

Berichtigung / Correction

A Molecular-Dynamics Simulation of the Complex Formation between Methyl (*R*)/(*S*)-2-Chloropropionate and Heptakis(3-*O*-acetyl-2,6-di-*O*-pentyl)- β -cyclodextrin

J. E. H. Köhler*, M. Hohla, M. Richters, W. A. König

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On page 124 the tables below their corresponding captions have inadvertently been exchanged; the following assignments of captions and tables are correct:

Table 1. Averaged (20–30 ps) molecular dimensions [$\text{\AA}$] of **1** and (*R*)/(*S*)-**2** and of their complexes at 300 K

Averaged distances	(<i>R</i>)-2 - 1	(<i>S</i>)-2(Cl-in) - 1	(<i>S</i>)-2(Cl-out) - 1	Empty CD
				Free enantiomer
CD length				
O(4,6) - O(1,3)	9.755 ± 0.573	10.112 ± 0.365	9.963 ± 0.592	10.164 ± 0.927
O(4,6) - O(3,5)	8.771 ± 0.471	9.647 ± 0.319	9.186 ± 0.472	11.089 ± 0.879
average length	9.263 ± 0.522	9.880 ± 0.342	9.574 ± 0.532	10.626 ± 0.903
CD width				
O(1,2) - O(6,7)	10.642 ± 0.290	10.123 ± 0.313	10.479 ± 0.386	8.322 ± 1.150
O(1,2) - O(5,7)	10.127 ± 0.314	9.995 ± 0.242	10.003 ± 0.334	8.296 ± 0.863
average width	10.385 ± 0.302	10.059 ± 0.278	10.241 ± 0.360	8.309 ± 1.006
CD				
total average	9.824 ± 0.412	9.969 ± 0.310	9.908 ± 0.446	9.468 ± 0.954
Enantiomer				(<i>R</i>) 4.574 ± 0.246
length	5.018 ± 0.081	4.818 ± 0.200	4.667 ± 0.229	
C(1)- C(4)				(<i>S</i>) 4.814 ± 0.246

Table 2. Averaged (20–30 ps) molecular dimensions [$\text{\AA}$] of **1** and (*R*)/(*S*)-**2** and of their complexes at 333 K

Averaged distances	(R)-2 - 1	(S)-2 - 1	Empty CD
			Free enantiomer
CD length			
O(4,6) - O(1,3)	9.624 ± 0.354	10.573 ± 0.354	10.504 ± 0.510
O(4,6) - O(3,5)	8.647 ± 0.311	9.870 ± 0.327	10.331 ± 0.454
average length	9.136 ± 0.333	10.221 ± 0.341	10.418 ± 0.482
CD width			
O(1,2) - O(6,7)	10.534 ± 0.233	9.976 ± 0.292	9.287 ± 0.481
O(1,2) - O(5,7)	10.218 ± 0.207	9.681 ± 0.354	9.236 ± 0.454
average width	10.376 ± 0.220	9.829 ± 0.323	9.262 ± 0.468
CD			
total average	9.756 ± 0.277	10.025 ± 0.332	9.840 ± 0.475
Enantiomer length			(R) 4.622 ± 0.297
C(1) - C(4)	4.934 ± 0.162	4.375 ± 0.211	(S) 4.608 ± 0.307

Redaktion
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