Supporting Information

Cyclic Monoterpenes Trapped in a Polyaromatic Capsule: Unusual Selectivity, Isomerization, and Volatility Suppression

Ryuki Sumida, Yuya Tanaka, Keita Niki, Yoshihisa Sei, Shinji Toyota, and Michito Yoshizawa*

Laboratory for Chemistry and Life Science, Institute of Innovative Research, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan
Department of Chemistry, School of Science, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152–8551, Japan

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- Cartesian coordinates of **ACI**, **TBI-a**, **TBI-b**, and **MTO** without/within **1**

Materials and methods

NMR: Bruker AVANCE III HD 500 (500 MHz; TMS (δ = 0.00 ppm) in $CDCl_3$ was used as an external standard for host-guest studies in D_2O), ESI-TOF MS: Bruker micrOTOF II, X-ray: Bruker AXS D8 VENTURE/PHOTON 100 diffractometer, FT-IR: SHIMADZU IRSprit, ITC: MicroCal system, VP-ITC model, TG-DTA: SHIMADZU DTG-60, Molecular mechanics calculation (geometry optimization): Dassault Systèmes Co., Materials Studio, Forcite module (version 5.5.3), CONFLEX Co., Conflex 8, Rev. C program, DFT calculation: Gaussian 16(rev. C01), Spartan'10 (Wavefunction, Inc.).

Solvents and reagents: TCI Co., Ltd., FUJIFILM Wako Chemical Co., Kanto Chemical Co., Inc., Sigma-Aldrich Co., and Cambridge Isotope Laboratories, Inc. Ultra-pure water (Milli-Q) was used for the ITC analysis. Capsule **1** was synthesized according to a previously reported procedure.[S1]

References

[S1] M. Yamashina, Y. Sei, M. Akita, M. Yoshizawa, *Nat. Commun.* **2014**, *5*, 4662.

[S2] S. H. Yalkowsky, Y. He, P. Jain, *Handbook of Aqueous Solubility Data*, CRC Press, 2nd Ed., 2010.

[S3] The Human Metabolome Database, *p*-Menthane (HMDB0031455), https://hmdb.ca/metabolites/HMDB0031455.

[S4] European Chemicals Agency, CLH report, alpha-terpinene, https://echa.europa.eu/documents/10162/d5e38899-0537-3d67-c1a7-8922b01f0ec9.

[S5] a) Sigma-Aldrich, MSDS, (–)-menthone, *p*-cymene.

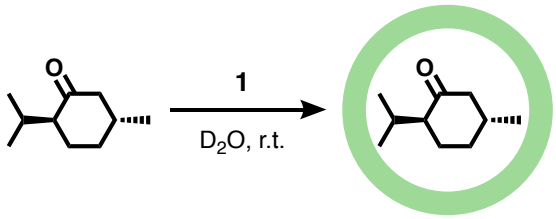
[S6] Tokyo Chemical Industry Co., Ltd., SDS, (–)-menthol, (+)-camphor.

[S7] a) TGSC Information System, *p*-menthane, http://www.thegoodscentscompany.com/data/rw1023491.html; b) TGSC Information System, (–)-borneol, http://www.thegoodscentscompany.com/data/rw1011571.html c) TGSC Information System, alpha-terpinene, http://www.thegoodscentscompany.com/data/rw1016031.html.

[S8] M. J. Frisch et al., Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford, Connecticut, **2016**.

[S9] E. F. C. Byrd et al., *J. Phys. Chem. A* **2017**, *121*, 2265.

Formation of 1•MTO RS085



Capsule **1** (1.0 mg, 0.26 μmol) and (–)-menthone (**MTO**; 0.1 mg, 0.91 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. After removal of excess **MTO** under vacuum, the quantitative formation of 1:1 host-guest complex **1•MTO** was confirmed by NMR and ESI-TOF MS analyses. ^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.65 (m, 3H, **MTO**), –2.56 (br, 1H, **MTO**), –2.44 (m, 3H, **MTO**), –2.34 (br, 1H, **MTO**), –2.29 (m, 3H, **MTO**), –1.74 (br, 1H, **MTO**), –1.57 (br, 1H, **MTO**), –1.20 (br, 2H, **MTO**), –1.10 (br, 1H, **MTO**), –0.87 (br, 1H, **MTO**), –0.71 (br, 1H, **MTO**), 2.48 (m, 24H, **1**), 3.12 (m, 16H, **1**), 3.49 (s, 12H, **1**), 3.95 (m, 8H, **1**), 4.01 (m, 8H, **1**), 4.08 (m, 8H, **1**), 4.50 (m, 4H, **1**), 4.60 (m, 4H, **1**), 5.98 (s, 4H, **1**), 6.59 (s, 8H, **1**), 6.78 (s, 8H, **1**), 7.01 (d, J = 8.7 Hz, 8H, **1**), 7.24 (s, 8H, **1**), 7.53 (br, 8H, **1**), 7.68 (d, J = 8.1 Hz, 8H, **1**), 7.77 (br, 8H, **1**), 7.99 (br, 16H, **1**), 8.35 (dd, J = 6.8, 6.8 Hz, 8H, **1**), 8.56 (d, J = 7.2 Hz, 8H, **1**), 9.32 (s, 8H, **1**). ^{1}H DOSY NMR (500 MHz, D_2O, 25 ºC): $D = 9.57 \times 10^{-11}$ m^2 s^{-1}. ESI-TOF MS (H_2O): m/z 1947.7 [**1•MTO** – 2•NO_3^-]$^{2+}$, 1277.8 [**1•MTO** – 3•NO_3^-]$^{3+}$, 942.9 [**1•MTO** – 4•NO_3^-]$^{4+}$.

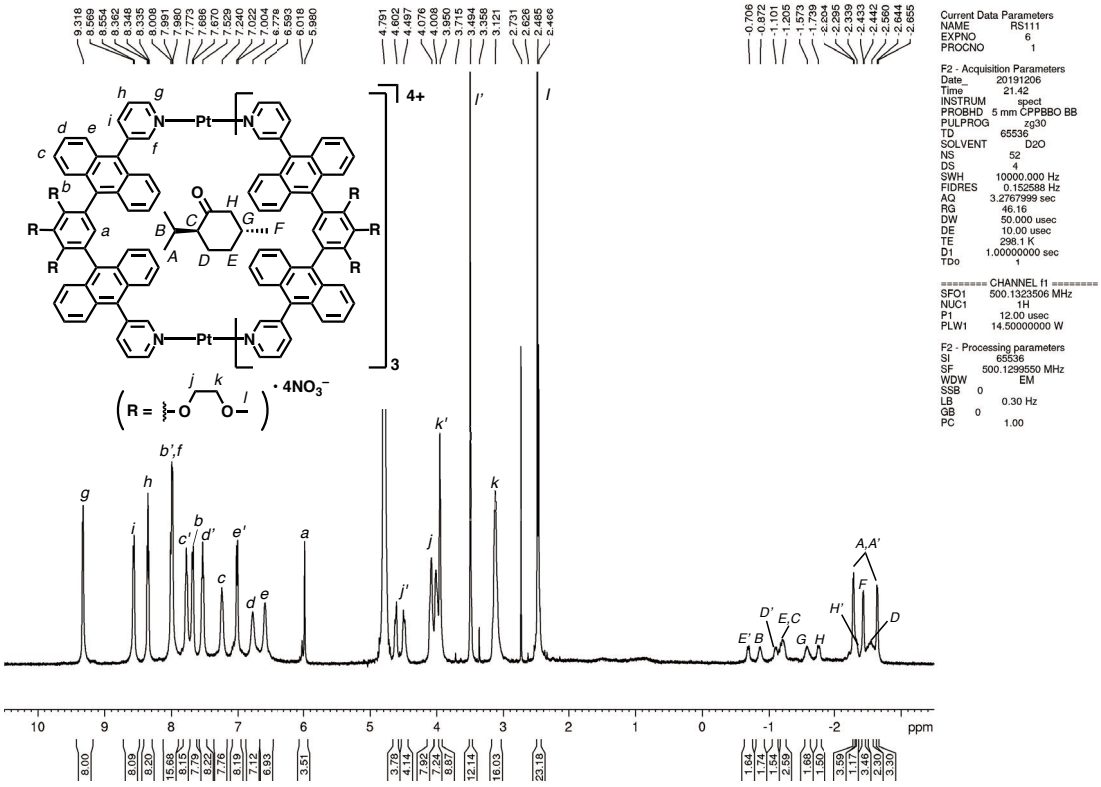


Figure S1. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTO**.

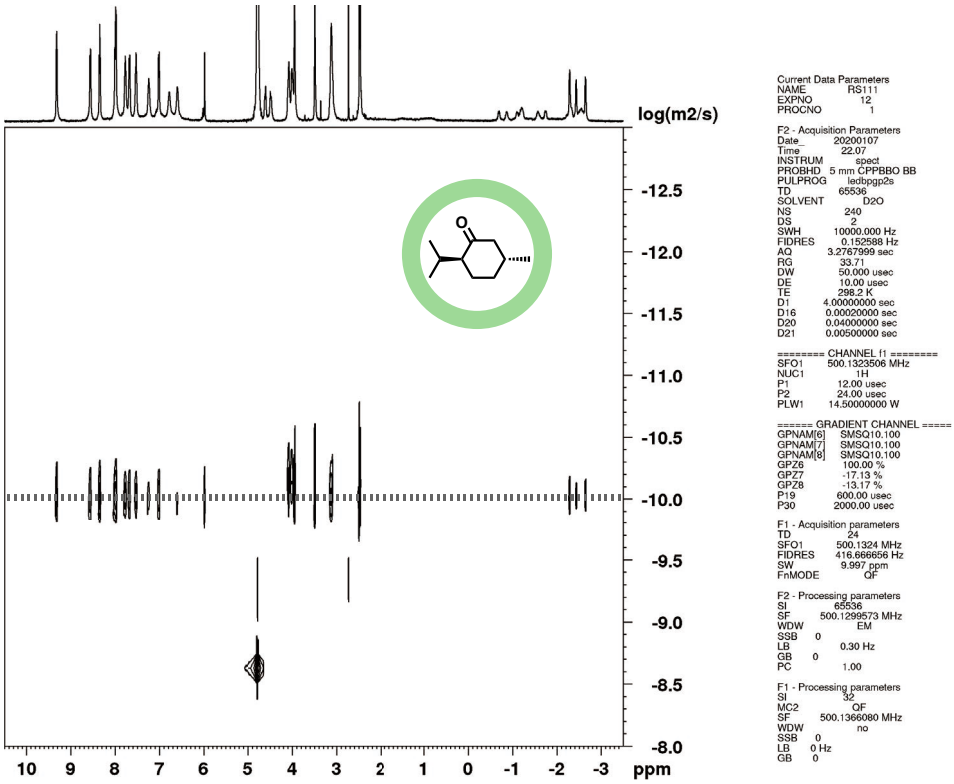


Figure S2. ^{1}H DOSY NMR spectrum (500 MHz, D_2O, 298 K) of **1•MTO**.

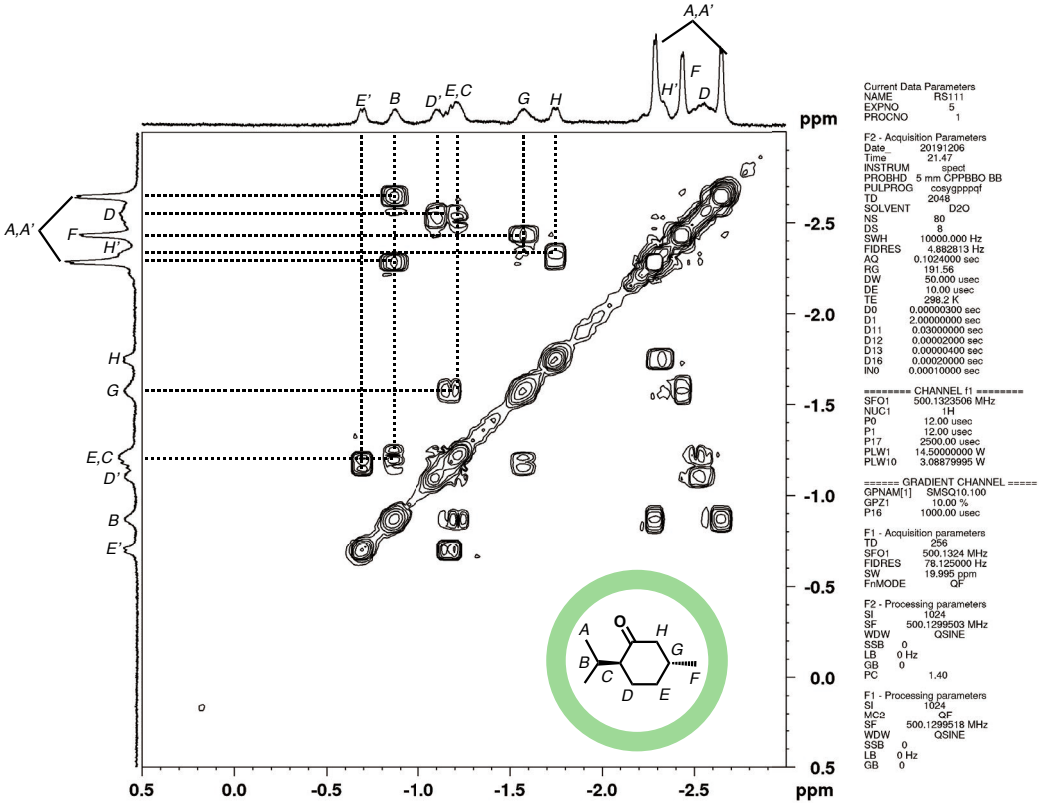


Figure S3a. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTO**.

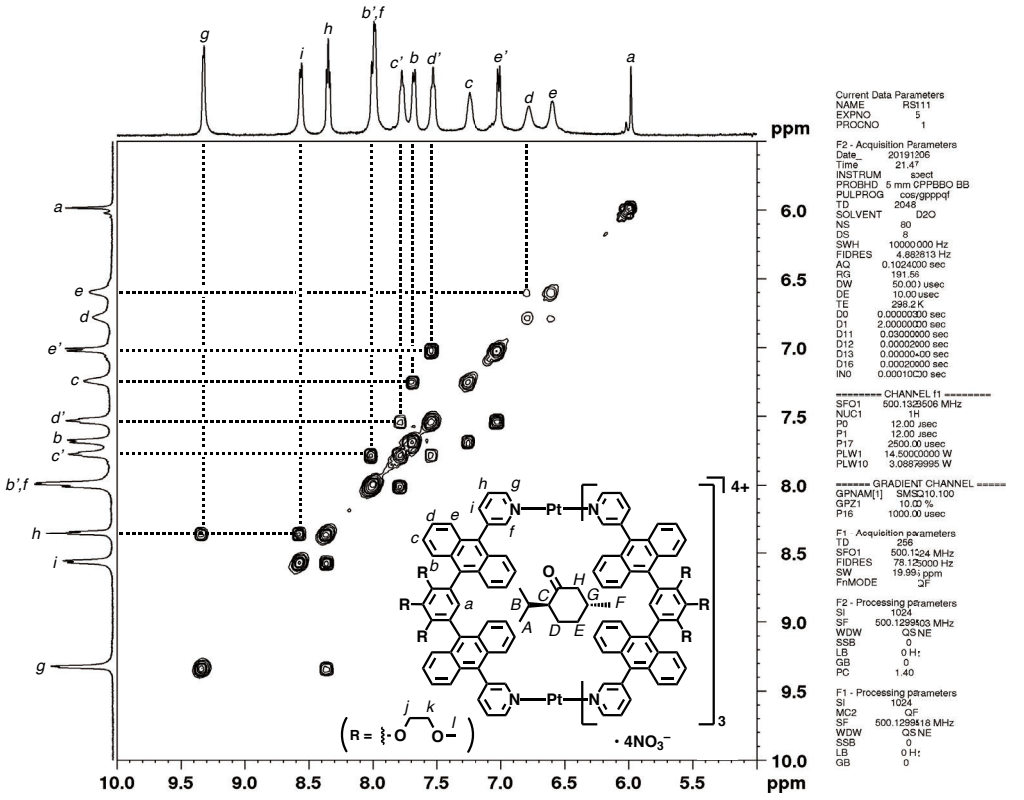


Figure S3b. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTO**.

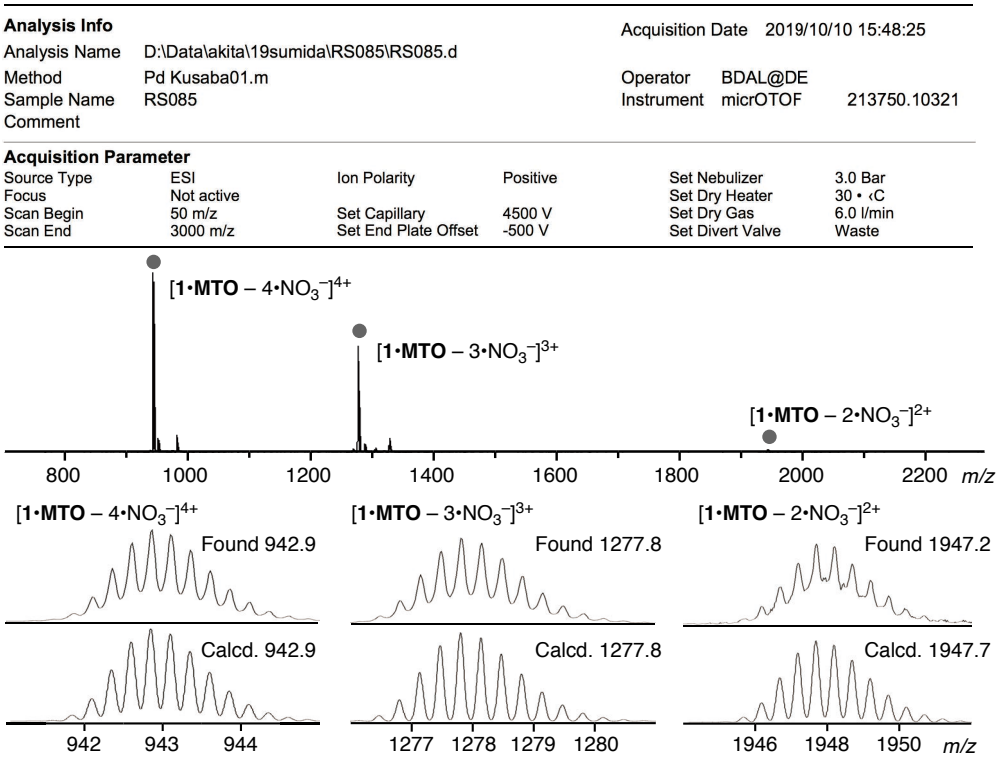
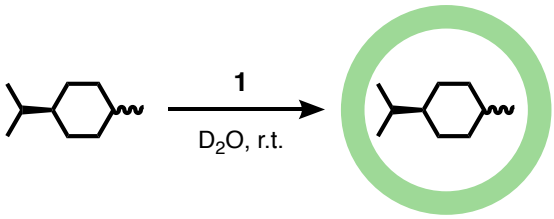


Figure S4. ESI-TOF MS spectrum (H_2O) of **1•MTO**.

