Supplementary Materials for

The Asymmetry is Derived from Mechanical Interlocking of Achiral Axle and Achiral Ring Components

–Syntheses and Properties of Optically Pure [2]Rotaxanes with Mechanical Chirality–

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1. Procedures for the determination of binding constants of rotaxane $\mathbf{5}_{2nd}$ with PGO

1-1 Rotaxane $\mathbf{5}_{2nd}$ with (*R*)-PGO

A solution of $\mathbf{5}_{2nd}$ (0.57 mM) and a solution of (*R*)-PGO (46.2 mM) each in C_6D_6 were prepared. An initial ^{1}H NMR spectrum of $\mathbf{5}_{2nd}$ was recorded. Samples were made by adding the guest solutions to a 650 μL of the host solution. Namely, 20, 40, 60, 80, 100, 120, 140, 190, 240, 340, and 440 μL portions of the guest solution were added. Then, spectra of these samples were recorded. The association constant was calculated by the non-liner least-squares method[1-3] following the chemical shifts of one of the aromatic protons of $\mathbf{5}_{2nd}$ shown in Scheme 1 as H^e.

1-2 Rotaxane $\mathbf{5}_{2nd}$ with (*S*)-PGO

A solution of $\mathbf{5}_{2nd}$ (0.57 mM) and a solution of (*S*)-PGO (56.8 mM) each in C_6D_6 were prepared. An initial ^{1}H NMR spectrum of $\mathbf{5}_{2nd}$ was recorded. Samples were made by adding the guest solutions to a 650 μL of the host solution. Namely, 15, 30, 50, 70, 100, 130, 170, 210, 250, 290, and 330 μL portions of the guest solution were added. Then, spectra of these samples were recorded. The association constant was calculated by the non-liner least-squares method[1-3] following the chemical shifts of one of the aromatic protons of $\mathbf{5}_{2nd}$ shown in Scheme 1 as H^e.

2. Table S1 Tabulated ^{1}H NMR titration data of Rotaxane $\mathbf{5_{2nd}}$ with (*R*)-PGO

Table S1. Tabulated ^{1}H NMR titration data of Rotaxane $\mathbf{5_{2nd}}$ with (*R*)-PGO in $CDCl_3$ at 30 ºC, calculated binding constant, and calculated chemical shift of the complex.

	$[H]_t$ (mM) [a]	$[G]_t$ (mM) [b]	$[G]_t / [H]_t$ [c]	δ (ppm) [d]
1	0.570	0.00	0.0	8.522
2	0.553	1.38	2.5	8.504
3	0.537	2.68	5.0	8.492
4	0.522	3.91	7.5	8.481
5	0.507	5.07	10.0	8.475
6	0.494	6.17	12.5	8.468
7	0.481	7.21	15.0	8.462
8	0.469	8.20	17.5	8.458
9	0.441	10.5	23.7	8.450
10	0.416	12.5	30.0	8.445
11	0.374	15.9	42.5	8.438
12	0.340	18.7	54.9	8.433
				δ_{comp}=8.394
				K=125±3

[a] Total concentration of Rotaxane $\mathbf{5_{2nd}}$.

[b] Total concentration of (*R*)-PGO.

[c] The ratio of Rotaxane $\mathbf{5_{2nd}}$ over (*R*) -PGO.

[d] Observed chemical shifts of one of the phenyl proton H^d of Rotaxane $\mathbf{5_{2nd}}$.

3. Figure S1 ^{1}H NMR titration curve for the complexation of Rotaxane $\mathbf{5_{2nd}}$ with (*R*)-PGO

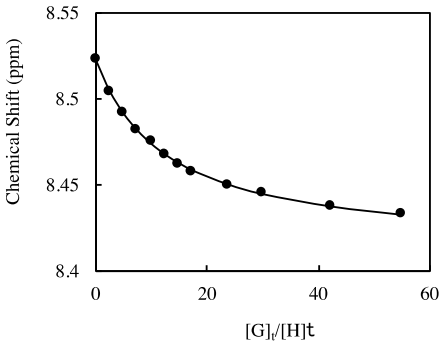

Figure S1. ^{1}H NMR titration curve for the complexation of Rotaxane $\mathbf{5_{2nd}}$ with (*R*)-PGO at 30 ºC.

4. Table S2 Tabulated ^{1}H NMR titration data of Rotaxane $\mathbf{5_{2nd}}$ with (*S*)-PGO

Table S2. Tabulated ^{1}H NMR titration data of Rotaxane $\mathbf{5_{2nd}}$ with (*S*)-PGO in $CDCl_3$ at 30 °C, calculated binding constant, and calculated chemical shift of the complex.

	$[H]_t$ (mM) [a]	$[G]_t$ (mM) [b]	$[G]_t / [H]_t$ [c]	δ (ppm) [d]
1	0.570	0.00	0.0	8.522
2	0.557	1.28	2.3	8.510
3	0.545	2.51	4.6	8.499
4	0.529	4.06	7.7	8.488
5	0.514	5.52	10.7	8.481
6	0.494	7.57	15.3	8.471
7	0.475	9.47	19.9	8.465
8	0.452	11.8	26.1	8.457
9	0.431	13.9	32.2	8.450
10	0.411	15.8	38.3	8.447
11	0.394	17.5	44.5	8.444
12	0.378	19.1	50.6	8.440
				δ_{comp}=8.390
				K=84.7±4.0

[a] Total concentration of Rotaxane $\mathbf{5_{2nd}}$.

[b] Total concentration of (*S*)-PGO.

[c] The ratio of Rotaxane $\mathbf{5_{2nd}}$ over (*S*) -PGO.

[d] Observed chemical shifts of one of the phenyl proton H^d of Rotaxane $\mathbf{5_{2nd}}$.

5. Figure S2 ^{1}H NMR titration curve for the complexation of Rotaxane 5_{2nd} with (*S*)-PGO

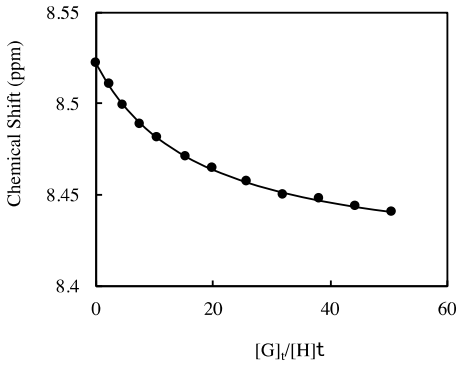

Figure S2. ^{1}H NMR titration curve for the complexation of Rotaxane $\mathbf{5_{2nd}}$ with (*S*)-PGO at 30 °C.

6. References

1. Hirose, K. (2001) A practical guide for the determination of binding constants, *J. Incl. Phenom.*, 39, 3-4, 193-209 Doi 10.1023/A:1011117412693.
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3. Hirose, K., Quantitative analysis of binding properties. in *Analytical methods in supramolecular chemistry*, ed. Schalley, C.A., Wiley-VCH Verlag GmbH & Co. KGaA, 2012, pp. 27-66, 9783527644131.