121

2.5 Crystallographic data for compound (*R*,*R*)-11

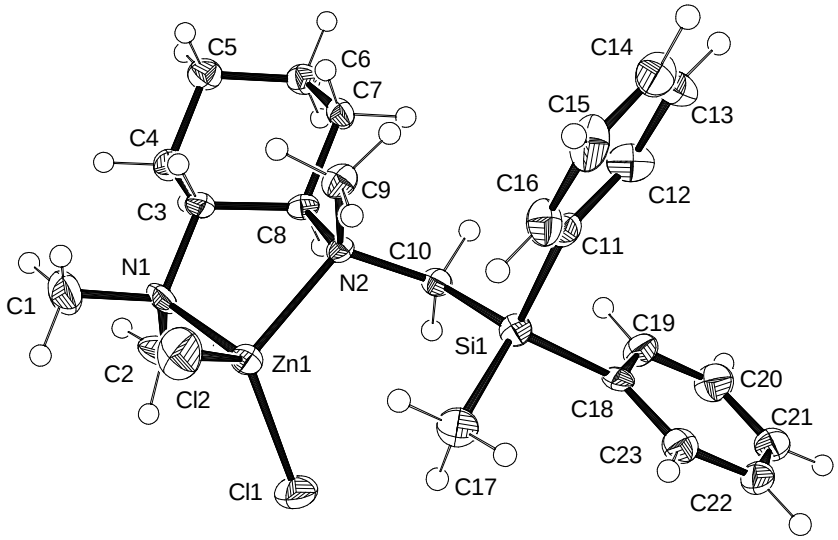

Figure 11 ORTEP plot of (*R*,*R*)-**11** at 50 % probability level.

Table S13 Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for compound (*R*,*R*)-**11**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	8138(1)	8987(1)	9214(1)	24(1)
Cl(1)	9858(1)	8751(2)	8500(1)	39(1)
Cl(2)	7042(1)	11058(1)	8837(1)	44(1)
Si(1)	7294(1)	6226(1)	6876(1)	21(1)
N(2)	7196(2)	6882(3)	9170(2)	15(1)
C(10)	7591(2)	5767(3)	8311(2)	18(1)
N(1)	8291(2)	8687(4)	10845(2)	26(1)

C(8)	7394(2)	6149(3)	10245(2)	16(1)
C(3)	7425(3)	7421(4)	11116(3)	19(1)
C(1)	7997(3)	10189(4)	11399(3)	44(1)
C(6)	6770(2)	4161(5)	11611(2)	24(1)
C(11)	5757(3)	5898(4)	6514(2)	22(1)
C(12)	5296(3)	4373(4)	6505(2)	33(1)
C(5)	6733(3)	5443(3)	12452(2)	24(1)
C(7)	6536(2)	4858(3)	10527(2)	21(1)
C(9)	5969(2)	7275(3)	8992(2)	23(1)
C(4)	7635(2)	6675(4)	12205(2)	22(1)
C(13)	4182(3)	4121(6)	6178(2)	37(1)
C(18)	8122(3)	4744(4)	6113(3)	18(1)
C(19)	8474(3)	3275(4)	6523(3)	26(1)
C(16)	5051(3)	7135(4)	6186(2)	27(1)
C(15)	3930(3)	6855(5)	5870(3)	35(1)
C(14)	3499(3)	5355(5)	5870(3)	35(1)
C(17)	7731(2)	8244(3)	6479(2)	29(1)
C(20)	9034(3)	2165(4)	5910(3)	33(1)
C(2)	9486(3)	8235(4)	11127(3)	46(1)
C(22)	8921(2)	3871(6)	4425(2)	26(1)
C(23)	8364(3)	5000(4)	5039(3)	26(1)
C(21)	9245(3)	2472(4)	4861(3)	29(1)

Table S14 Anisotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	28(1)	19(1)	26(1)	1(1)	5(1)	-4(1)
Cl(1)	26(1)	51(1)	39(1)	-3(1)	8(1)	-9(1)
Cl(2)	62(1)	22(1)	48(1)	4(1)	7(1)	10(1)
Si(1)	20(1)	21(1)	22(1)	-1(1)	0(1)	2(1)
N(2)	12(2)	14(2)	19(2)	-2(1)	1(1)	3(1)
C(10)	12(2)	13(2)	27(2)	-5(2)	5(2)	2(2)
N(1)	31(2)	18(2)	29(2)	2(2)	-2(1)	-14(2)
C(8)	10(2)	19(2)	20(2)	5(2)	2(2)	4(2)
C(3)	16(2)	16(2)	23(2)	2(2)	4(2)	-4(2)
C(1)	65(3)	26(3)	40(3)	-5(2)	11(2)	-15(2)
C(6)	22(2)	25(2)	26(2)	4(2)	2(1)	0(2)
C(11)	25(2)	28(2)	14(2)	0(2)	3(2)	-1(2)