Formation of 1•MTA RS016



Capsule **1** (1.0 mg, 0.26 μmol) and *p*-menthane (**MTA**; 0.06 mg, 0.43 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The quantitative formation of 1:1 host-guest complex **1•MTA** was confirmed by NMR and ESI-TOF MS analyses.

^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.44 (br, 3H, **MTA**), –2.35 (br, 3H, **MTA**), –2.31 (br, 2H, **MTA**), –2.17 (br, 3H, **MTA**), –2.01 (br, 2H, **MTA**), –1.93 (br, 2H, **MTA**), –1.78 (br, 1H, **MTA**), –1.69 (br, 1H, **MTA**), –1.61 (br, 1H, **MTA**), –1.47 (br, 1H, **MTA**), –1.38 (br, 1H, **MTA**), 2.51 (m, 24H, **1**), 3.15 (m, 16H, **1**), 3.51 (s, 12H, **1**), 3.97 (br, 8H, **1**), 4.04 (m, 8H, **1**), 4.11 (m, 8H, **1**), 4.51 (m, 4H, **1**), 4.64 (m, 4H, **1**), 6.10 (s, 4H, **1**), 6.49 (d, J = 9.4 Hz, 5H, **1**), 6.58 (d, J = 9.3 Hz, 3H, **1**), 6.88 (br, 8H, **1**), 7.07 (br, 8H, **1**), 7.41 (br, 8H, **1**), 7.57 (br, 16H, **1**), 7.69 (d, J = 9.3 Hz, 8H, **1**), 7.83 (br, 8H, **1**), 8.07 (br, 8H, **1**), 8.42 (dd, J = 6.6, 7.7 Hz, 8H, **1**), 8.68 (br, 8H, **1**), 9.24 (d, J = 5.0 Hz, 8H, **1**). ESI-TOF

MS (H_2O): *m/z* 1940.2 [**1•MTA** – 2•NO_3^-]$^{2+}$, 1273.2 [**1•MTA** – 3•NO_3^-]$^{3+}$, 939.2 [**1•MTA** – 4•NO_3^-]$^{4+}$.

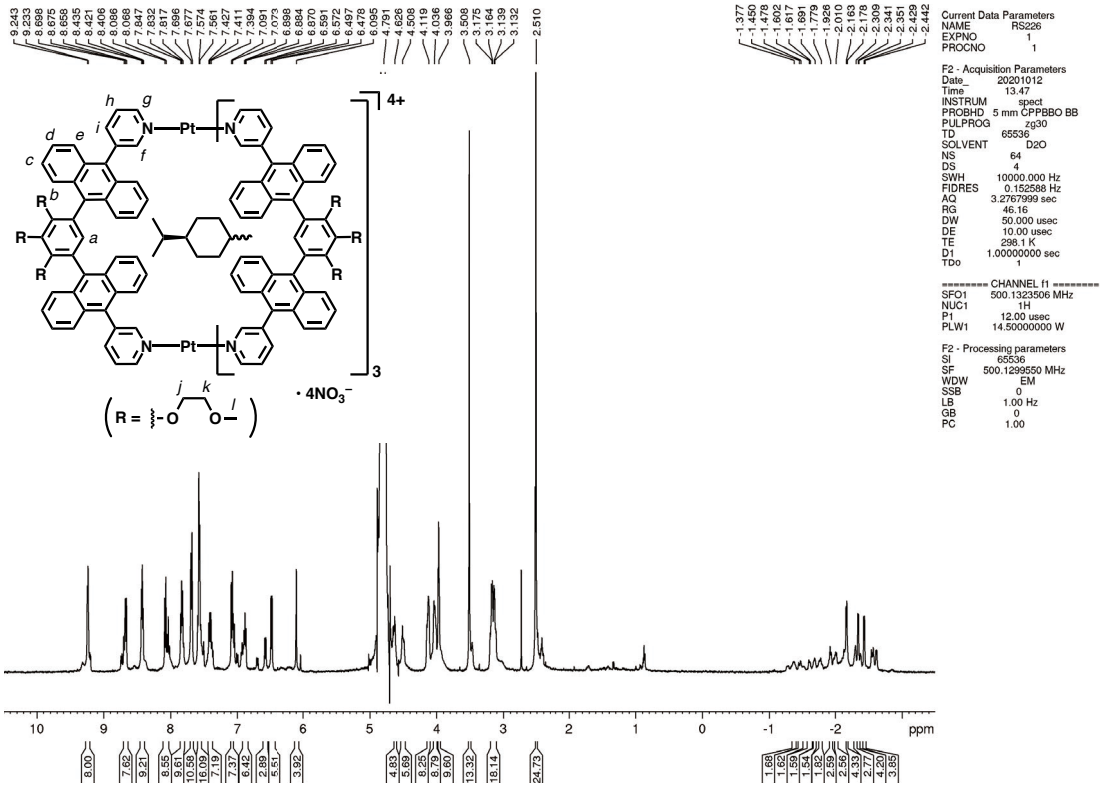


Figure S5. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTA**.

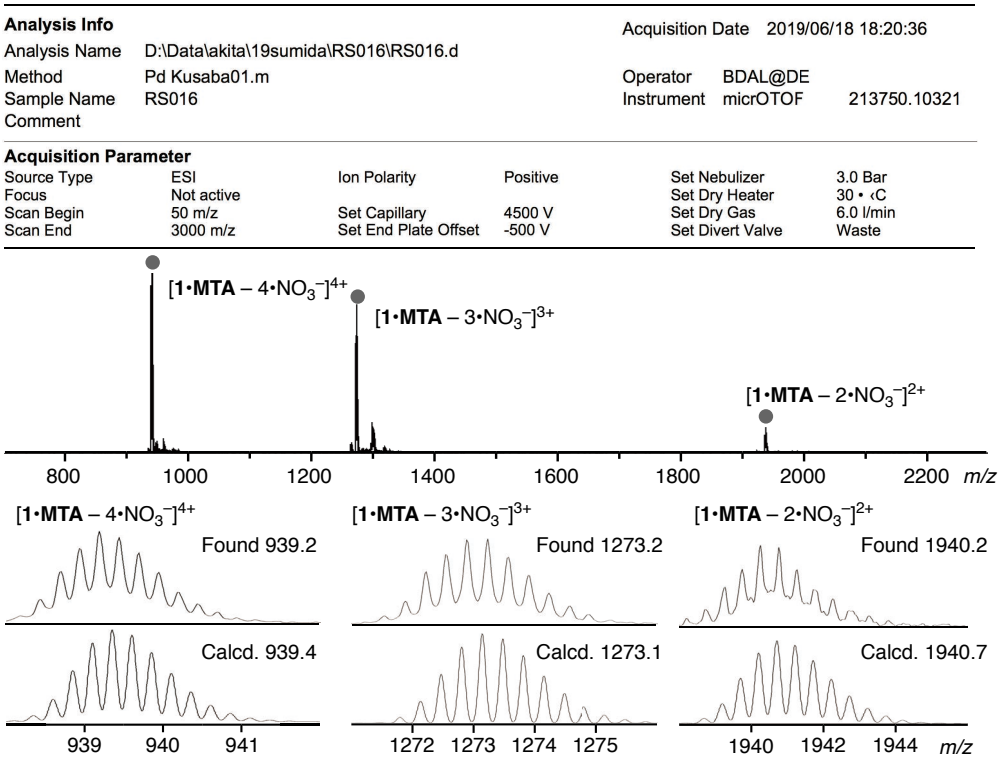
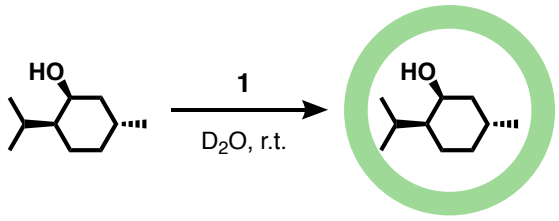


Figure S6. ESI-TOF MS spectrum (H_2O) of **1•MTA**.

Formation of 1•MTL RS018, 019



Capsule **1** (1.5 mg, 0.39 μmol) and (–)-menthol (**MTL**; 0.6 mg, 3.8 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The quantitative formation of 1:1 host-guest complex **1•MTL** was confirmed by NMR and ESI-TOF MS analyses. In the same way, 1:1 host-guest complex **1**•(+)-menthol was quantitatively formed from **1** (1.0 mg, 0.26 μmol) and (+)-menthol (0.4 mg, 2.6 μmol) and the ^{1}H NMR spectrum was comparable to that of **1•MTL**.

^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.52 (br, 8H, **MTL**), –2.38 (br, 5H, **MTL**), –2.09 (br, 1H, **MTO**), –1.92 (br, 2H, **MTL**), –1.77 (br, 1H, **MTL**), –1.60 (br, 1H, **MTL**), –1.32 (br, 1H, **MTL**), –1.22 (br, 1H, **MTL**), 2.55 (br, 24H, **1**), 3.19 (br, 16H, **1**), 3.52 (s, 12H, **1**), 3.98 (br, 8H, **1**), 4.11 (m, 16H, **1**), 4.58 (m, 8H, **1**), 5.91 (s, 4H, **1**), 6.91 (br, 16H, **1**), 7.17 (br, 8H, **1**), 7.50 (br, 16H, **1**), 7.70 (br, 16H, **1**), 7.81 (br, 8H, **1**), 7.97 (br, 8H, **1**), 8.40 (br, 8H, **1**), 8.71 (br, 8H, **1**), 9.17 (br, 8H, **1**). ESI-TOF MS (H_2O): *m/z* 1948.1

[**1•MTL** – 2•NO_3^-]$^{2+}$, 1278.2 [**1•MTL** – 3•NO_3^-]$^{3+}$, 943.4 [**1•MTL** – 4•NO_3^-]$^{4+}$.

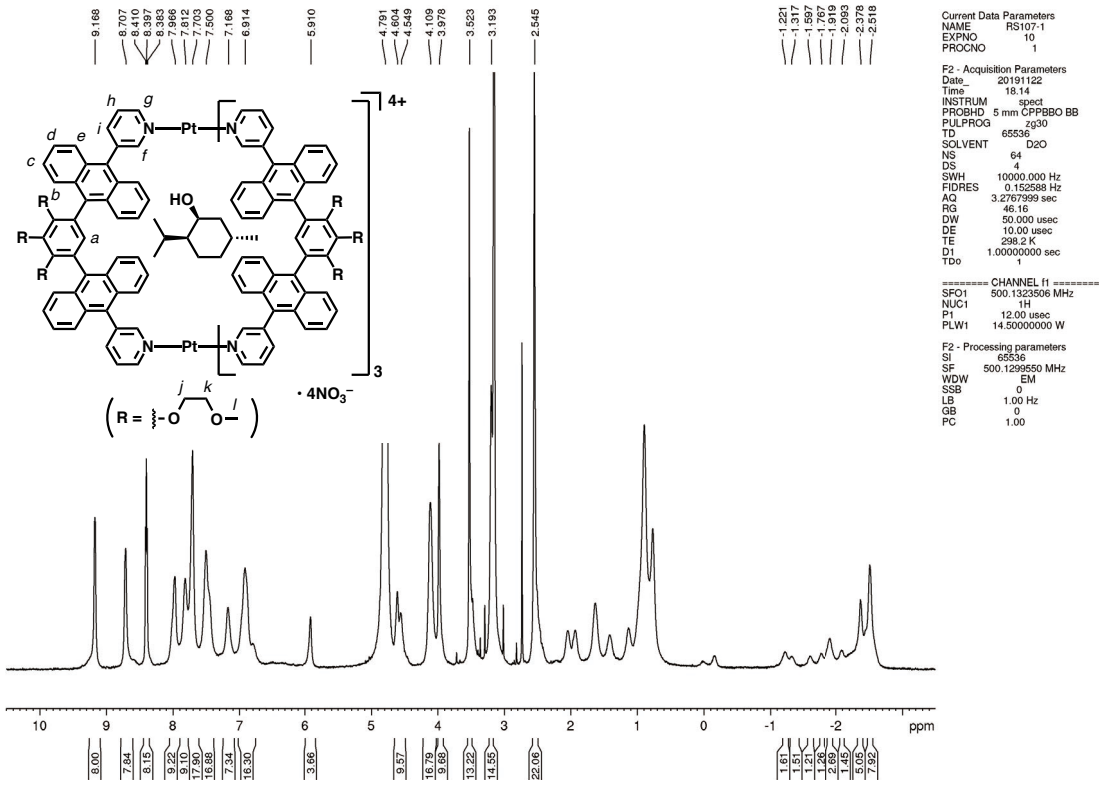


Figure S7a. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTL**.

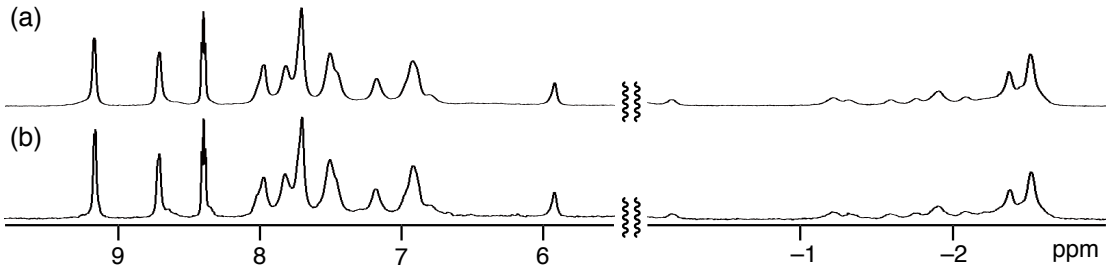


Figure S7b. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of a) **1•MTL** and b) **1**•(+)-menthol.

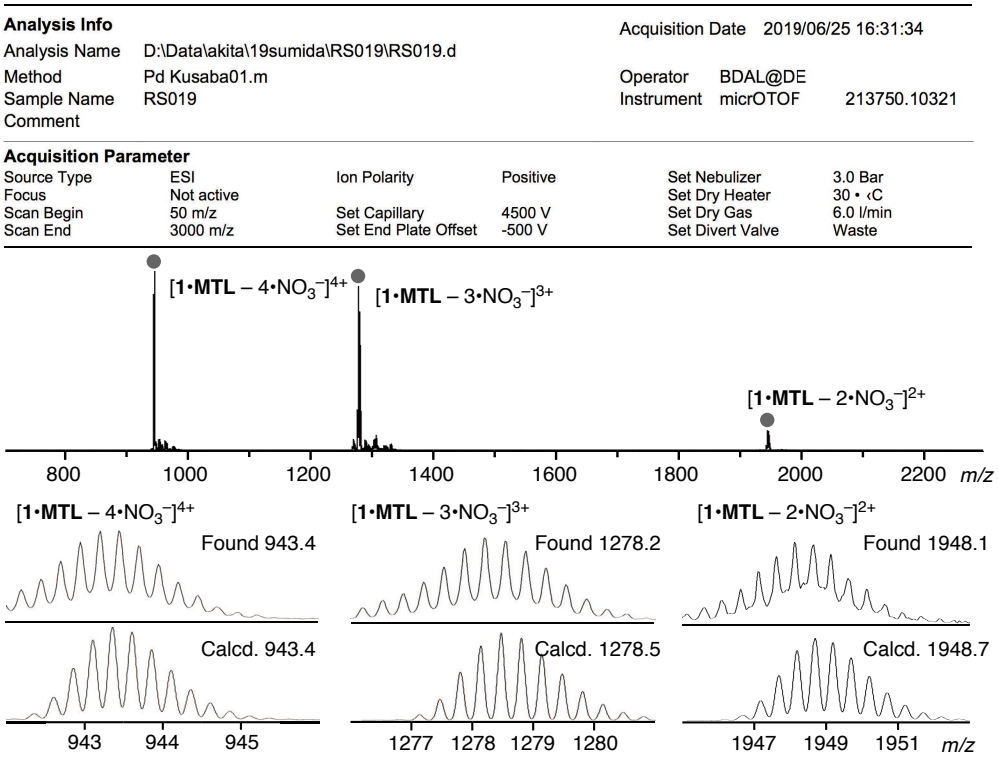
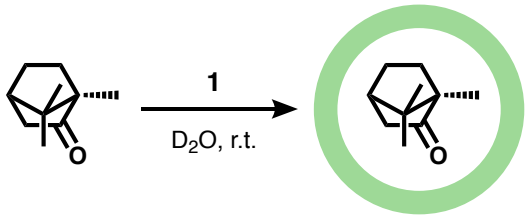


Figure S8. ESI-TOF MS spectrum (H_2O) of **1•MTL**.

Formation of 1•CMP RS086



Capsule **1** (1.0 mg, 0.26 μmol) and (–)-camphor (**CMP**; 0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. After removal of excess **CMP** under vacuum, the quantitative formation of 1:1 host-guest complex **1•CMP** was confirmed by NMR and ESI-TOF MS analyses.

^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.79 (br, 6H, **CMP**), –2.53 (br, 3H, **CMP**), –2.31 (br, 2H, **CMP**), –1.96 (br, 1H, **CMP**), –1.80 (br, 1H, **CMP**), –1.54 (br, 2H, **CMP**), –1.19 (br, 1H, **CMP**), 2.41 (br, 24H, **1**), 3.02 (br, 16H, **1**), 3.46 (s, 12H, **1**), 3.87 (m, 8H, **1**), 3.92 (m, 8H, **1**), 4.01 (m, 8H, **1**), 4.43 (m, 4H, **1**), 4.63 (m, 4H, **1**), 6.21 (s, 16H, **1**), 6.29 (s, 4H, **1**), 6.93 (br, 8H, **1**), 7.06 (d, J = 9.0 Hz, 8H, **1**), 7.51 (dd, J = 8.2, 7.1 Hz, 8H, **1**), 7.70 (br, 16H, **1**), 8.00 (br, 16H, **1**), 8.34 (dd, J = 6.6, 6.8 Hz, 8H, **1**), 8.47 (d, J = 7.2 Hz, 8H, **1**), 9.35 (d, J = 5.5 Hz, 8H, **1**). ESI-TOF MS (H_2O): m/z 1946.7 [**1•CMP** – 2•NO_3^-]$^{2+}$, 1277.1 [**1•CMP** – 3•NO_3^-]$^{3+}$, 942.4 [**1•CMP** – 4•NO_3^-]$^{4+}$.

