Electronic Supplementary Material (ESI) for Chemical Communications

Möbius Molekules with Twists and Writhes

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Supporting Information

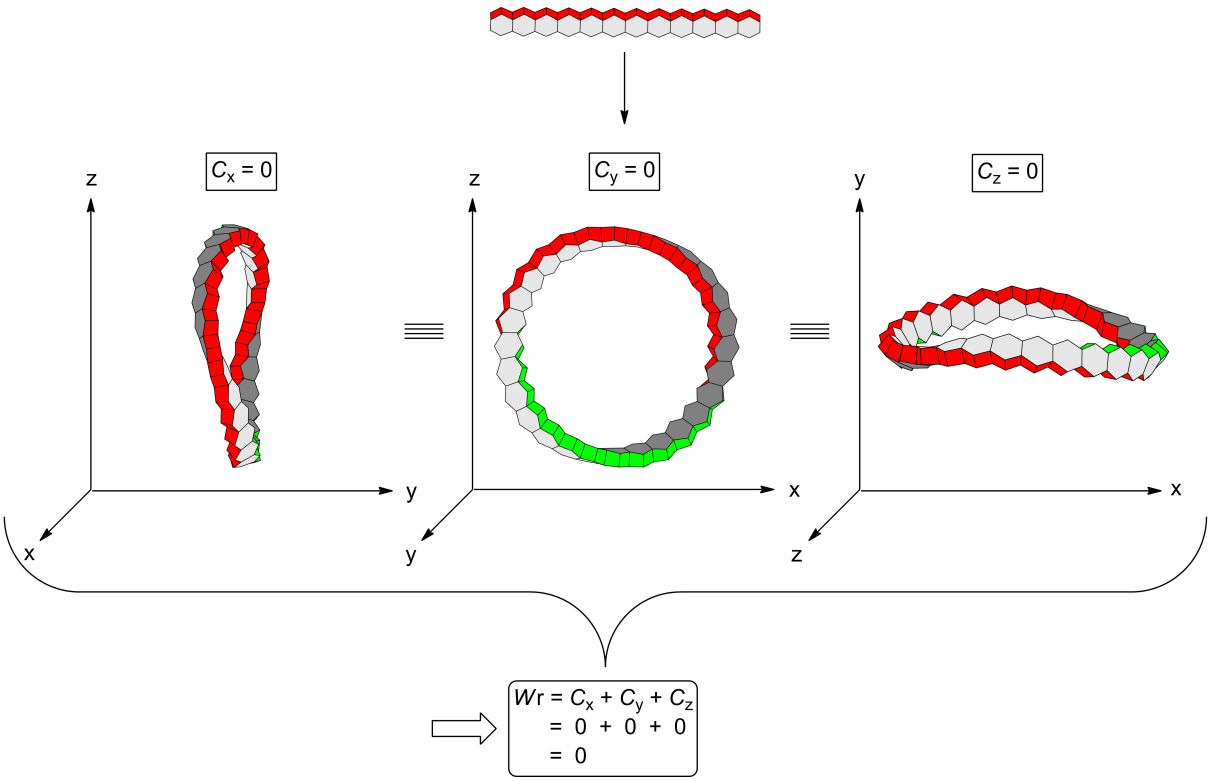

Figure S1: Construction of a Möbius bands with $L_k = 2$ from a linear precursor. a) Möbius ribbon with $T_w = 2$ and $W_r = 0$. The writhe is defined as the sum of self-crossings ($W_r = C_x + C_y + C_z$) if the object is viewed parallel to the three Cartesian axes (x, y, and z).