C(12)	22(2)	36(3)	40(2)	11(2)	-4(2)	3(2)
C(5)	27(2)	23(2)	22(2)	4(2)	-2(2)	-2(2)
C(7)	24(2)	17(2)	22(2)	-1(2)	2(2)	-4(2)
C(9)	16(2)	25(2)	27(2)	1(2)	1(2)	7(2)
C(4)	25(2)	23(2)	17(2)	1(2)	2(2)	0(2)
C(13)	28(2)	38(3)	46(2)	-4(3)	-1(2)	-18(3)
C(18)	11(2)	25(2)	20(2)	1(2)	0(2)	-8(2)
C(19)	30(3)	30(2)	18(2)	0(2)	4(2)	0(2)
C(16)	30(2)	23(2)	29(2)	-7(2)	-4(2)	5(2)
C(15)	32(3)	39(3)	33(2)	-9(2)	-13(2)	25(2)
C(14)	16(2)	56(3)	34(3)	-15(2)	-8(2)	8(2)
C(17)	28(2)	26(2)	32(2)	2(2)	0(2)	1(2)
C(20)	35(2)	28(2)	36(3)	1(2)	8(2)	3(2)
C(2)	34(2)	65(3)	38(3)	14(2)	-14(2)	-27(2)
C(22)	18(2)	36(2)	24(2)	-7(3)	4(2)	-6(3)
C(23)	18(2)	26(2)	33(3)	-1(2)	-7(2)	-3(2)
C(21)	16(2)	33(2)	37(3)	-8(2)	6(2)	1(2)

Table S15 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for compound (*R*,*R*)-**11**.

	x	y	z	U(eq)
H(10A)	7252	4719	8461	21
H(10B)	8428	5650	8391	21
H(8)	8166	5644	10231	20
H(3)	6657	7935	11133	22
H(1A)	7241	10548	11166	66
H(1B)	8566	10999	11228	66
H(1C)	7991	10010	12167	66
H(6A)	7531	3651	11617	29
H(6B)	6192	3342	11771	29
H(12)	5752	3503	6725	39
H(5A)	6880	4977	13160	29
H(5B)	5968	5941	12459	29
H(7A)	5755	5308	10513	25
H(7B)	6570	4008	9988	25
H(9A)	5894	7947	8362	34
H(9B)	5673	7838	9612	34
H(9C)	5534	6298	8886	34
H(4A)	8399	6174	12218	26

H(4B)	7624	7509	12756	26
H(13)	3885	3076	6168	45
H(19)	8322	3036	7245	31
H(16)	5340	8184	6180	33
H(15)	3460	7713	5652	42
H(14)	2732	5168	5657	43
H(17A)	7587	8389	5718	43
H(17B)	8546	8388	6627	43
H(17C)	7290	9024	6881	43
H(20)	9273	1192	6215	40
H(2A)	10018	8992	10809	69
H(2B)	9647	7172	10856	69
H(2C)	9579	8245	11900	69
H(22)	9074	4080	3699	31
H(23)	8141	5971	4721	31
H(21)	9619	1703	4438	34

Table S16. Crystal data and structure refinement of all zinc(II) bromide complexes.

Compound	(*R*,*R*)-**5**·$ZnCl_2$	(*R*,*R*)-**6**·$ZnCl_2$
CCDC-No.	CCDC 851905	CCDC 851906
Formula	$C_{18}H_{32}SiN_2ZnCl_2$	$C_{23}H_{34}Cl_2N_2SiZn$
Formula weight [g·mol^{-1}]	440.82	502.88
Temperature [K]	173(2)	173(2)
Wave length [Å]	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1$ (4)	$P2_1$ (4)
a [Å]	a = 11.3678(13)	a = 11.7147(11)
b [Å]	b = 8.2162(9)	b = 8.4569(8)
c [Å]	c = 11.6616(17)	c = 12.6064(12)
β [°]	β = 95.005(13)	β = 90.317(8)
Volume [Å^3]	1085.0(2)	1248.9(2)
Z	Z = 2	Z = 2
Calc. density [Mg·m^{-3}]	1.349	1.337
μ ($Mo_{K\alpha}$) [mm^{-1}]	1.436	1.257
F(000)	4646	528
Crystal dimensions [mm]	0.30 x 0.20 x 0.10	0.30 x 0.10 x 0.10
Theta range [°]	2.40 to 24.99	2.37 to 25.00
Index ranges	$-13 \le h \le 13$	$-13 \le h \le 13$
	$-9 \le k \le 9$	$-10 \le k \le 9$
	$-13 \le l \le 13$	$-14 \le l \le 14$
Reflections collected	9876	11941
Independent reflections	3321 [R_{int} = 0.1124]	4202 [R_{int} = 0.0473]
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameter	3321 / 1 / 222	4202 / 1 / 266
Goodness-of-fit on F^2	1.004	0.829
Final R indices [2sigma(I)]	*R*1 = 0.0709	*R*1 = 0.0293
	w*R*2 = 0.1271	w*R*2 = 0.0345
R indices (all data)	*R*1 = 0.1327	*R*1 = 0.0463
	w*R*2 = 0.1384	w*R*2 = 0.0355
Absolute structure parameter	–0.08(3)	–0.014(9)