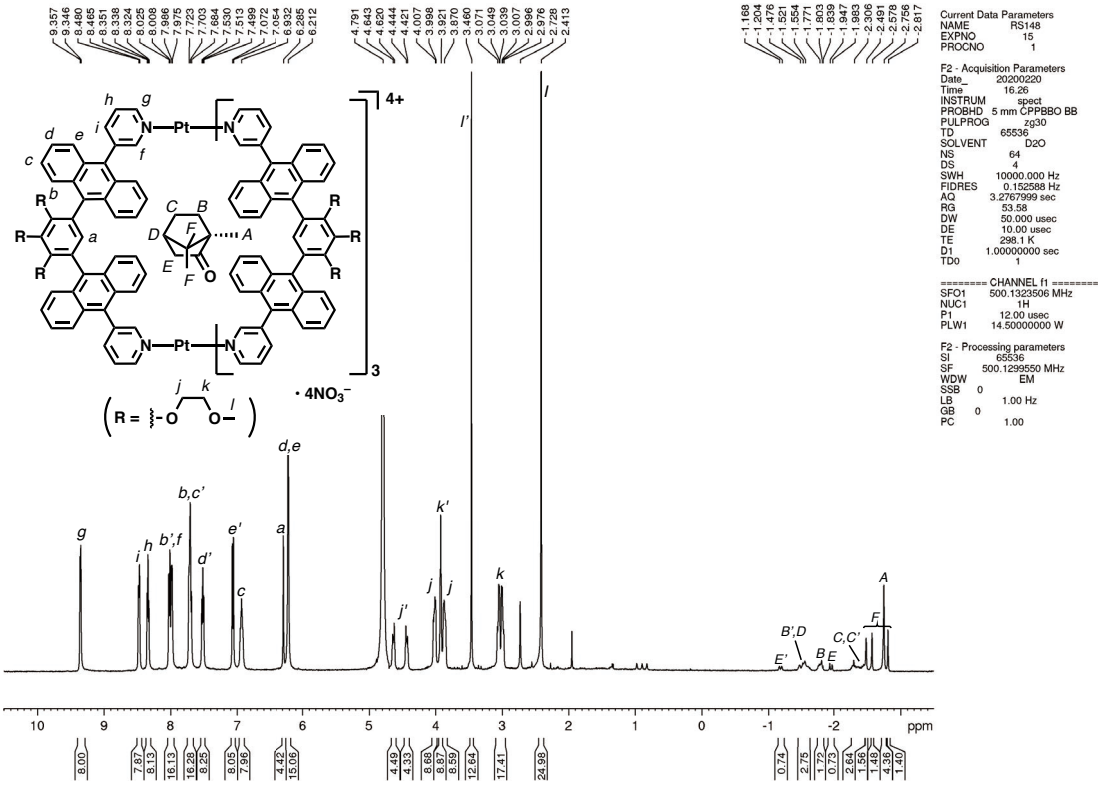


Figure S9. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1•CMP**.

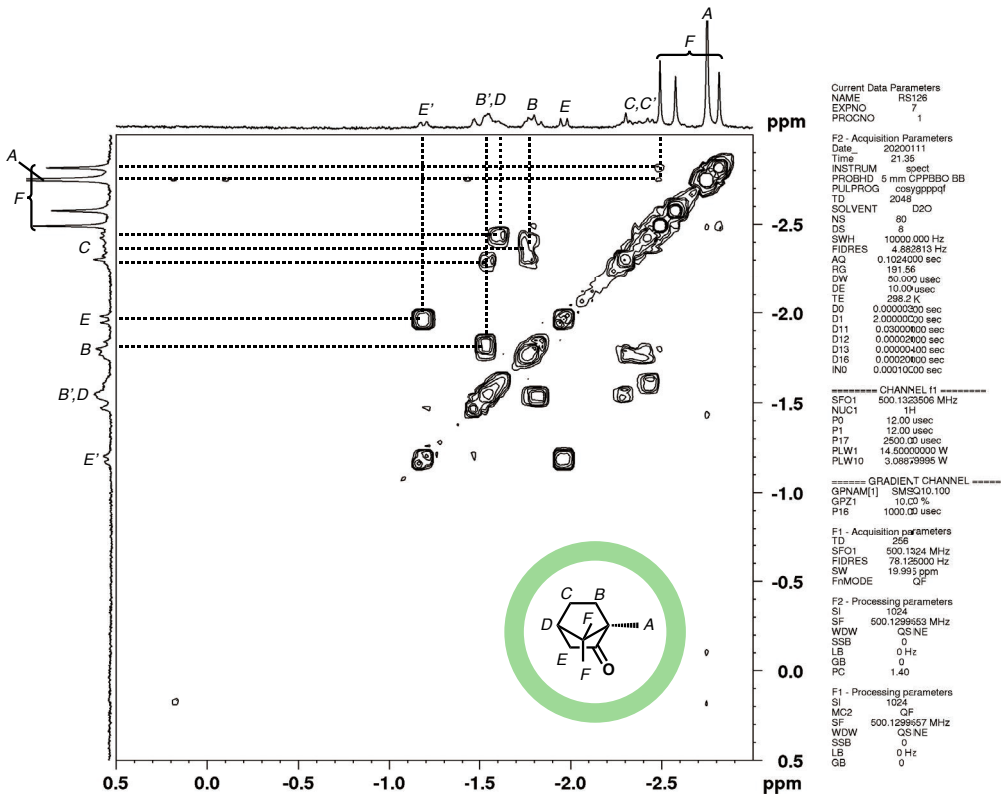


Figure S10. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, D_2O, r.t.) of **1•CMP**.

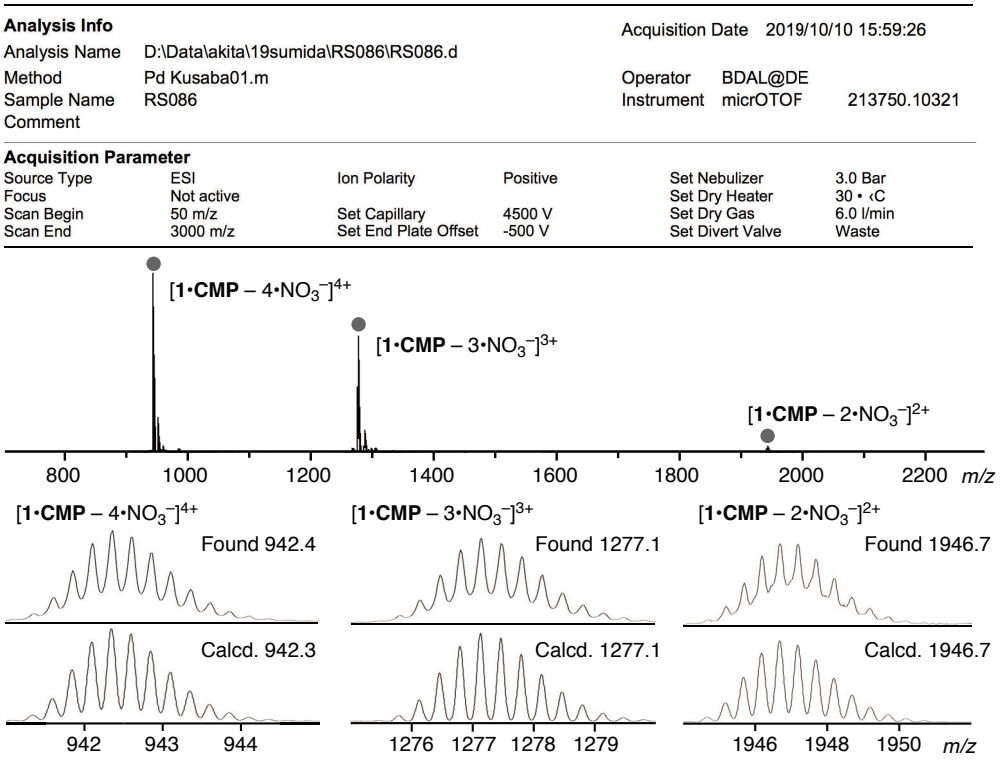
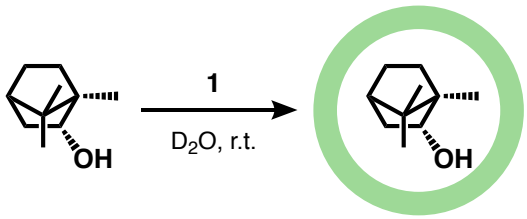


Figure S11. ESI-TOF MS spectrum (H_2O) of **1•CMP**.

Formation of 1•BNL RS045



Capsule **1** (1.0 mg, 0.26 μmol) and (–)-borneol (**BNL**; 0.3 mg, 1.7 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. After removal of excess **BNL** under vacuum, the quantitative formation of 1:1 host-guest complex **1•BNL** was confirmed by NMR and ESI-TOF MS analyses.

^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.67 (br, 3H, **BNL**), –2.58 (br, 4H, **BNL**), –2.28 (br, 3H, **BNL**), –2.18 (br, 1H, **BNL**), –2.10 (br, 2H, **BNL**), –1.68 (br, 2H, **BNL**), –1.55 (br, 1H, **BNL**), –1.21 (br, 2H, **BNL**), 2.42 (br, 24H, **1**), 3.02 (br, 16H, **1**), 3.46 (s, 12H, **1**), 3.86 (br, 8H, **1**), 3.92 (br, 8H, **1**), 4.01 (m, 8H, **1**), 4.43 (m, 4H, **1**), 4.63 (m, 4H, **1**), 6.23 (br, 16H, **1**), 6.36 (br, 4H, **1**), 6.93 (br, 8H, **1**), 7.08 (d, J = 8.9 Hz, 8H, **1**), 7.53 (dd, J = 8.2, 6.9 Hz, 8H, **1**), 7.71 (br, 16H, **1**), 7.92 (br, 8H, **1**), 8.02 (d, J = 8.5 Hz, 8H, **1**), 8.35 (dd, J = 6.6, 6.5 Hz, 8H, **1**), 8.50 (d, J = 7.8 Hz, 8H, **1**), 9.33 (d, J = 5.5 Hz, 8H, **1**). ESI-TOF MS (H_2O): m/z 1948.2 [**1•BNL** – 2•NO_3^-]$^{2+}$, 1278.1 [**1•BNL** – 3•NO_3^-]$^{3+}$,

942.9 [**1•BNL** – 4•NO_3^-]$^{4+}$.

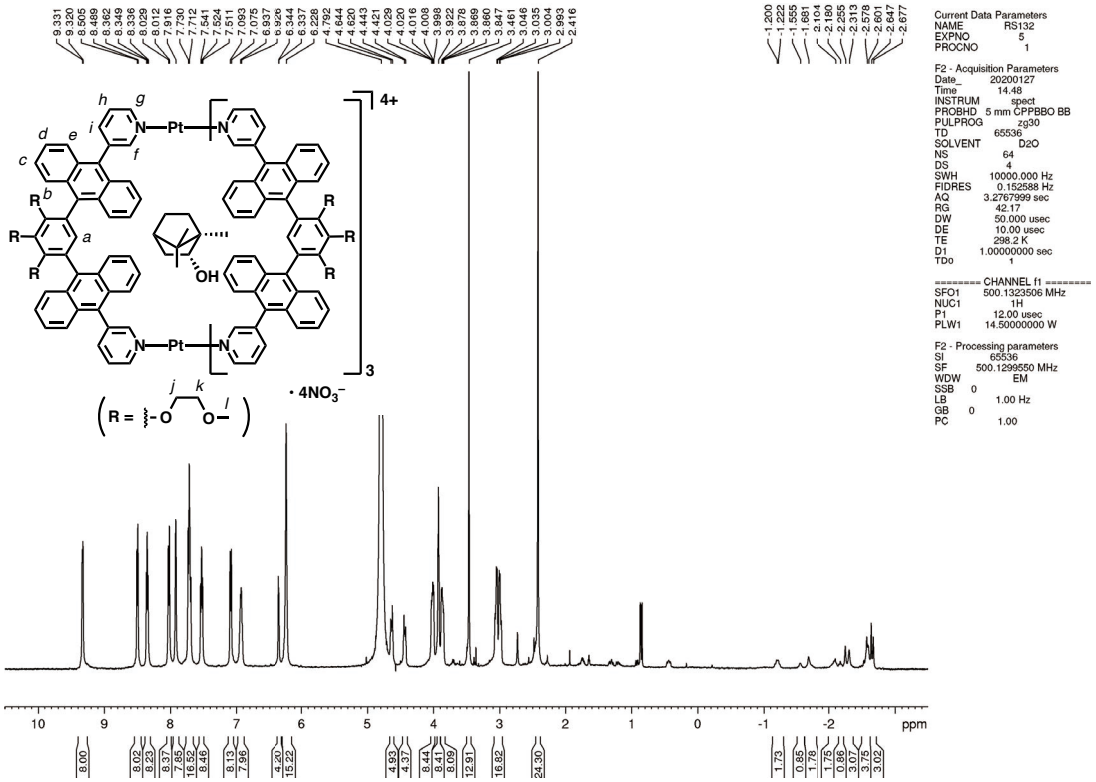


Figure S12. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1•BNL**.

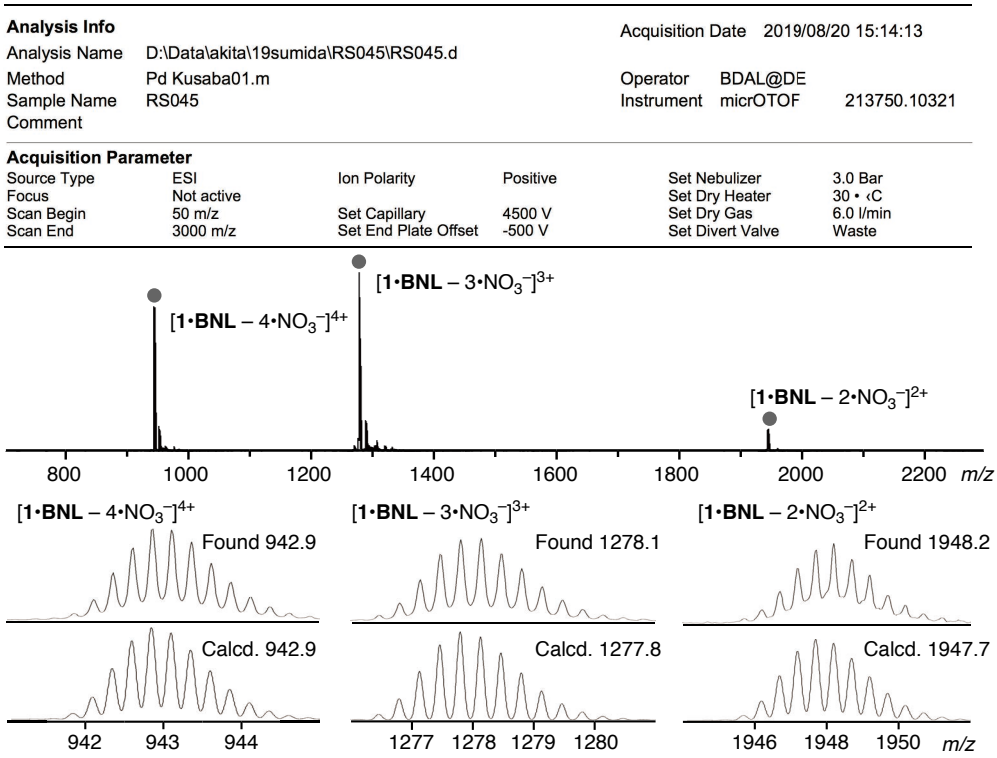
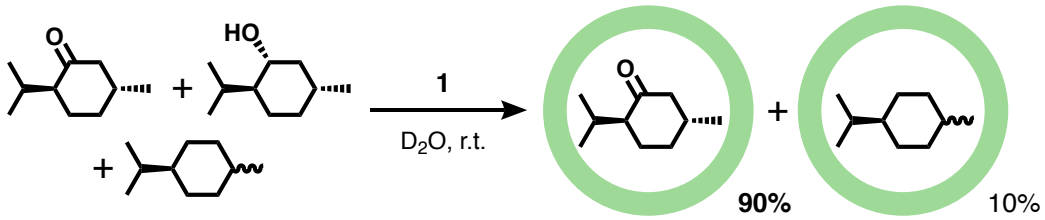


Figure S13. ESI-TOF MS spectrum (H_2O) of **1•BNL**.

Competitive binding of MTO, MTA, and MTL by 1 RS038



Capsule **1** (1.0 mg, 0.26 μmol), **MTO** (0.4 mg, 2.6 μmol), **MTA** (0.4 mg, 2.6 μmol) and **MTL** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The formation of complexes **1•MTO**, **1•MTA**, and **1•MTL** in a 90:10:0 ratio was confirmed by NMR analysis.

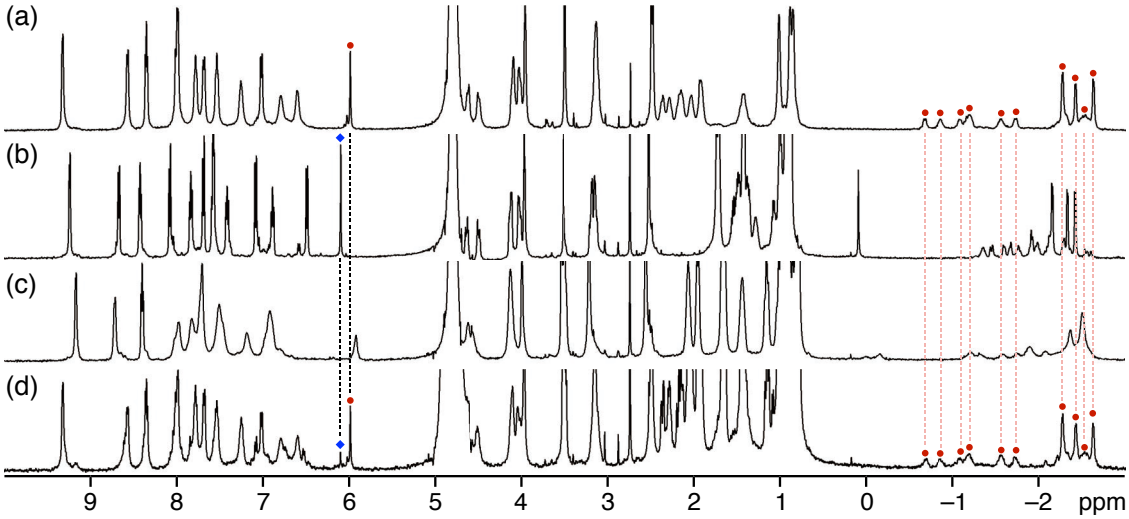
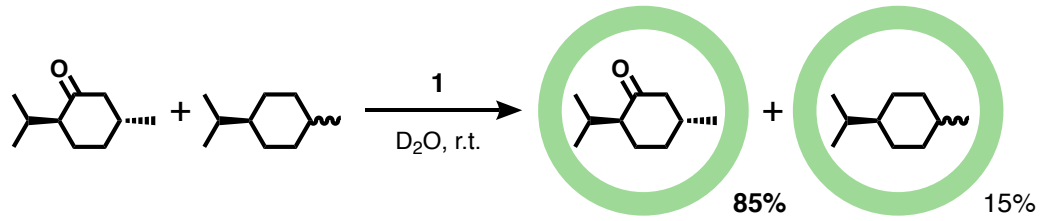


Figure S14. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO**, (b) **1•MTA**, (c) **1•MTL**, and (d) products after mixing **MTO**, **MTA**, and **MTL** with **1** at r.t. for 1 h.

