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How Can Rotaxanes Be Modified by Varying Functional Groups at the Axle?—A Combined Theoretical and Experimental Analysis of Thermochemistry and Electronic Effects

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All calculated entropy changes $T\Delta_R S^{ex}$ for the exchange reaction in Tables 8 and 9 given in this paper are more negative by a constant contribution of $-4.8\ kJ\,mol^{-1}$. The corrected values for the entropy contributions as well as the free energy changes are given in the corrected versions of Tables 8 and 9 shown below. The corrected values for the exchange formation are thus in even better agreement with the experimental data, whereas the values obtained from the COSMO interaction energies show larger discrepancies. The conclusions drawn in the original publication are not affected by these corrections in any way. The authors apologize for the oversight.

Table 8. Thermochemical quantities at $T=298.15$ K and $p=101\,325$ Pa. Complex **1–8** ($CHCl_3$) was used as the reaction partner for all other guests in the case of the exchange reaction. $\Delta_R G_{COSMO}$ denotes free reaction enthalpies based on the interaction energies ΔE^{cp}_{Cosmo} obtained from COSMO calculations ($\varepsilon=4.81$). All values in [$kJ\,mol^{-1}$].

		Formation				Exchange			
Guest	No.	$\Delta_R H^f$	$T\Delta_R S^f$	$\Delta_R G^f$	$\Delta_R G^f_{COSMO}$	$\Delta_R H^{ex}$	$T\Delta_R S^{ex}$	$\Delta_R G^{ex}$	$\Delta_R G^{ex}_{COSMO}$
				axle–wheel complexes					
MeO-	**1–2**	−29.7	−49.0	19.3	56.7	−29.9	−7.1	−22.8	−0.7
Cl-	**1–3**	−28.1	−50.6	22.4	59.4	−28.3	−8.6	−19.7	1.8
H-	**1–4**	−28.2	−50.4	22.2	59.3	−28.4	−8.5	−19.9	1.7
*t*Bu-	**1–5**	−28.2	−49.5	21.3	59.2	−28.4	−7.5	−20.9	1.5
NO_2-	**1–6**	−26.9	−52.1	25.1	63.0	−27.1	−10.1	−17.0	5.4
				solvent complexes					
CH_2Cl_2	**1–7**	−6.1	−41.5	35.5	–	−6.3	0.4	−6.7	–
$CHCl_3$	**1–8**	0.2	−46.7	46.9	62.4	0.0	0.0	0.0	0.0
H_2O	**1–9**	−14.4	−33.7	19.3	–	−14.6	8.3	−22.9	–
$(H_2O)_4$	**1–10**	−56.3	−52.7	−3.6	–	−56.5	−10.8	−45.7	–
				rotaxane mimics					
H(2-fold)	**12**	−29.0	−45.7	16.7	–	–	–	–	–
H(1-fold)	**13**	−16.0	−43.9	27.9	–	–	–	–	–

Table 9. Calculated electronic and thermochemical energies of the exchange reaction [Eq. (5)] at $T=298.15$ K and $p=101\,325$ Pa compared with the experimental free binding enthalpies ΔG^{exp}_1 at $T=303$ K. The chloroform complex **1–8** is chosen as the reaction partner for all axles. ΔE^{ZPE}_{adia} corresponds to the adiabatic interaction energy corrected for the zero-point energy (ZPE). All values in [$kJ\,mol^{-1}$].

Guest	No.	ΔE^{CP}_{adia}	ΔE^{CP}_{strain}	ΔE^{ZPE}_{adia}	$\Delta_R H$	$T\Delta_R S$	$\Delta_R G$	$\Delta_R G_{COSMO}$	ΔG^{exp}_1
MeO-	**1–2**	−37.9	−48.4	−35.8	−29.9	−7.1	−22.8	−0.7	−12.1
Cl-	**1–3**	−36.6	−47.2	−33.9	−28.3	−8.6	−19.7	1.8	−13.6
H-	**1–4**	−36.5	−46.9	−33.9	−28.4	−8.5	−19.9	1.7	−11.0
*t*Bu-	**1–5**	−36.0	−46.8	−34.6	−28.4	−7.5	−20.9	1.5	−11.4
NO_2-	**1–6**	−35.7	−46.6	−32.6	−27.1	−10.1	−17.0	5.4	−13.7

