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Absolute Asymmetric Synthesis of Stereochemically Labile Aldehyde Helicates and Subsequent Chirality Transfer Reactions

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- A. Tables of selected bond distances and angles for compounds **2** and **4-6**.
- B. Table showing the retention times for the chiral adducts.

Table A1. Selected bond lengths [Å] and angles [°] for **2**.

Al(1)-O(1)	1.707(4)	Al(1)-O(2)	1.706(4)
Al(1)-O(3)	1.713(4)	Al(1)-O(4)	1.852(4)
Al(2)-O(5)	1.704(4)	Al(2)-O(6)	1.700(4)
Al(2)-O(7)	1.720(4)	Al(2)-O(8)	1.846(4)
O(1)-C(18)	1.335(7)	O(2)-C(36)	1.353(7)
O(3)-C(54)	1.360(7)	O(4)-C(55)	1.258(7)
O(5)-C(79)	1.336(7)	O(6)-C(97)	1.355(7)
O(7)-C(115)	1.359(7)	O(8)-C(116)	1.236(8)
O(1)-Al(1)-O(2)	112.1(2)	O(2)-Al(1)-O(3)	109.2(2)
O(1)-Al(1)-O(3)	115.6(2)	O(2)-Al(1)-O(4)	106.8(2)
O(1)-Al(1)-O(4)	102.5(2)	O(3)-Al(1)-O(4)	110.2(2)
O(5)-Al(2)-O(6)	113.5(2)	O(6)-Al(2)-O(7)	110.8(2)
O(5)-Al(2)-O(7)	114.3(2)	O(6)-Al(2)-O(8)	105.3(2)
O(5)-Al(2)-O(8)	104.5(2)	O(7)-Al(2)-O(8)	107.6(2)

Table A2. Selected bond lengths [Å] and angles [°] for **4**.

Al(1)-O(1)	1.712(5)	Al(1)-O(2)	1.837(7)
O(1)-C(18)	1.339(8)	O(2)-C(19)	1.25(2)
O(1)-Al(1)-O(1) ^a	113.03(15)	O(1)-Al(1)-O(1) ^b	113.03(15)
O(1) ^a -Al(1)-O(1) ^b	113.03(15)	O(1)-Al(1)-O(2)	105.63(18)
O(1) ^a -Al(1)-O(2)	105.63(18)	O(1) ^b -Al(1)-O(2)	105.63(17)

Symmetry transformations used to generate equivalent atoms:

a) $-x+y, -x+1, z$; b) $-y+1, x-y+1, z$.

Table A3. Selected bond lengths [Å] and angles [°] for **5**.

Al(1)-O(1)	1.723(5)	Al(1)-O(2)	1.694(5)
Al(1)-O(3)	1.718(5)	Al(1)-O(4)	1.825(5)
Al(2)-O(6)	1.703(5)	Al(2)-O(7)	1.713(5)
Al(2)-O(8)	1.709(5)	Al(2)-O(9)	1.835(5)
O(1)-C(18)	1.349(7)	O(2)-C(36)	1.363(8)
O(3)-C(54)	1.351(8)	O(4)-C(55)	1.254(9)
O(6)-C(80)	1.349(7)	O(7)-C(98)	1.350(8)
O(8)-C(116)	1.338(8)	O(9)-C(117)	1.251(8)
O(2)-Al(1)-O(3)	113.1(2)	O(2)-Al(1)-O(1)	112.1(2)
O(3)-Al(1)-O(1)	112.1(3)	O(2)-Al(1)-O(4)	110.0(2)
O(3)-Al(1)-O(4)	103.9(2)	O(1)-Al(1)-O(4)	105.1(2)
O(6)-Al(2)-O(8)	110.0(2)	O(6)-Al(2)-O(7)	119.5(2)
O(8)-Al(2)-O(7)	112.2(2)	O(6)-Al(2)-O(9)	102.1(2)
O(8)-Al(2)-O(9)	106.5(2)	O(7)-Al(2)-O(9)	105.1(2)

Table A4. Selected bond lengths [Å] and angles [°] for **6**.

Al(1)-O(1)	1.701(8)	Al(1)-O(2)	1.714(7)
Al(1)-O(3)	1.732(7)	Al(1)-O(4)	1.849(7)
Al(2)-O(6)	1.710(8)	Al(2)-O(7)	1.702(7)
Al(2)-O(8)	1.737(7)	Al(2)-O(9)	1.856(7)
O(1)-C(18)	1.347(12)	O(2)-C(36)	1.353(12)
O(3)-C(54)	1.330(13)	O(4)-C(55)	1.254(12)
O(6)-C(80)	1.331(12)	O(7)-C(98)	1.358(12)
O(8)-C(116)	1.332(11)	O(9)-C(117)	1.232(12)
O(1)-Al(1)-O(2)	118.6(4)	O(1)-Al(1)-O(3)	107.8(4)
O(2)-Al(1)-O(3)	115.3(4)	O(1)-Al(1)-O(4)	103.2(3)
O(2)-Al(1)-O(4)	108.9(3)	O(3)-Al(1)-O(4)	101.0(3)
O(7)-Al(2)-O(6)	118.2(4)	O(7)-Al(2)-O(8)	113.5(3)
O(6)-Al(2)-O(8)	108.6(3)	O(7)-Al(2)-O(9)	110.7(3)
O(6)-Al(2)-O(9)	101.9(3)	O(8)-Al(2)-O(9)	102.2(3)

Table B. Retention times for the chiral adducts.

#	Adduct	GC Program ^a	Retention time (min)	
			t _{R1} ^b	t _{R2} ^b
1	3-phenylbutanal	1	18.3	19.4
2	4-phenylbut-3-en-2-ol	1	77.6	80.6
3	3-phenylpentanal	1	11.3	11.7
4	1-phenylpent-1-en-3-ol	1	54.4	56.8
5	3-phenylheptanal	1	16.6	17.6
6	1-phenylhept-1-en-3-ol	1	63.8	68.5
7	1-phenylethanol	2	5.1	5.6
8	1-phenylpropan-1-ol	3	21.2	22.6
9	1-phenylpentan-1-ol	2	8.2	8.8
10	1- <i>p</i> -tolylethanol	2	7.0	8.0
11	1- <i>p</i> -tolylpropan-1-ol	2	11.0	12.5
12	1-(4- <i>tert</i> -butylphenyl)ethanol	2	17.0	18.7
13	1-(4-methoxyphenyl)ethanol	2	17.2	19.0

^a1 = isothermal 90 °C, 2 = isothermal 115 °C, 3 = isothermal 110 °C. ^bOnly the absolute configuration of entries 7-11 was established, and for these alcohols the (R)-enantiomer elutes first. The configuration of the other alcohols relate to the first eluting peak in the chromatogram (which is not necessarily the same as for entries 7-11).