Competitive binding of MTO and MTA by 1 RS031



Capsule **1** (1.0 mg, 0.26 μmol), **MTO** (0.4 mg, 2.6 μmol), and **MTA** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The formation of complexes **1•MTO** and **1•MTA** in an 85:15 ratio was confirmed by NMR analysis.

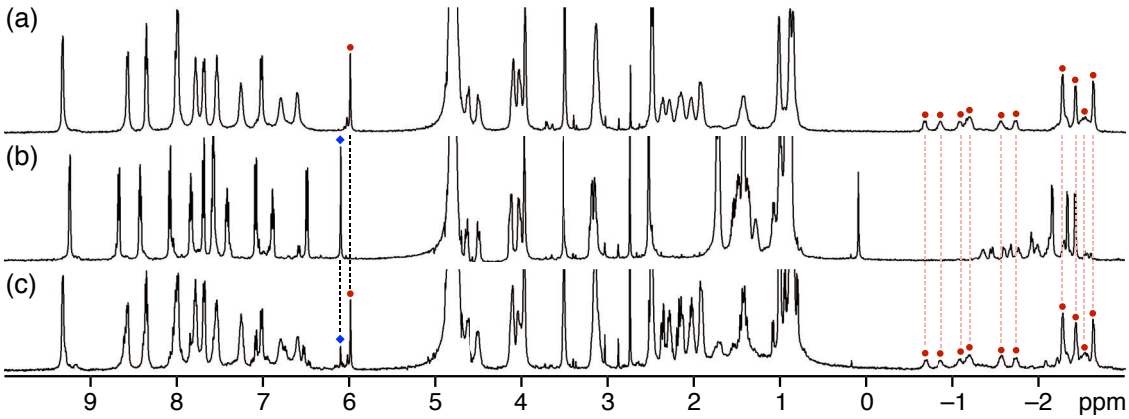
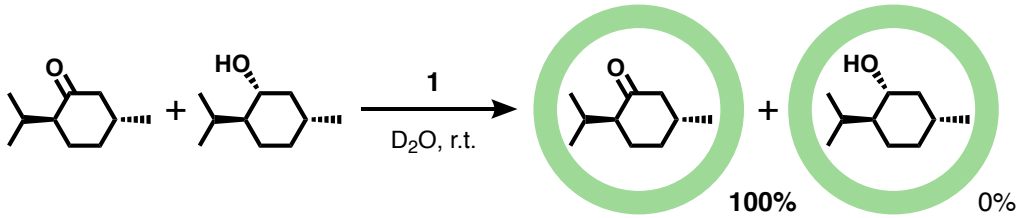


Figure S15. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO**, (b) **1•MTA**, and (c) products after mixing **MTO** and **MTA** with **1** at r.t. for 1 h.

Competitive binding of MTO and MTL by 1 RS029



Capsule **1** (1.0 mg, 0.26 μmol), **MTO** (0.4 mg, 2.6 μmol), and **MTL** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The exclusive formation of a **1•MTO** complex was confirmed by NMR and ESI-TOF MS analyses.

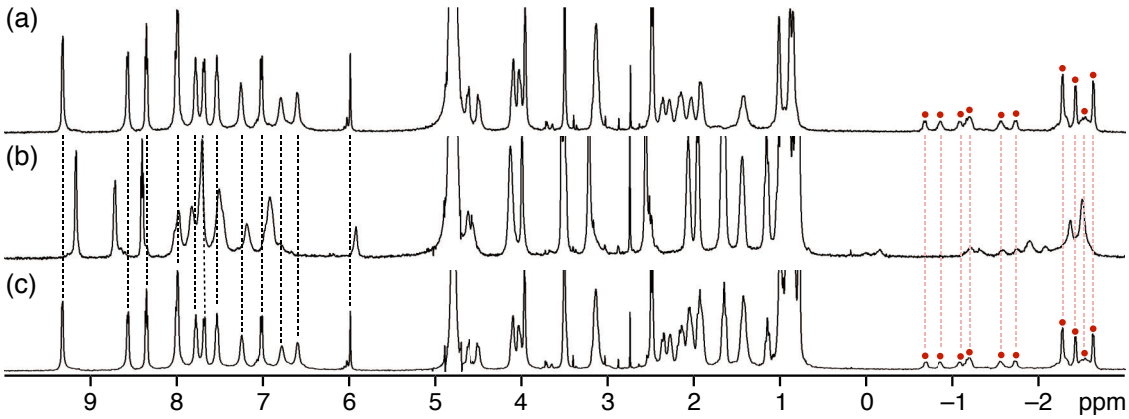


Figure S16a. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO**, (b) **1•MTL**, and (c) products after mixing **MTO** and **MTL** with **1** at r.t. for 1 h.

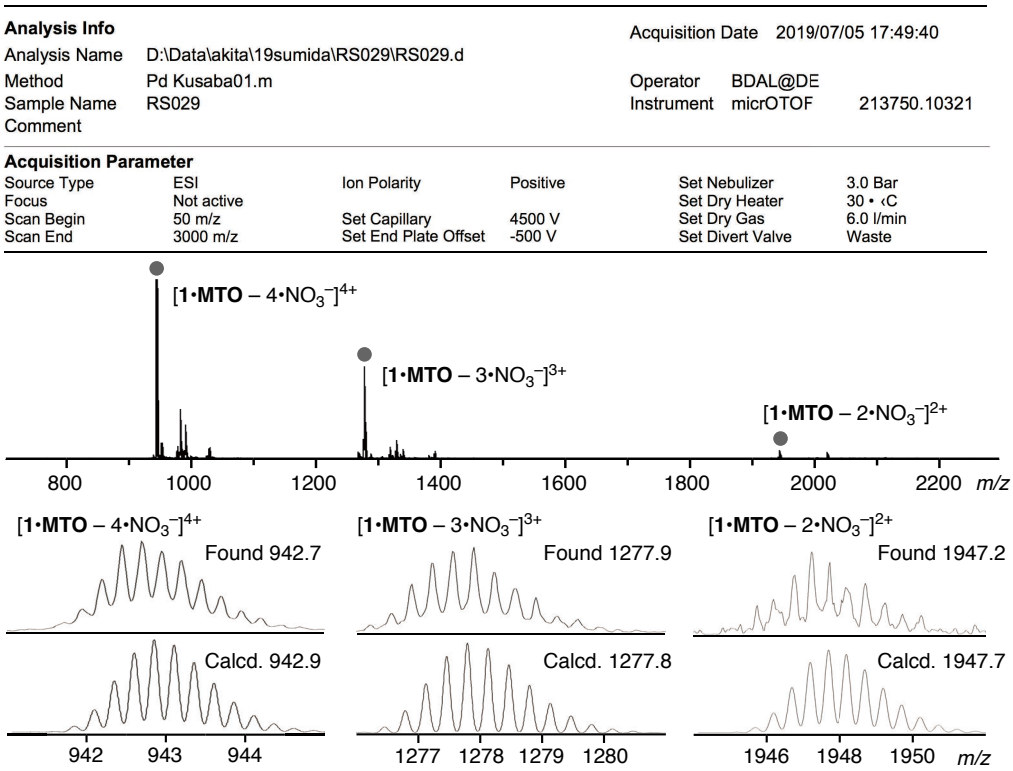
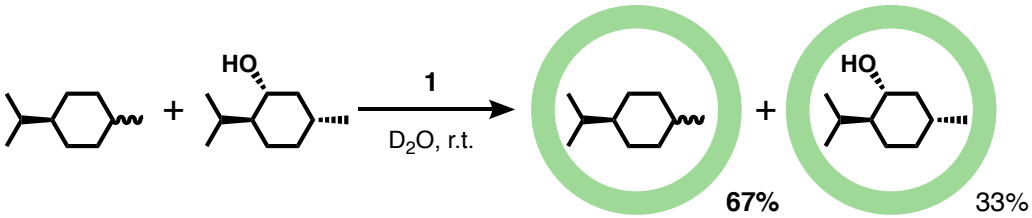


Figure S16b. ESI-TOF MS spectrum (H_2O) of products after mixing **MTO** and **MTL** with **1** at r.t. for 1 h.

Competitive binding of MTA and MTL by 1 RS030



Capsule **1** (1.0 mg, 0.26 μmol), **MTA** (0.4 mg, 2.6 μmol), and **MTL** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The formation of complexes **1•MTA** and **1•MTL** in a 67:33 ratio was confirmed by NMR analysis.

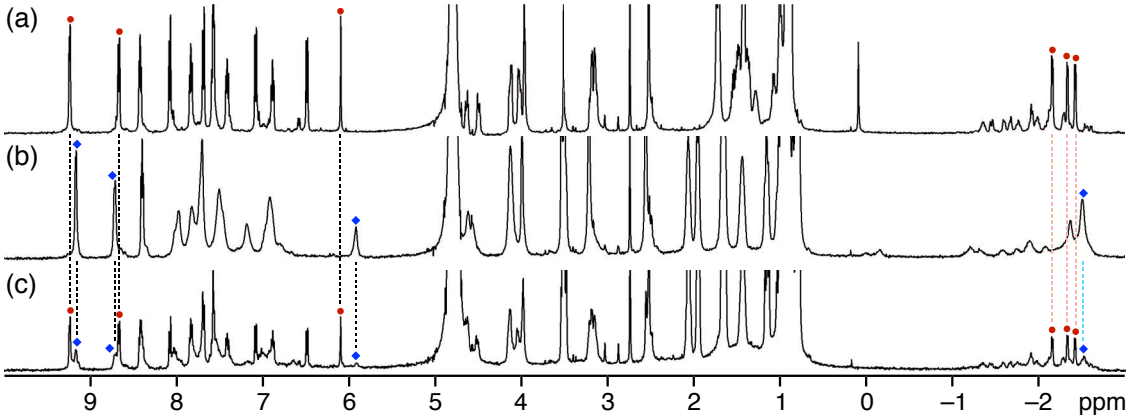
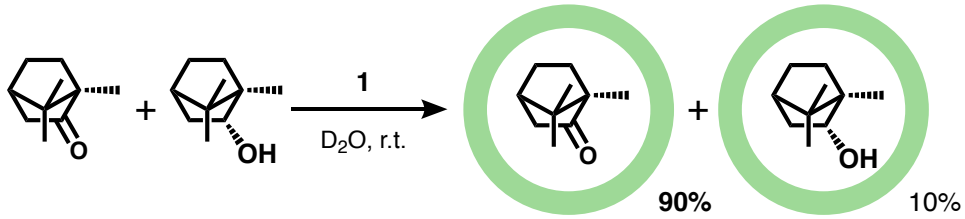


Figure S17. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTA**, (b) **1•MTL**, and (c) products after mixing **MTA** and **MTL** with **1** at r.t. for 1 h.

Competitive binding of CMP and BNL by 1 RS088



Capsule **1** (1.0 mg, 0.26 μmol), **CMP** (0.4 mg, 2.6 μmol), and **BNL** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The formation of complexes **1•CMP** and **1•BNL** in a 90:10 ratio was confirmed by NMR analysis.

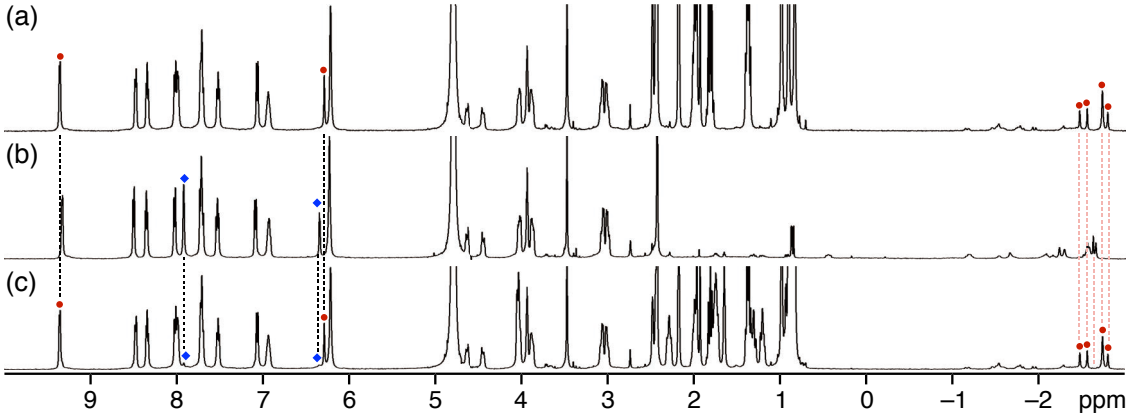
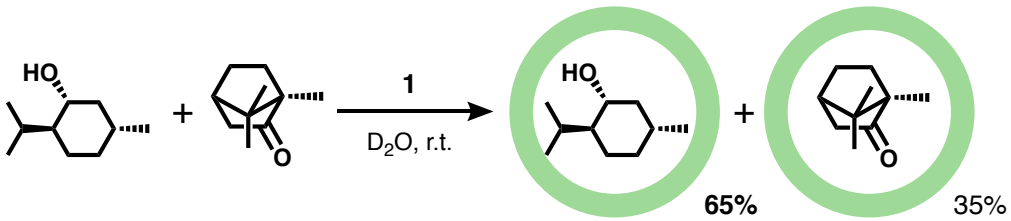


Figure S18. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•CMP**, (b) **1•BNL**, and (c) products after mixing **CMP** and **BNL** with **1** at r.t. for 1 h.

Competitive binding of MTL and CMP by 1 RS087



Capsule **1** (1.0 mg, 0.26 μmol), **MTL** (0.4 mg, 2.6 μmol), and **CMP** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The formation of complexes **1•MTL** and **1•CMP** in a 65:35 ratio was confirmed by NMR analysis.

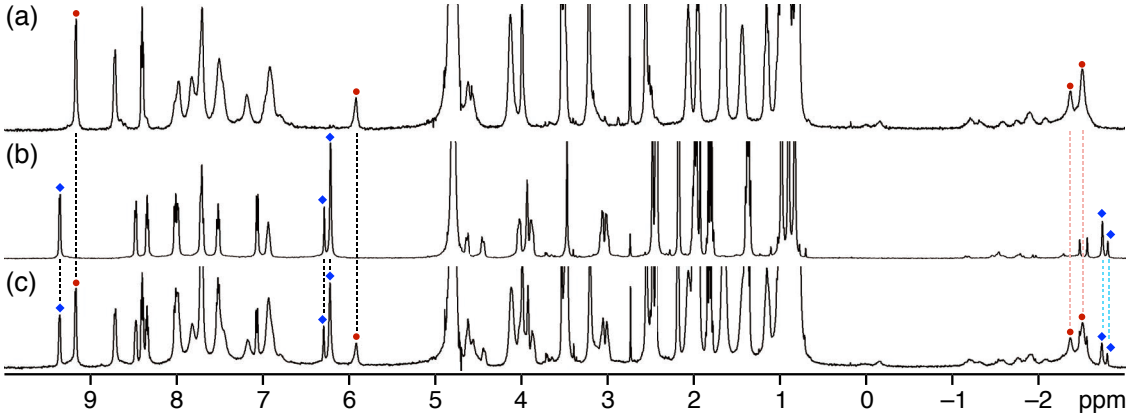


Figure S19. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTL**, (b) **1•CMP**, and (c) products after mixing **MTL** and **CMP** with **1** at r.t. for 1 h.

Thermodynamic studies of 1•MTO and 1•CMP RS215, 276

Isothermal titration calorimetry (ITC) measurements were performed by dropping H_2O solutions of **1** (0.75 mM, 273 μL) to a H_2O solution of **MTO** (0.045 mM, 1.46 mL) at 25 ºC and H_2O solutions of **CMP** (8.25 mM, 107 μL) to a H_2O solution of **1** (0.16 mM, 1.46 mL) at 25 ºC.

Table S1. Thermodynamic parameters and binding constants (K_a) for the formation of complexes **1•MTO** and **1•CMP**, as obtained by ITC experiments (H_2O, 298 K).

Complex	ΔH [kcal mol^{-1}]	$T\Delta S$ [kcal mol^{-1}]	ΔG [kcal mol^{-1}]	K_a / 10^5 [M^{-1}]
1•MTO	–20.2 ± 0.35	–12.3	–7.94	6.62 ± 8.81
1•CMP	–3.56 ± 0.11	3.78	–7.34	2.42 ± 0.63

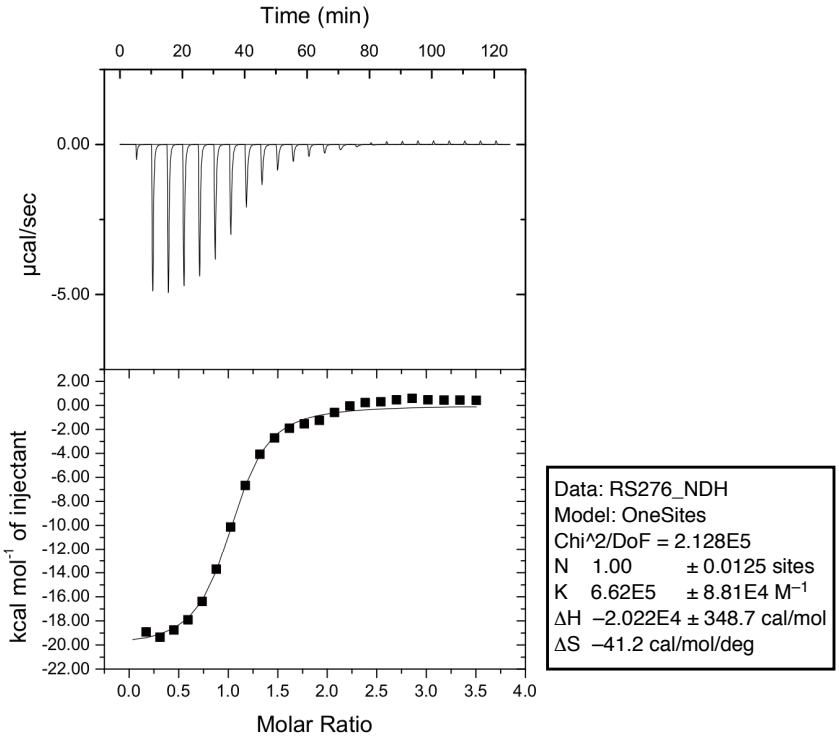


Figure S20. ITC thermograph (H_2O, 25 ºC) and its titration curve of **1** to **MTO**. The solid line represents the best-fitting curve obtained from the ‘‘one sites’’ model.