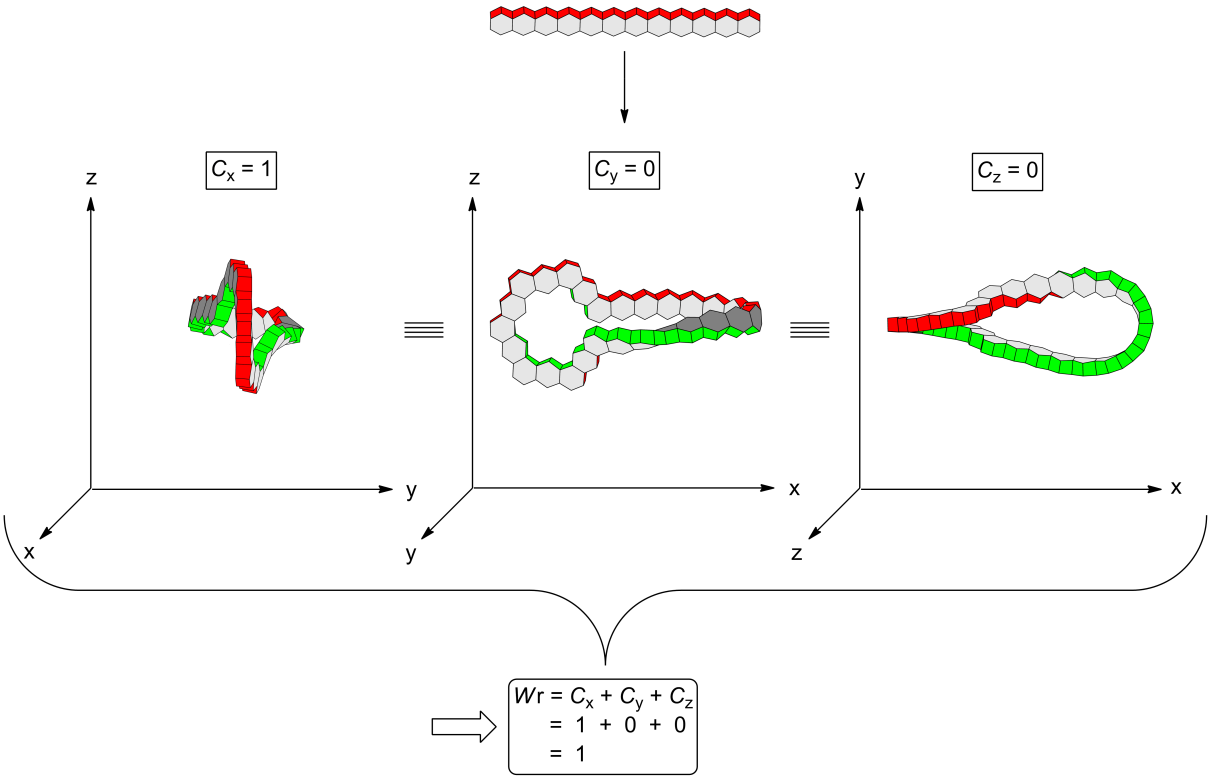

Figure S2: Construction of a Möbius bands with $L_k = 2$ from a linear precursor. Möbius ribbon with $T_w = 1$ and $W_r = 1$ The writhe is defined as the sum of positive and negative self-crossings ($W_r = C_x + C_y + C_z$) if the object is viewed parallel to the three Cartesian axes (x, y, and z).

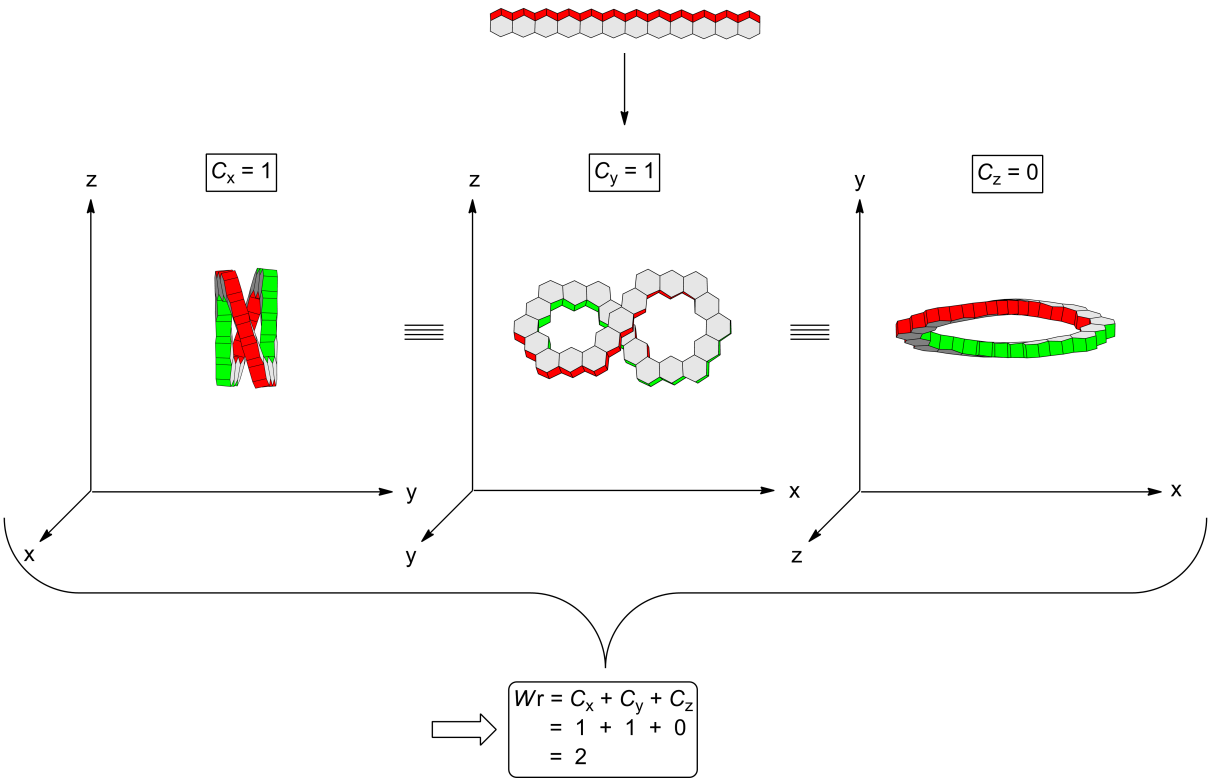

Figure S3: Construction of a Möbius bands with $L_k = 2$ from a linear precursor. Möbius ribbon with $T_w = 1$ and $W_r = 2$ (figure-eight). The writhe is defined as the sum of positive and negative self-crossings ($W_r = C_x + C_y + C_z$) if the object is viewed parallel to the three Cartesian axes (x, y, and z).