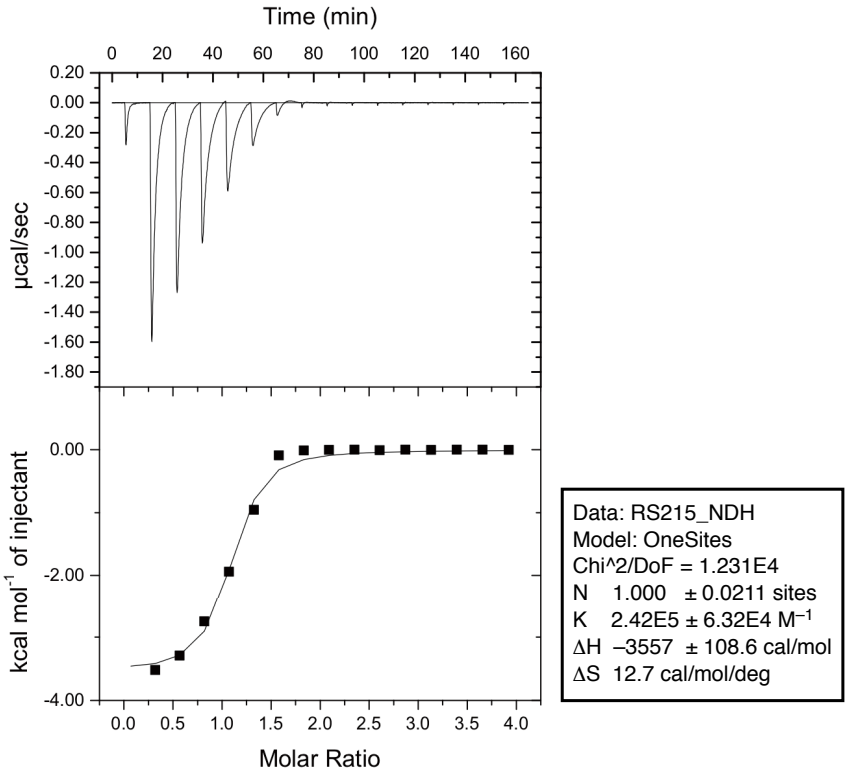
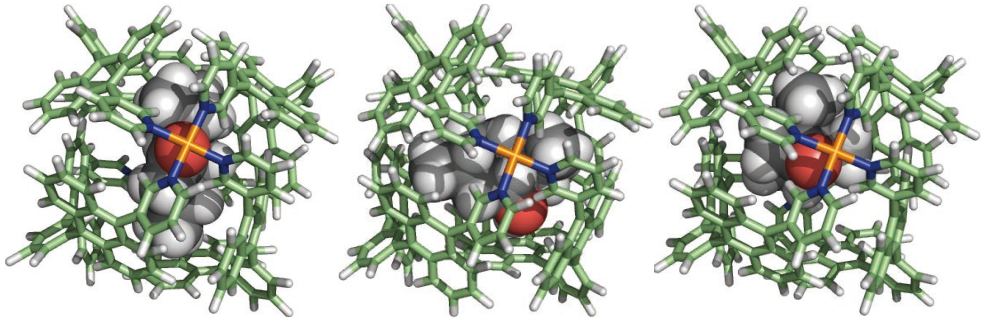


Figure S21. ITC thermograph (H_2O, 25 ºC) and its titration curve of **CMP** to **1**. The solid line represents the best-fitting curve obtained from the ‘‘one sites’’ model.



		1•MTO	1•MTL	1•CMP
CH-π interaction	≦ 3.6 Å	1	2	0
	3.7-4.0 Å	6	3	5
H••O=C interaction	≦ 3.9 Å	3	0	3

Figure S22. Optimized structures of **1•MTO**, **1•MTL**, and **1•CMP** (R = -H) and the numbers of CH-π and hydrogen-bonding interactions.

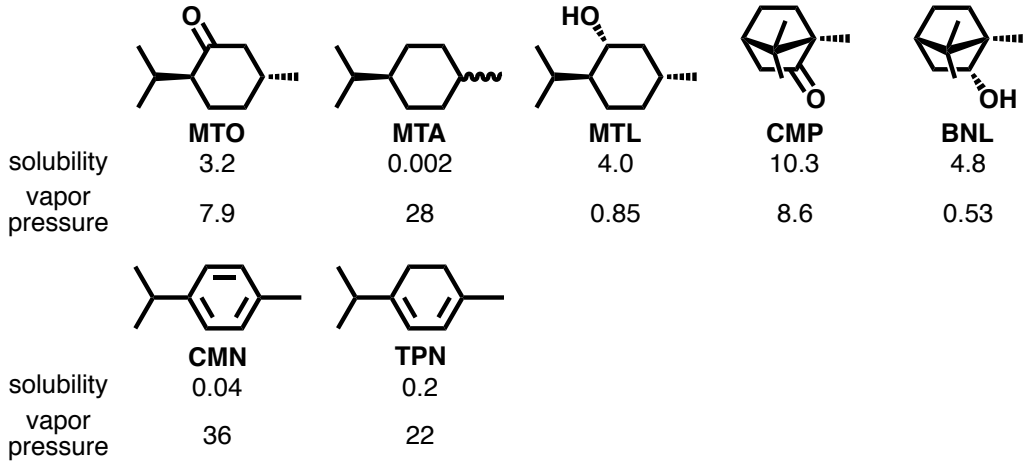
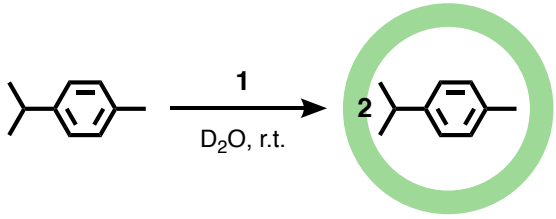


Figure S23. Water solubility (mM) and vapor pressure ($\times 10^{-4}$ atm) of CMTs (25 ºC).[S2-7]

Formation of 1•(CMN)$_2$ RS113



Capsule **1** (1.0 mg, 0.26 μmol) and *p*-cymene (**CMN**; 0.4 mg, 2.7 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 40 min. The quantitative formation of 1:2 host-guest complex **1**•(**CMN**)$_2$ was confirmed by NMR and ESI-TOF MS analyses.

^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.44 (d, J = 6.4 Hz, 6H, **CMN**), –2.37 (d, J = 6.5 Hz, 6H, **CMN**), –1.59 (s, 6H, **CMN**), –0.73 (br, 2H, **CMN**), 2.51 (s, 24H, **1**), 3.52 (s, 12H, **1**), 3.57 (d, J = 7.8 Hz, 4H, **CMN**), 3.99 (br, 8H, **1**), 4.08 (m, 8H, **1**), 4.13 (m, 8H, **1**), 4.50 (m, 4H, **1**), 4.54 (m, 4H, **1**), 6.21 (s, 4H, **1**), 6.60 (d, J = 8.7 Hz, 8H, **1**), 6.87 (d, J = 8.9 Hz, 8H, **1**), 6.97 (dd, J = 7.7, 7.4 Hz, 8H, **1**), 7.04 (s, 8H, **1**), 7.39 (dd, J = 7.6, 7.6 Hz, 8H, **1**), 7.49 (dd, J = 7.8, 7.3 Hz, 8H, **1**), 7.81 (br, 16H, **1**), 8.08 (d, J = 8.8 Hz, 8H, **1**), 8.31 (dd, J = 6.8, 6.8 Hz, 8H, **1**), 8.63 (d, J = 7.8 Hz, 8H, **1**), 9.01 (d, J = 5.6 Hz, 8H, **1**). ESI-TOF MS (H_2O): m/z 2004.8 [**1**•(**CMN**)$_2$ – 2•NO_3^-]$^{2+}$, 1315.6 [**1**•(**CMN**)$_2$ – 3•NO_3^-]$^{3+}$, 971.2 [**1**•(**CMN**)$_2$ – 4•NO_3^-]$^{4+}$.

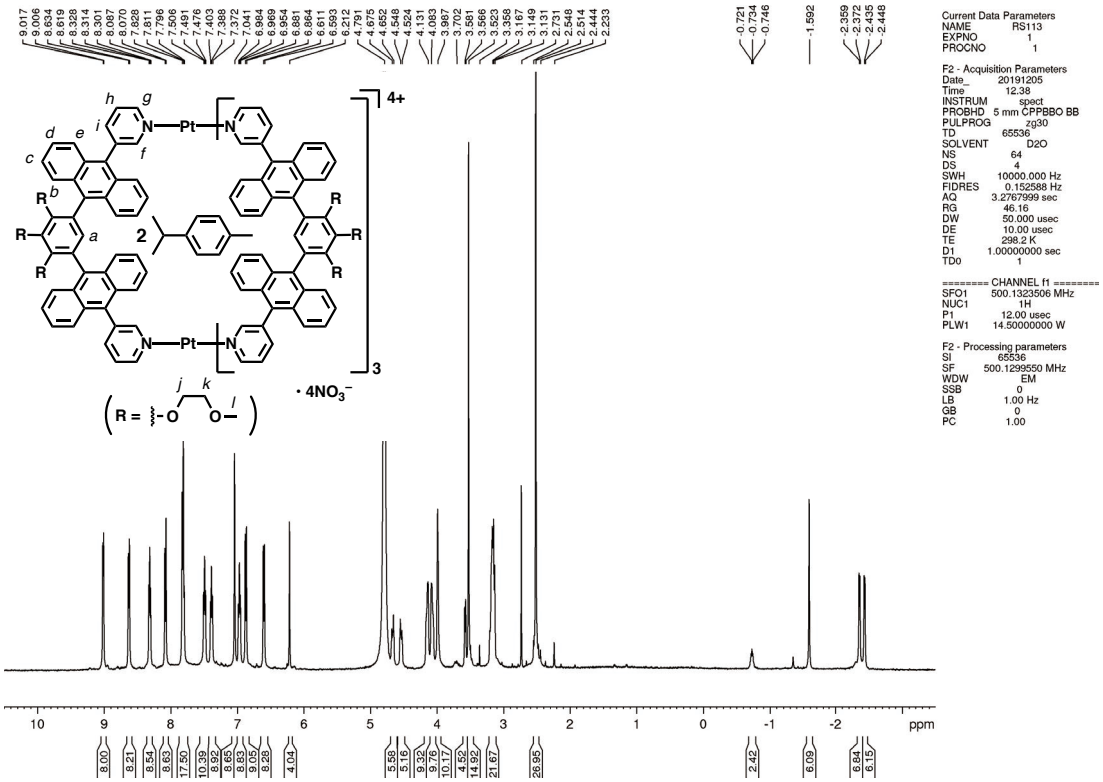


Figure S24. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1**•(**CMN**)$_2$.

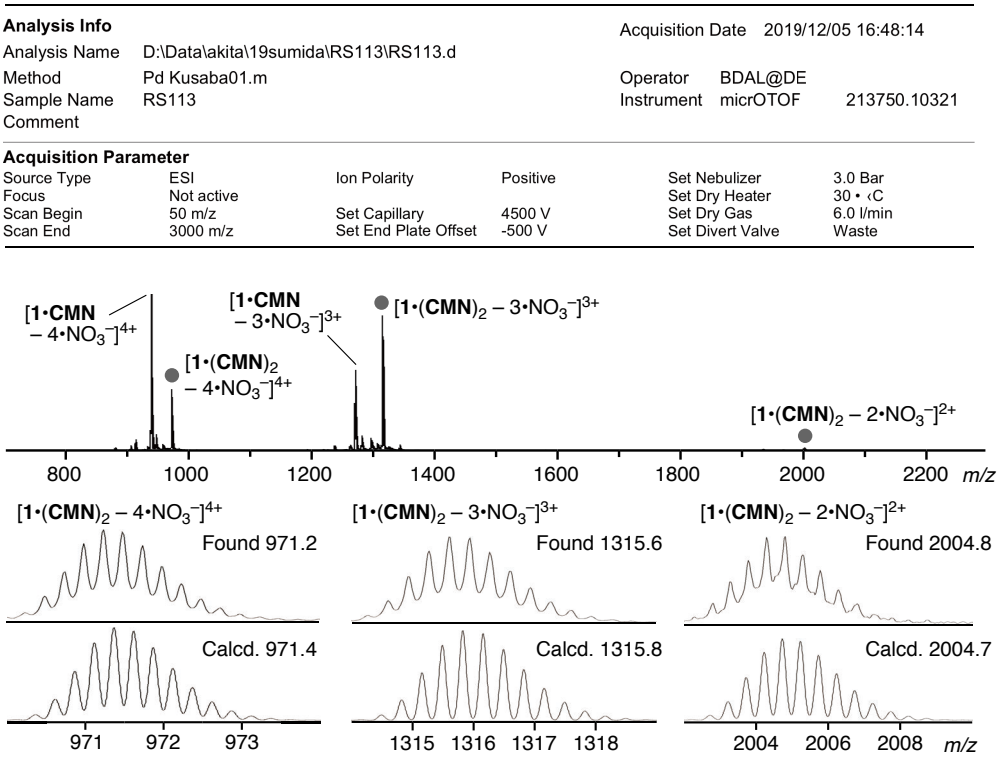
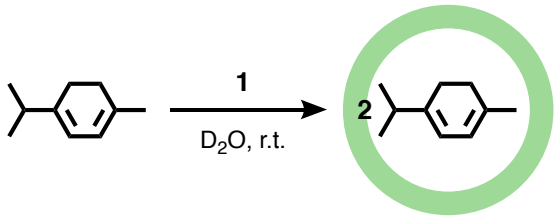


Figure S25. ESI-TOF MS spectrum (H_2O) of **1**•(**CMN**)$_2$.

Formation of 1•(TPN)$_2$ RS114



Capsule **1** (1.0 mg, 0.26 μmol) and α-terpinene (**TPN**; 0.4 mg, 2.7 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 40 min. The quantitative formation of 1:2 host-guest complex **1**•(**TPN**)$_2$ was confirmed by NMR and ESI-TOF MS analyses.

^{1}H NMR (500 MHz, D_2O, r.t.): δ –2.49 (br, 1H, **TPN**), –2.66 (br, 1H, **TPN**), –2.55 (d, J = 6.4 Hz, 6H, **TPN**), –2.48 (d, J = 5.8 Hz, 6H, **TPN**), –2.37 (br, 1H, **TPN**), –2.15 (br, 1H, **TPN**), –1.94 (s, 6H, **TPN**), –1.70 (br, 2H, **TPN**), –1.46 (m, 2H, **TPN**), –1.36 (m, 2H, **TPN**), –1.07 (m, 2H, **TPN**), –0.94 (m, 2H, **TPN**), 2.50 (m, 24H, **1**), 3.15 (m, 16H, **1**), 3.51 (s, 12H, **1**), 3.97 (br, 8H, **1**), 4.03 (m, 8H, **1**), 4.11 (m, 8H, **1**), 4.51 (m, 4H, **1**), 4.64 (m, 4H, **1**), 6.07 (s, 4H, **1**), 6.59 (d, J = 9.0 Hz, 1H, **1**), 6.99 (br, 16H, **1**), 7.36 (br, 8H, **1**), 7.48 (s, 8H, **1**), 7.53 (dd, J = 7.7, 7.7 Hz, 8H, **1**), 7.73 (d, J = 9.4 Hz, 8H, **1**), 7.81 (dd, J = 7.5, 7.7 Hz, 8H, **1**), 8.05 (d, J = 8.7 Hz, 8H, **1**), 8.38 (dd, J = 6.9, 6.4 Hz, 8H, **1**), 8.66 (br, 8H, **1**), 9.17 (br, 8H, **1**). ESI-TOF MS (H_2O): m/z 2006.8 [**1**•(**TPN**)$_2$ – 2•NO_3^-]$^{2+}$, 1316.9 [**1**•(**TPN**)$_2$ – 3•NO_3^-]$^{3+}$, 972.2 [**1**•(**TPN**)$_2$ – 4•NO_3^-]$^{4+}$.

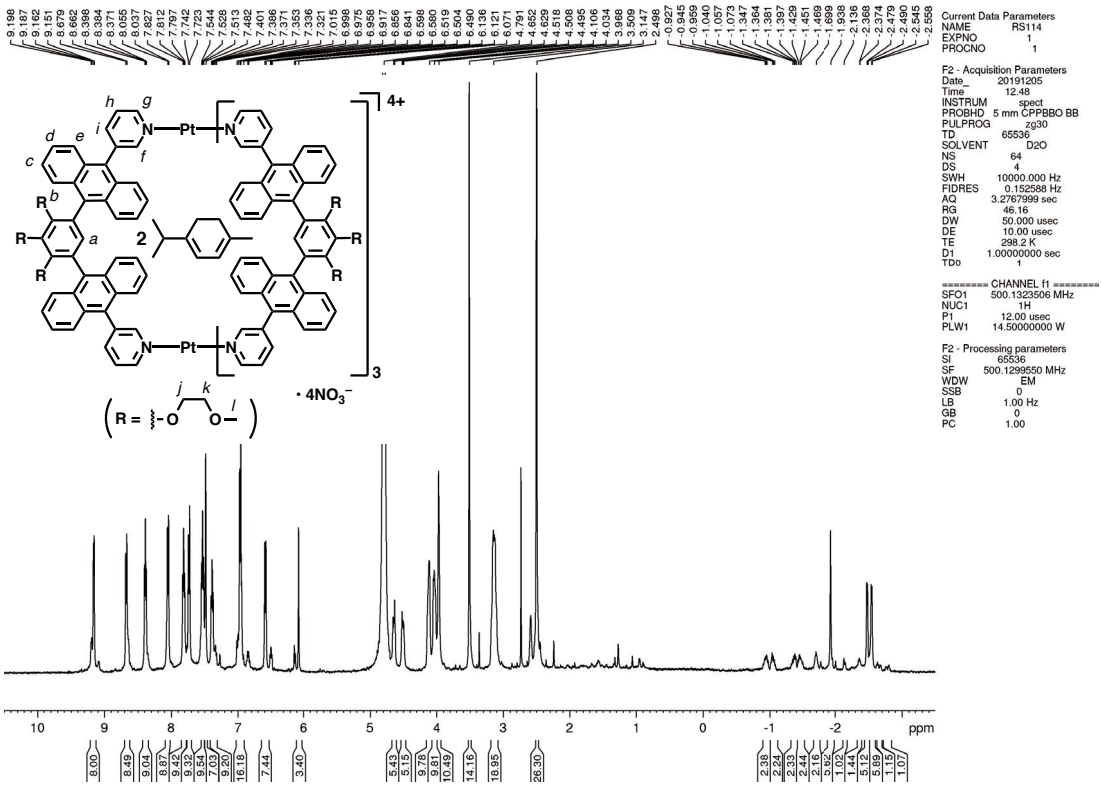


Figure S26. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1**•(**TPN**)$_2$.