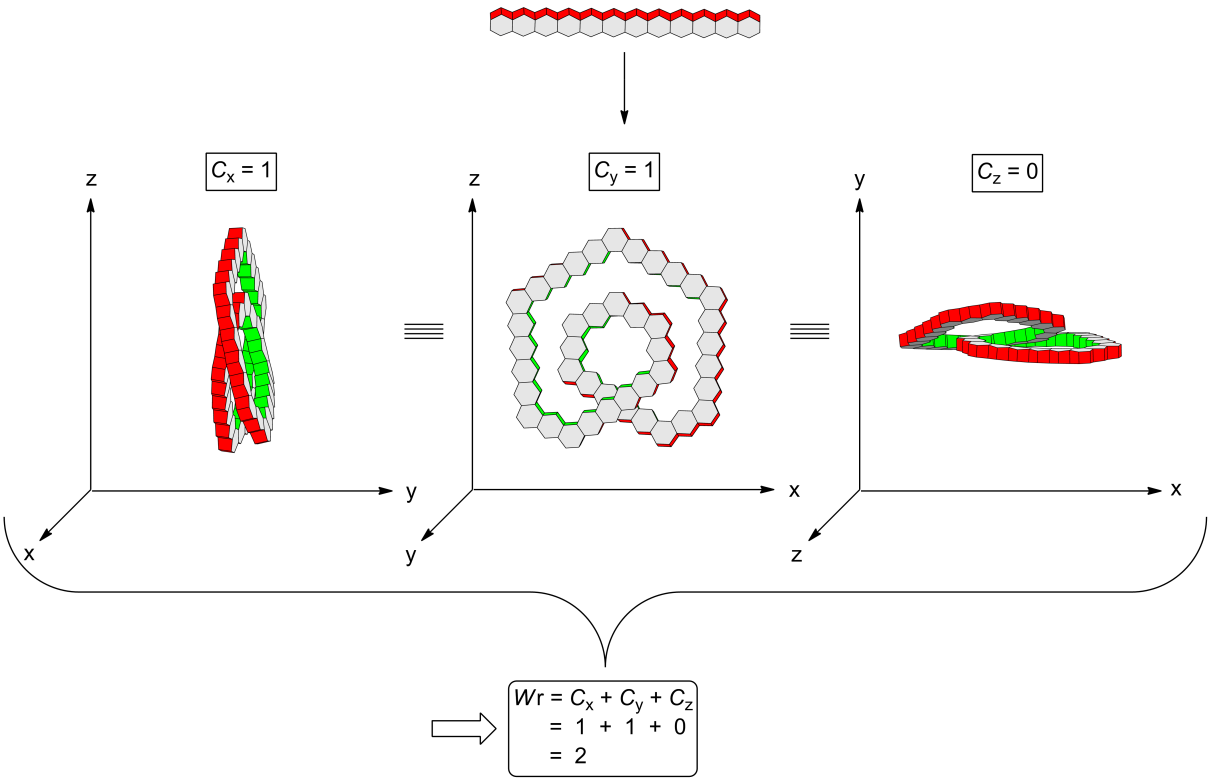

Figure S4: Construction of a Möbius bands with $L_k = 2$ from a linear precursor. Möbius ribbon with $T_w = 0$ and $W_r = 2$ (loop). The writhe is defined as the sum of positive and negative self-crossings ($W_r = C_x + C_y + C_z$) if the object is viewed parallel to the three Cartesian axes (x, y, and z).

Table S1: Complete list of calculated and experimental topological parameters of the calculated most stable isomers of [16]annulene derivative.

Entry	E_{rel} [a,b] [kcal / mol]	E_{rel} [a,c] [kcal /mol]	Configu-ration[a]	Topological parameters[a,d]				Com-pound
					L_k [Pi]	T_w [Pi]	W_r [Pi]	
1	0.00	0.00	*syn-tZcZcEt*	Calc.	1	0.63	0.37	
2	0.29	1.75	*anti-tEcZcEt*	Calc.	1	0.79	0.21	
3	0.56	0.30	*syn-cZtEcZt*	Calc.	1	0.88	0.12	
4	0.56	0.89	*syn-cEtZcZt*	Calc.	1	0.77	0.23	
5	2.47	4.95	*anti-cEtZcEt*	Calc.	1	0.90	0.10	
6	2.76	1.96	*anti-tZtEcZt*	Calc.	1	0.94	0.06	
7	2.77	1.90	*anti-tZcZcZt*	Calc.	1	0.48	0.52	**1** (C_2)
				Exp.	1	0.46	0.54	
8	4.16	3.26	*syn-tEcZcEt*	Calc.	0	0.00	0.00	
9	6.71	5.23	*syn-tZcZcEc*	Calc.	1	0.61	0.39	
10	6.91	5.29	*syn-tZtZtZt*	Calc.	0	0.00	0.00	**2** (C_s)
				Exp.	0	0.04	-0.04	
11	8.36	10.74	*anti-tEcEtZc*	Calc.	1	0.88	0.12	
12	9.30	8.86	*syn-tEtZcZc*	Calc.	1	0.62	0.38	
13	9.34	13.06	*anti-cEtZtEc*	Calc.	1	0.92	0.08	
14	11.20	10.25	*anti-tZtZcZc*	Calc.	1	0.68	0.32	
15	11.20	10.25	*anti-cZcZcZc*	Calc.	1	0.68	0.32	
16	11.74	11.56	*syn-cEtZtEc*	Calc.	0	0.00	0.00	
17	12.38	9.53	*syn-cZtZcZc*	Calc.	1	0.71	0.29	
18	12.38	9.53	*syn-cZcZtZc*	Calc.	1	0.71	0.29	
19	14.25	13.96	*syn-cZtEcEc*	Calc.	1	0.84	0.16	
20	16.20	15.00	*syn-cEcZcZc*	Calc.	1	0.47	0.53	
21	23.49	24.35	*anti-cZcEcEc*	Calc.	1	0.80	0.20	
22	23.80	27.58	*anti-tEtEtEt*	Calc.	0	-0.02	0.02	
23	27.10	33.46	*syn-tEtEcEt*	Calc.	0	0.05	-0.05	
24	28.27	33.01	*anti-tEcEcEt*	Calc.	0	-0.07	0.07	
25	30.73	34.84	*anti-cEcZcEt*	Calc.	1	0.63	0.37	

[a] For details regarding the calculations and notations of entry 1-25 see reference 26; [b] E_{rel} B3LYP/6-31G*; [c] E_{rel} KMLYP/6-31G*; [d] All topological parameters were obtained using the unpublished program anewwrithm by F. Köhler and R. Herges.