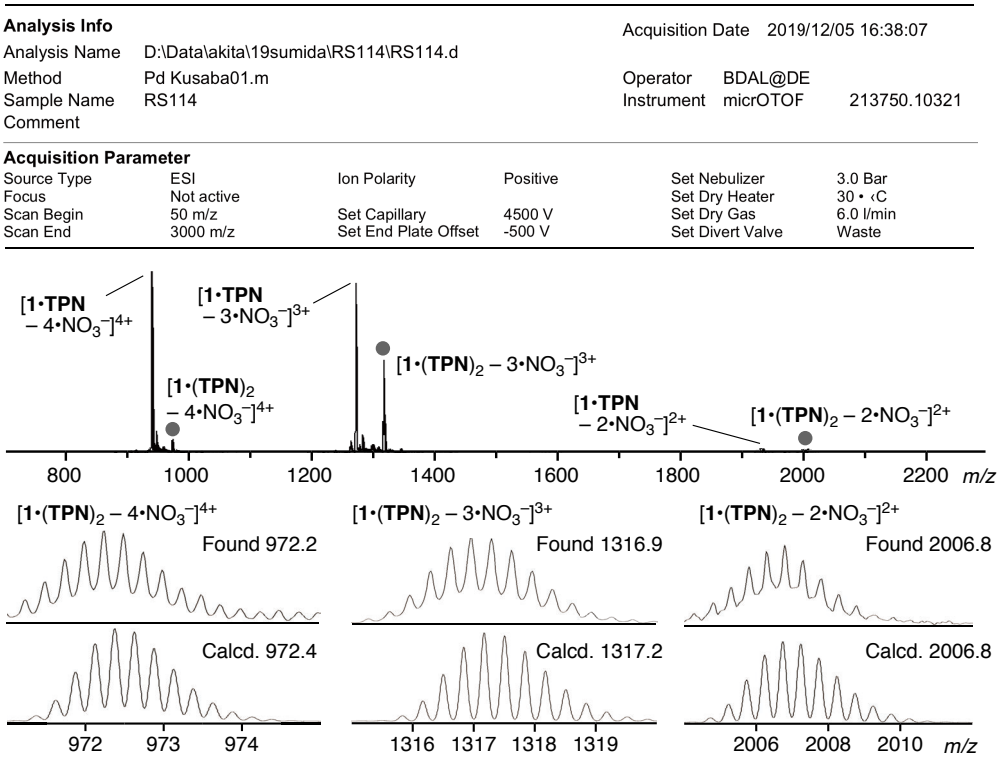
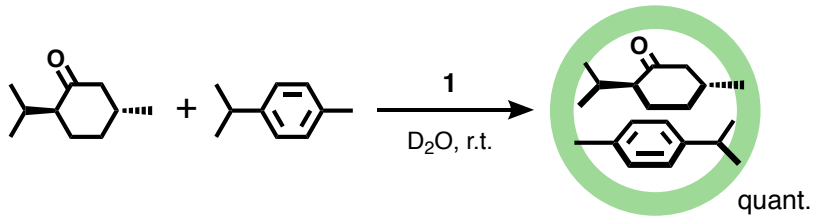


Figure S27. ESI-TOF MS spectrum (H_2O) of **1**•(**TPN**)$_2$.

Pair-selective formation of 1•(MTO•CMN) RS146, 172, 176, 190



Capsule **1** (1.0 mg, 0.26 μmol), **MTO** (0.4 mg, 2.6 μmol), and **CMN** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The selective formation of a **1•(MTO•CMN)** complex was confirmed by NMR and ESI-TOF MS analyses. Furthermore, encapsulated guests **MTO** and **CMN** could be extracted from **1•(MTO•CMN)** with $CDCl_3$. In the same way, from **1** (1.0 mg, 0.26 μmol), **CMN** (0.4 mg, 2.6 μmol), and **CMP** (0.4 mg, 2.6 μmol), the formation of complexes **1•(CMN)**$_2$ and **1•CMP** in an 88:12 ratio was confirmed by NMR analysis. ESI-TOF MS (H_2O): *m/z* 2014.6 [**1•(MTO•CMN)** – 2•NO_3^-]$^{2+}$, 1322.4 [**1•(MTO•CMN)** – 3•NO_3^-]$^{3+}$, 976.6 [**1•(MTO•CMN)** – 4•NO_3^-]$^{4+}$.

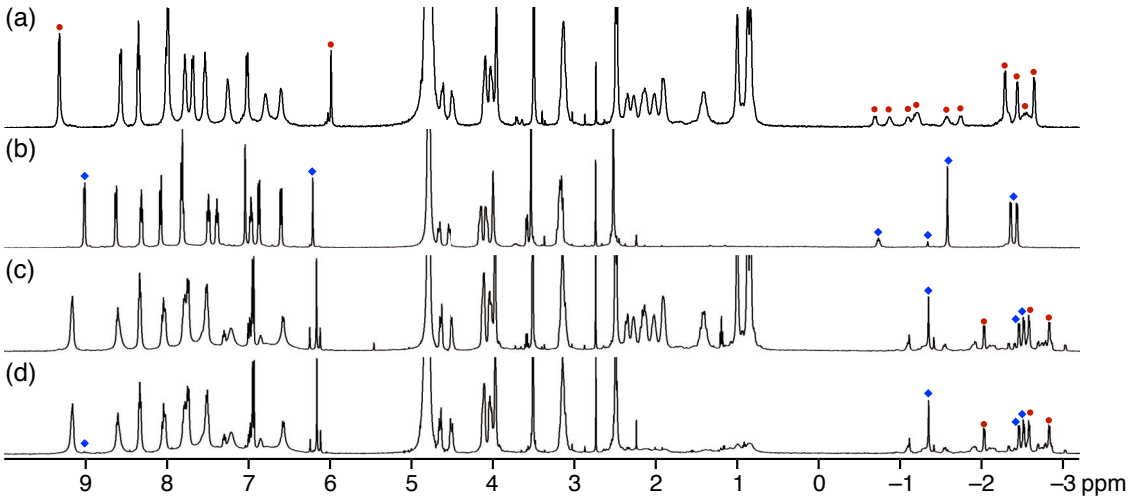


Figure S28a. ^1H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO**, (b) **1•(CMN)**$_2$, and **1•(MTO•CMN)** obtained from mixtures of **1**, **MTO**, and **CMN** in (c) a 1:10:10 and (d) 1:10:50 ratio.

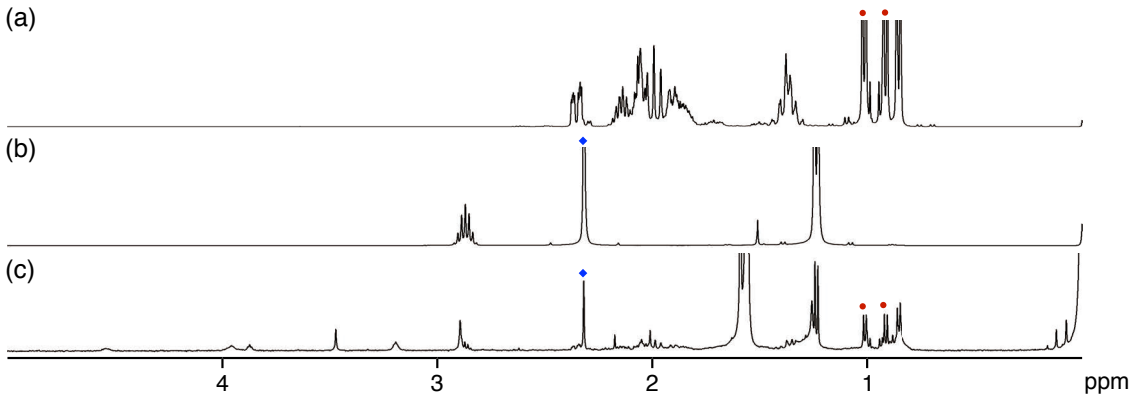


Figure S28b. ^{1}H NMR spectra (400 MHz, $CDCl_3$, r.t.) of (a) **MTO**, (b) **CMN**, and (c) guests extracted from isolated **1•(MTO•CMN)**.

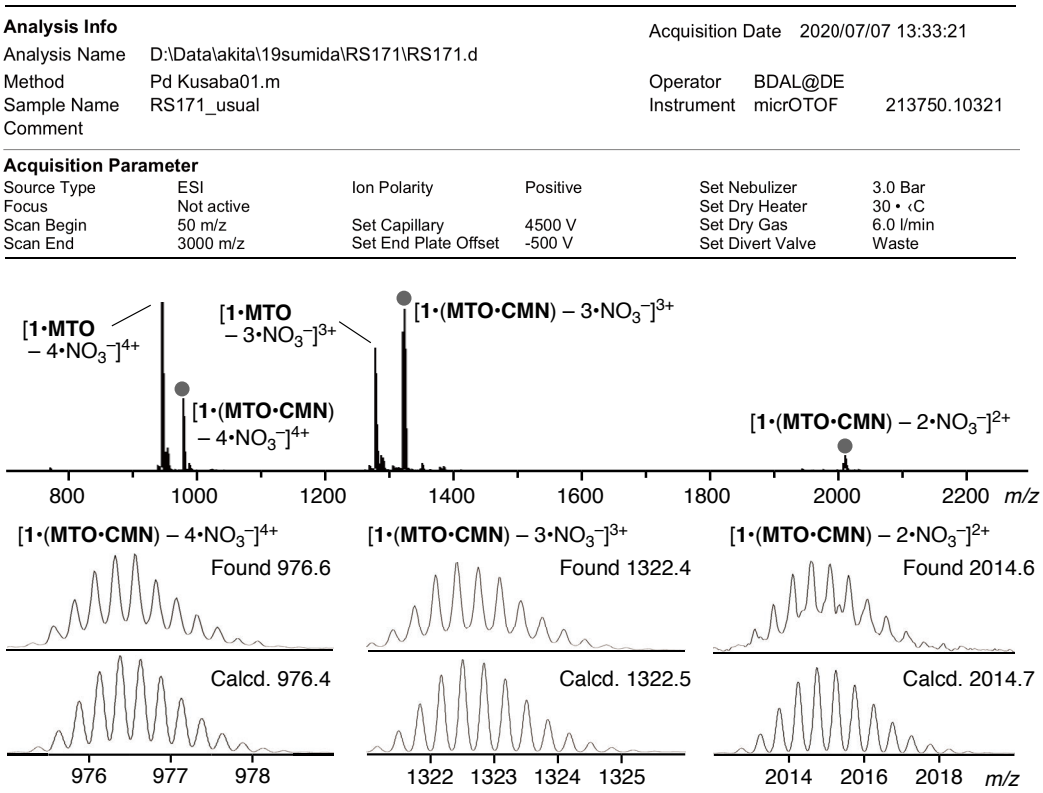


Figure S29. ESI-TOF MS spectrum (H_2O) of **1•(MTO•CMN)**.

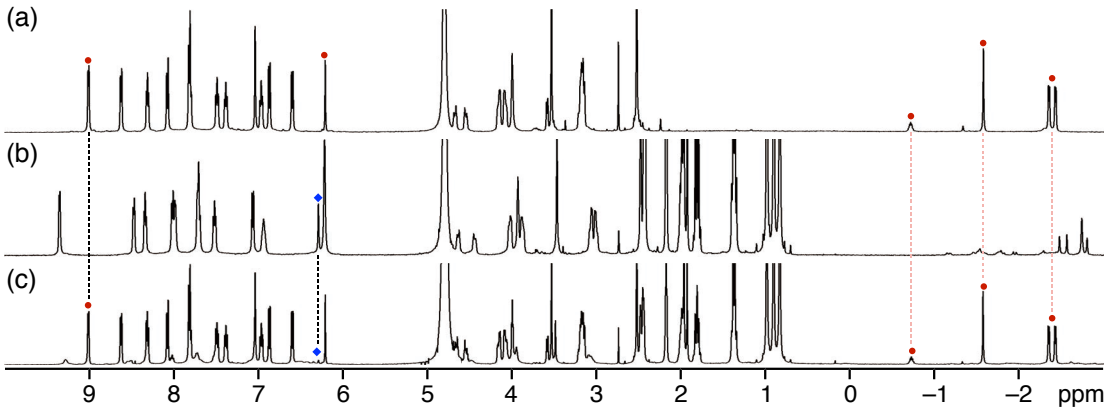


Figure S30. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1**•(**CMN**)$_2$, (b) **1**•**CMP**, and (c) products obtained from a mixture of **1**, **CMN**, and **CMP** at r.t. for 1 h.

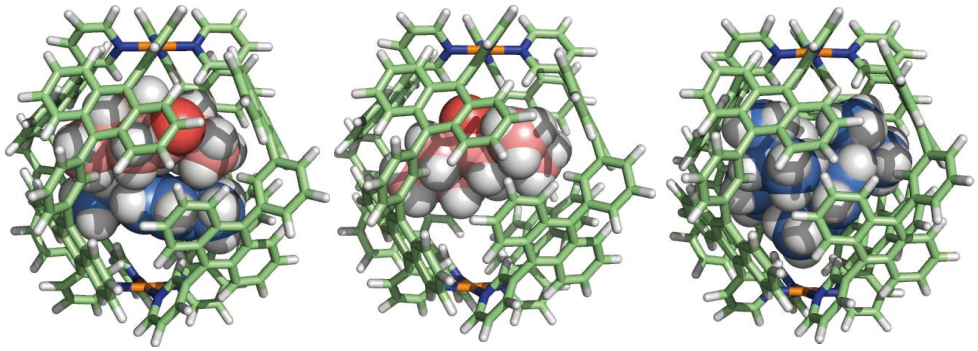
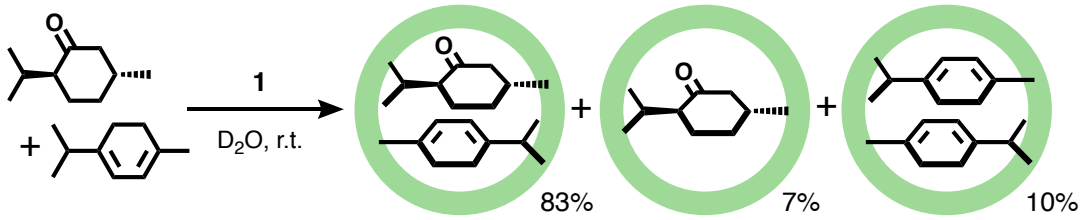


Figure S31. Optimized structures of host-guest complexes **1**•(**MTO**•**CMN**), **1**•(**MTO**), and **1**•(**CMN**)$_2$, and the energies of the sets of **1**•(**MTO**•**CMN**) + **CMN**, **1**•(**MTO**) + 2 × **CMN**, and **1**•(**CMN**)$_2$ + **MTO** (R = -H).

Pair-selective formation of 1•(MTO•TPN) RS160



Capsule **1** (1.0 mg, 0.26 μmol), **MTO** (0.4 mg, 2.6 μmol), and **TPN** (0.4 mg, 2.6 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. The selective formation of a **1**•(**MTO**•**TPN**) complex (83% selectivity) was confirmed by NMR and ESI-TOF MS analyses.

ESI-TOF MS (H_2O): *m/z* 2015.8 [**1**•(**MTO**•**TPN**) – 2•NO_3^-]$^{2+}$, 1323.2 [**1**•(**MTO**•**TPN**)

– 3•NO_3^-]$^{3+}$, 976.9 [**1**•(**MTO**•**TPN**) – 4•NO_3^-]$^{4+}$.

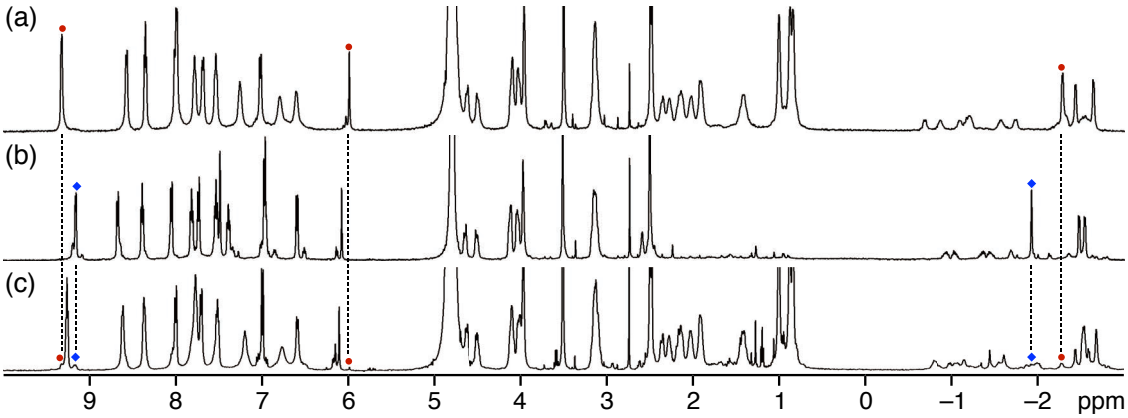


Figure S32. H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1**•**MTO**, (b) **1**•(**TPN**)$_2$, and (c) **1**•(**MTO**•**TPN**).

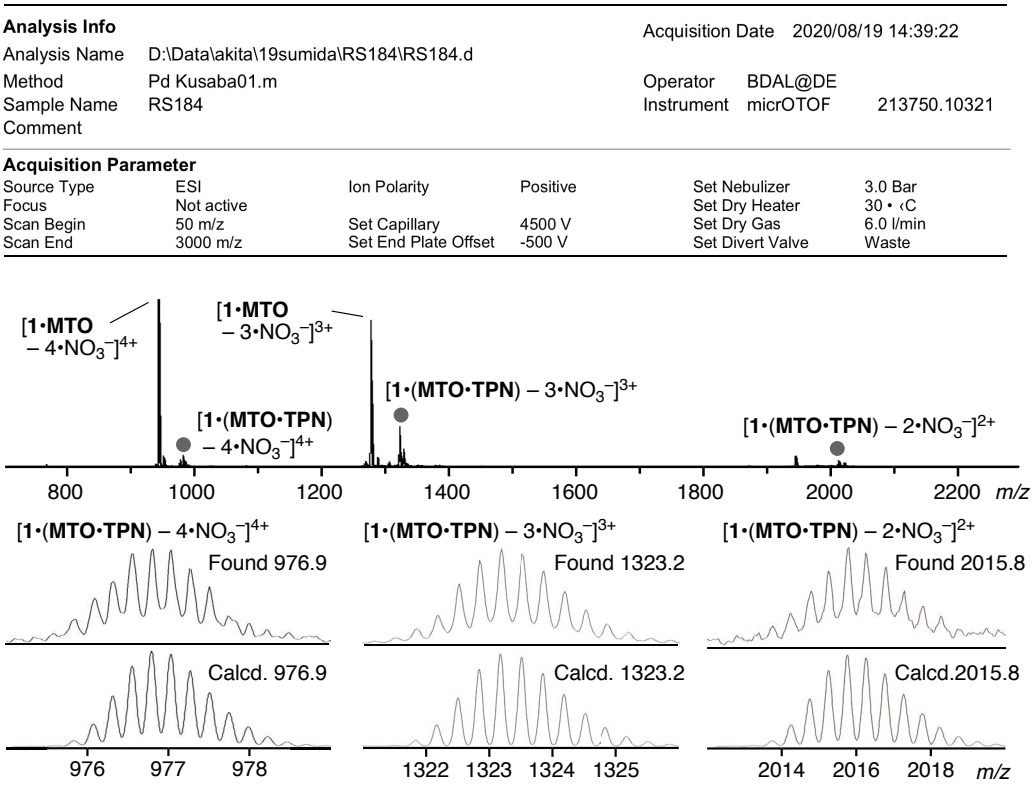


Figure S33. ESI-TOF MS spectrum (H_2O) of **1**•(**MTO**•**TPN**).

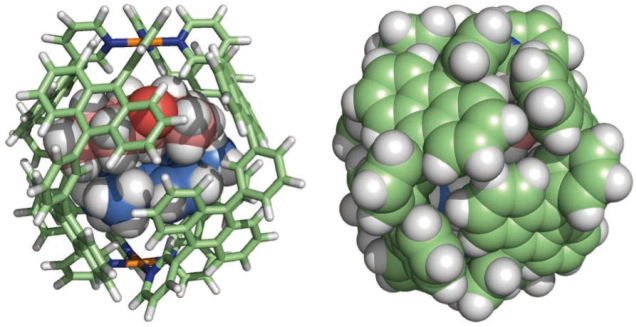


Figure S34. Optimized structure of **1**•(**MTO**•**TPN**) (R = -H).

Thermal isomerization of MTO within 1 RS277, 278, 279, 292, 304

Capsule **1** (1.0 mg, 0.26 μmol) and **MTO** (0.1 mg, 0.91 μmol) were added to a 2 mL test tube containing D_2O (0.5 mL). The mixture was stirred at r.t. for 1 h. After confirming of the quantitative formation of **1**•**MTO** by ^1H NMR analysis, the D_2O solution of **1**•**MTO** was stirred at 100 ºC for 8 h. The quantitative isomerization of **MTO** within **1** was confirmed by NMR and ESI-TOF MS analyses. When the resultant solution was stood at 30 ºC for 144 h, the quantitative regeneration of **1**•**MTO** was revealed by ^1H NMR analysis. The reversible isomerization of **MTO** was repeated three times within **1**.

The time-course profiles of the regeneration of **MTO** within **1** were investigated at 30, 40, and 50 ºC by ^1H NMR analysis. The NMR sample of **1**•**MTO** was prepared from **1** (1.0 mg, 0.26 μmol), **MTO** (0.2 mg, 1.3 μmol), and D_2O (0.5 mL).

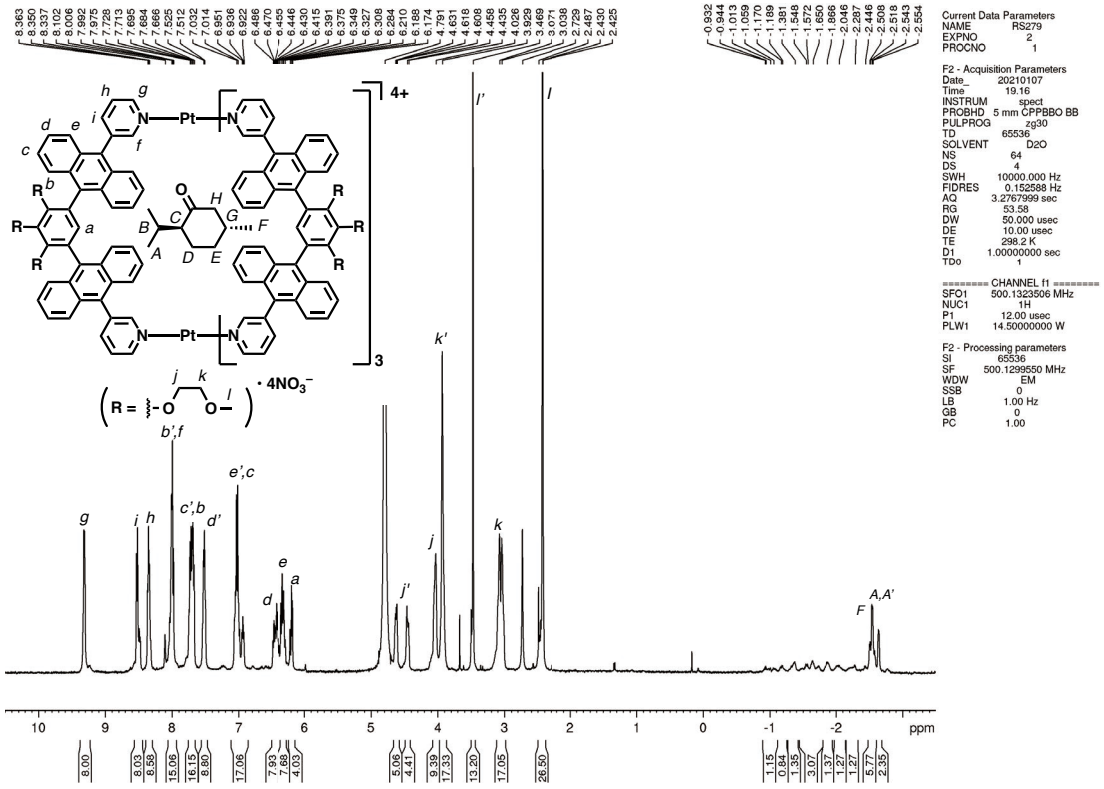


Figure S35a. ^{1}H NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTO** after heating at 100 ºC for 8 h.

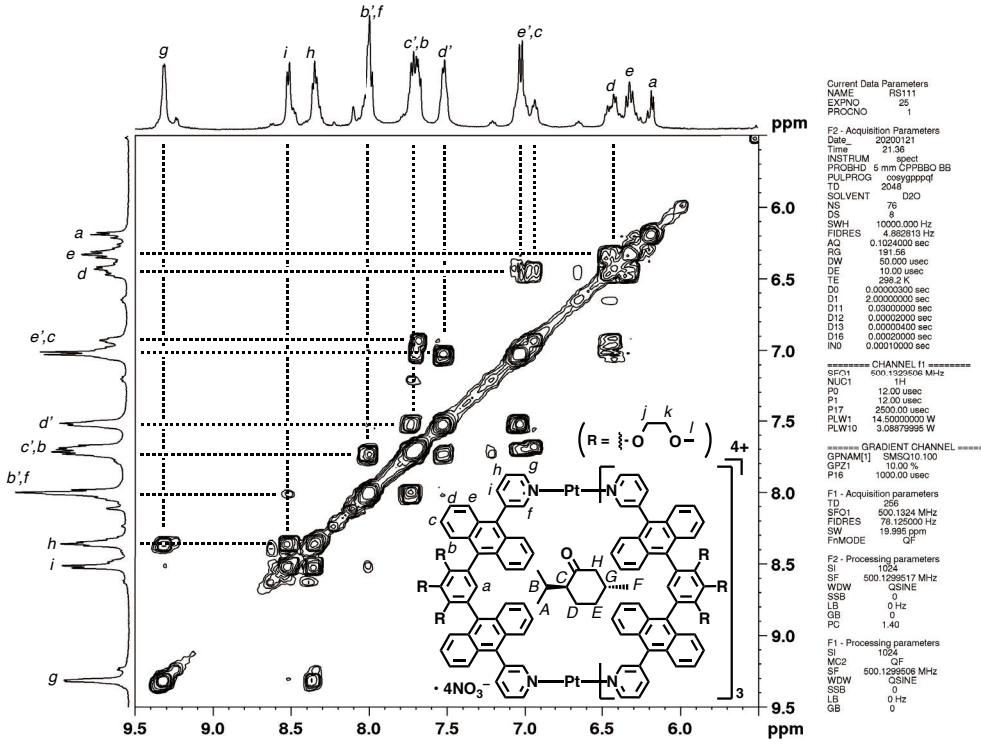


Figure S35b. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, D_2O, r.t.) of **1•MTO** after heating at 100 ºC for 8 h.

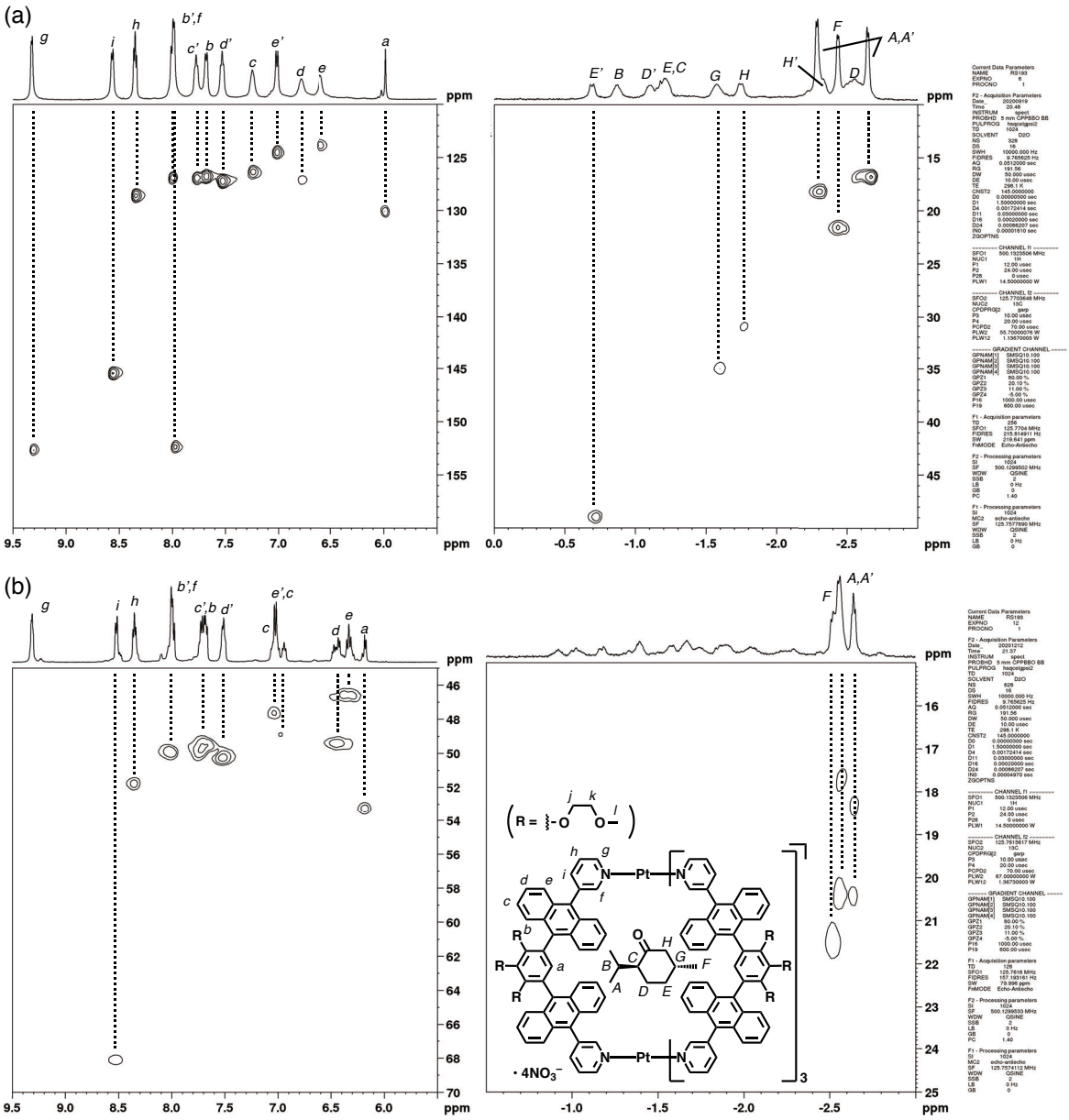


Figure S35c. HSQC spectra (500 MHz, D_2O, r.t.) of **1•MTO** (a) before and (b) after heating at 100 ºC for 8 h.

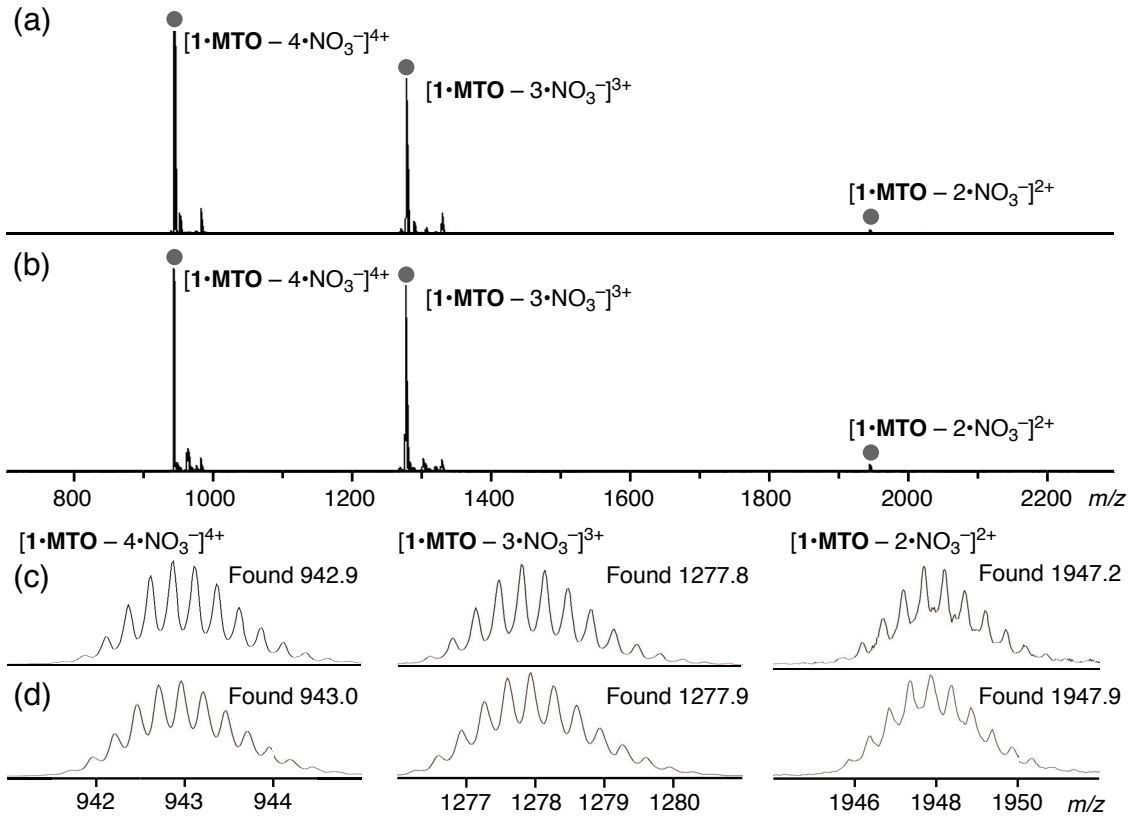


Figure S35d. ESI-TOF MS spectra of **1•MTO** (a) before and (b) after heating at 100 ºC for 8 h and the expansion of each signal (c) before and (d) after heating.

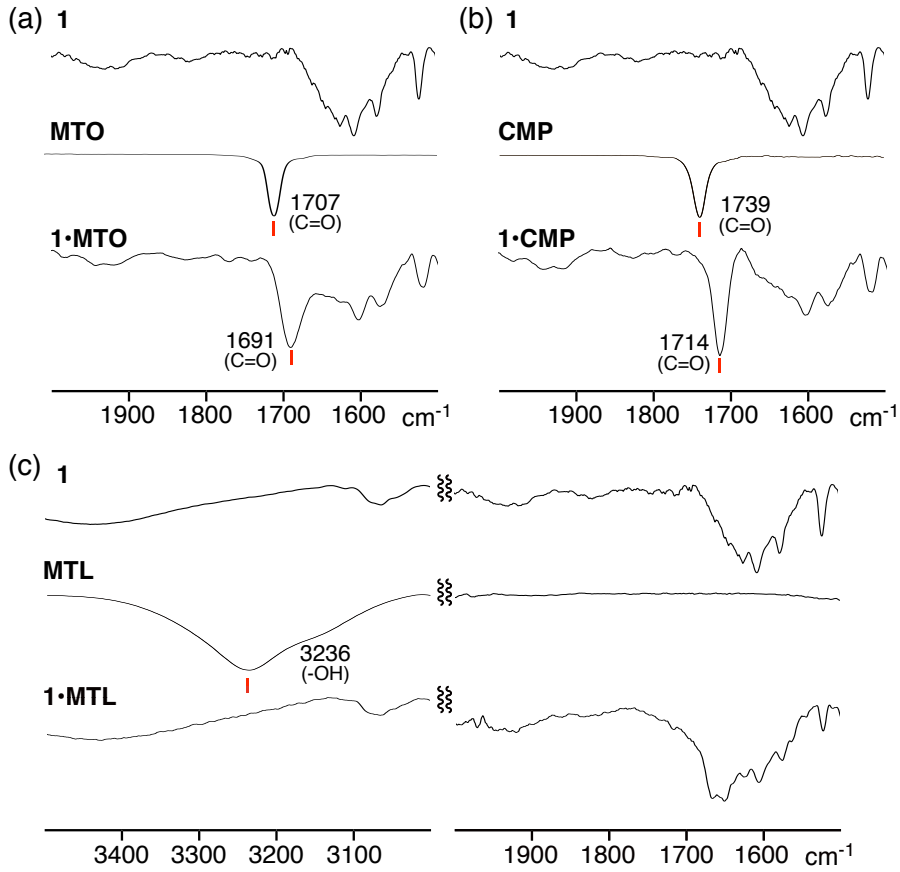


Figure S36a. FT-IR spectra of (a) **1•MTO**, (b) **1•CMP**, and (c) **1•MTL**.

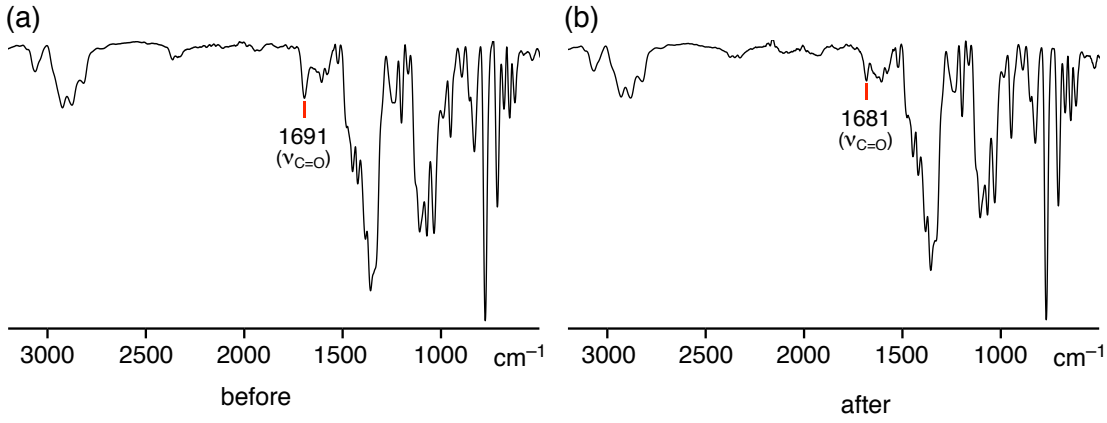


Figure S36b. FT-IR spectra of **1•MTO** (a) before and (b) after heating at 100 ºC for 8 h.

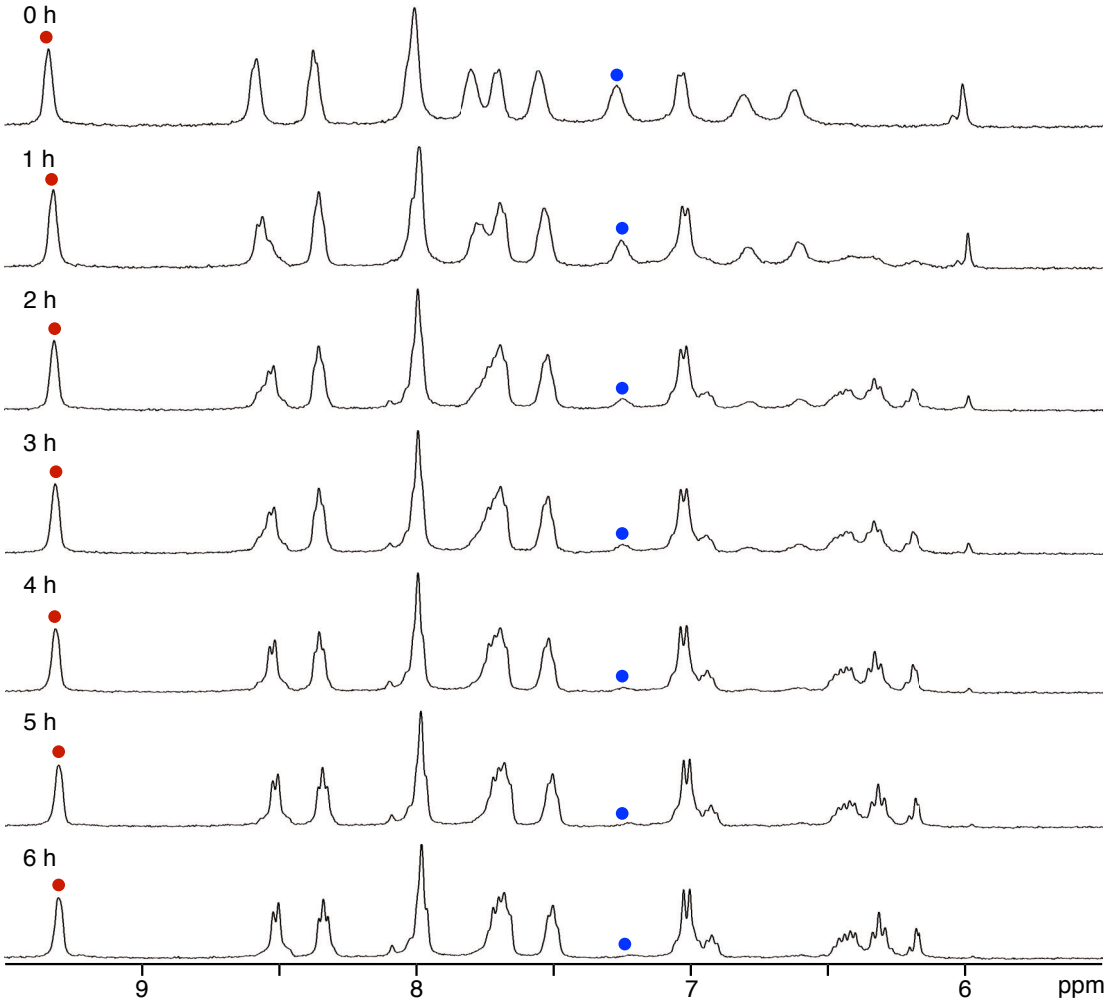


Figure S37a. Time-dependent ^{1}H NMR spectra (400 MHz, D_2O, r.t.) of **1•MTO** in D_2O before/after heating 100 ℃ for 6 h.

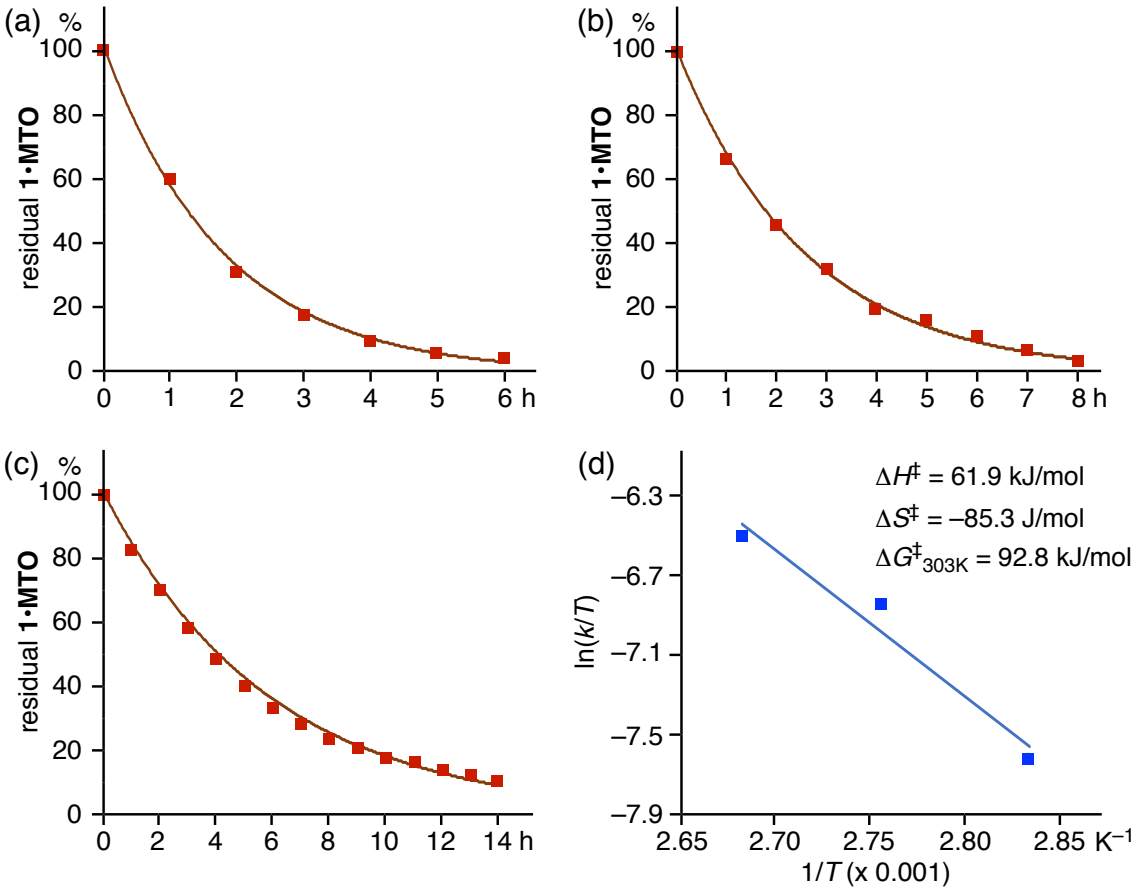


Figure S37b. Time-course isomerization profiles (%) of **MTO** within **1** at (a) 80, (b) 90, and (c) 100 ºC on the basis of the time-dependent ^{1}H NMR spectra, and (d) the Eyring plots.

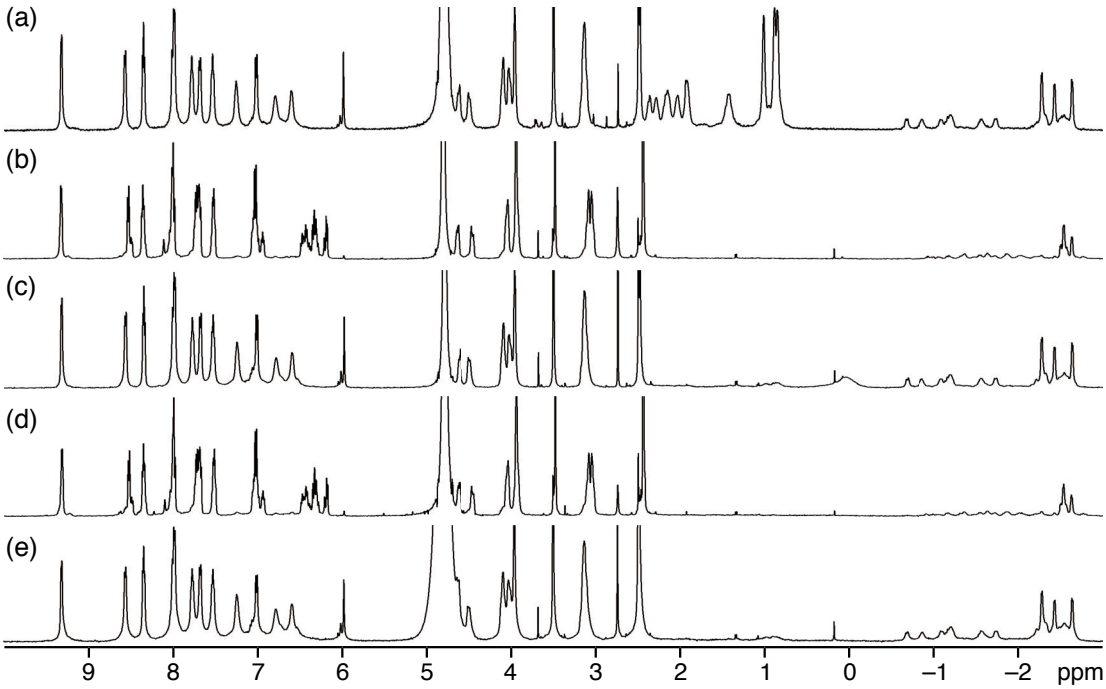


Figure S37c. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO** (and free **MTO**) and the compound after subsequent (b) 8 h heating at 100 ºC, (c) 144 h standing at 30 ºC, (d) 8 h heating at 100 ºC, and (e) 168 h standing at 30 ºC.

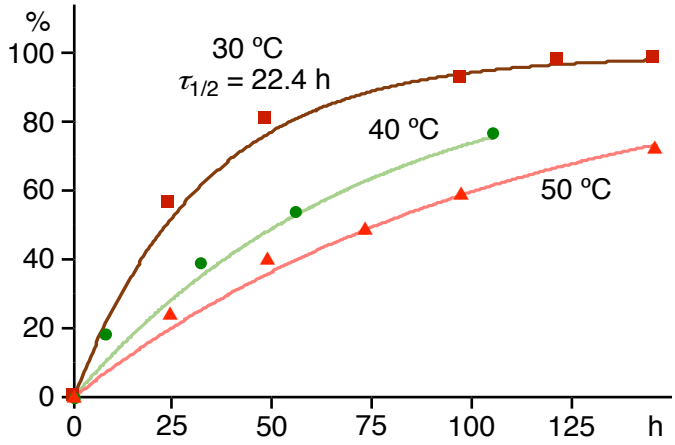


Figure S37d. Time-course profiles of the regeneration of **MTO** (%) within **1** in water at 30, 40, and 50 ºC, after heating of **1•MTO** at 100 ºC for 8 h.

Table S2. Crystal data and structure refinement for **1•MTO**.

Identification code	RS214menthone	
Empirical formula	$C_{222}H_{202}N_9O_{28}Pt_2$	
Formula weight	3808.52	
Temperature	93(2) K	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 18.7348(5) Å	α = 93.167(3)°
	b = 21.8196(9) Å	β = 101.052(3)°
	c = 27.4073(11) Å	γ = 107.422(3)°
Volume	10415.3(7) Å^3	
Z	2	
Density (calculated)	1.214 Mg/m^3	
Absorption coefficient	3.008 mm^{-1}	
F(000)	3919.0	
Crystal size	0.76 × 0.44 × 0.24 mm^3	
Theta range for data collection	5.066 to 150.57°	
Index ranges	-22 ≤ h ≤ 23, -27 ≤ k ≤ 27, -33 ≤ l ≤ 31	
Reflections collected	139099	
Independent reflections	40686 [R_{int} = 0.1525, R_{sigma} = 0.1376]	
Completeness to theta = 66.9682°	99.74 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.485 and 0.255	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	40686/3484/2450	
Goodness-of-fit on F^2	0.967	
Final R indices [I>2sigma(I)]	R_1 = 0.0917, wR_2 = 0.2324	
R indices (all data)	R_1 = 0.1741, wR_2 = 0.2877	
Largest diff. peak and hole	2.02 and –2.51 e.Å^{-3}	

The supplementary crystallographic data (CCDC 2058897) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam. ac.uk/data_request/cif.

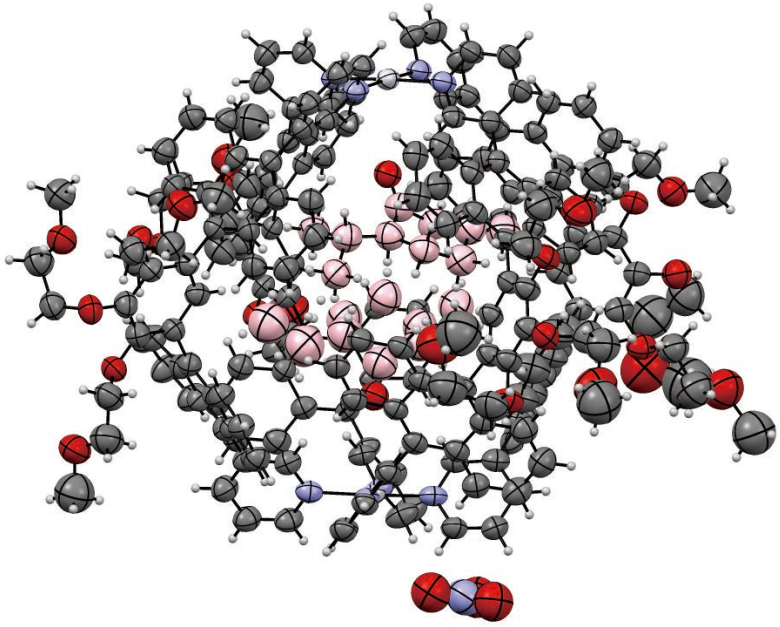


Figure S38a. ORTEP drawing of **1•MTO** (The thermal ellipsoids are drawn at 50% probability).

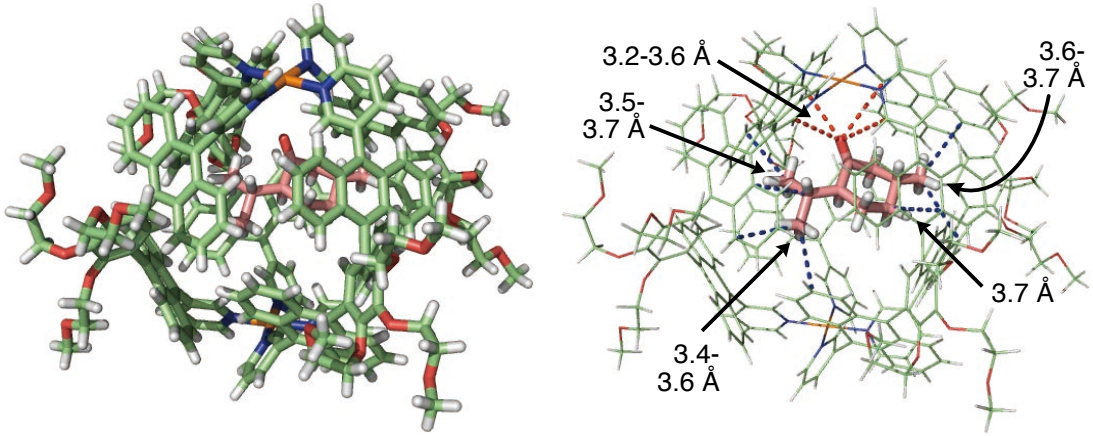


Figure S38b. Crystal structure (stick representation) of **1•MTO** and highlighted host-guest interactions (blue dot lines: CH-π interactions, red dot lines: hydrogen-bonding interactions). The counterion and one of the two disordered guests are omitted for clarity.

Table S3. Crystal data and structure refinement for **1•CMP**.

Identification code	RS214camphor	
Empirical formula	$C_{215.33}H_{189.33}N_{10}O_{30.5}Pt_2$	
Formula weight	3975.29	
Temperature	90 K	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 18.6373(5) Å	α = 93.016(2)°
	b = 22.0540(5) Å	β = 101.669(2)°
	c = 27.1149(5) Å	γ = 106.888(2)°
Volume	10369.9(4) Å^3	
Z	2	
Density (calculated)	1.215 Mg/m^3	
Absorption coefficient	3.033 mm^{-1}	
F(000)	3903.0	
Crystal size	0.07 × 0.065 × 0.04 mm^3	
Theta range for data collection	5.066 to 142.6°	
Index ranges	-21 ≤ h ≤ 22, -27 ≤ k ≤ 26, -33 ≤ l ≤ 31	
Reflections collected	62197	
Independent reflections	34891 [R_{int} = 0.0743, R_{sigma} = 0.0908]	
Completeness to theta = 66.97°	90.32 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.886 and 0.809	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	34891/3418/2400	
Goodness-of-fit on F^2	0.915	
Final R indices [I>2sigma(I)]	R_1 = 0.0779, wR_2 = 0.2310	
R indices (all data)	R_1 = 0.1037, wR_2 = 0.2538	
Largest diff. peak and hole	2.98 and –1.50 e.Å^{-3}	

The supplementary crystallographic data (CCDC 2059097) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam. ac.uk/data_request/cif.

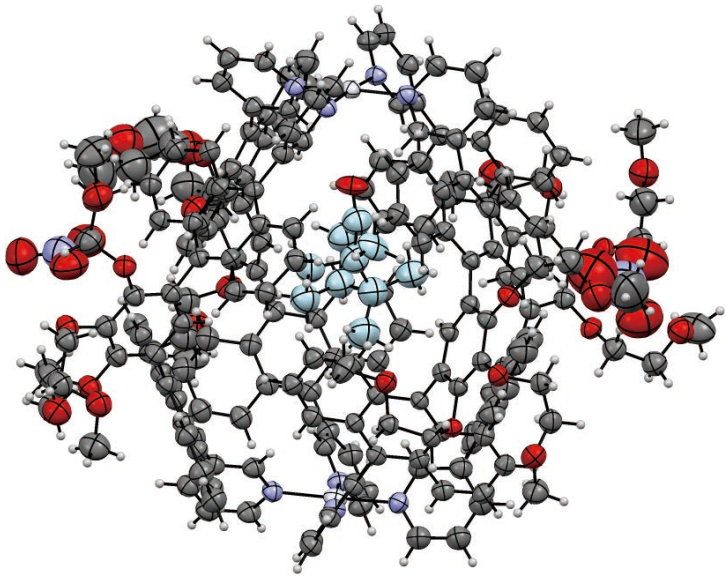


Figure S39a. ORTEP drawing of **1•CMP** (The thermal ellipsoids are drawn at 50% probability).

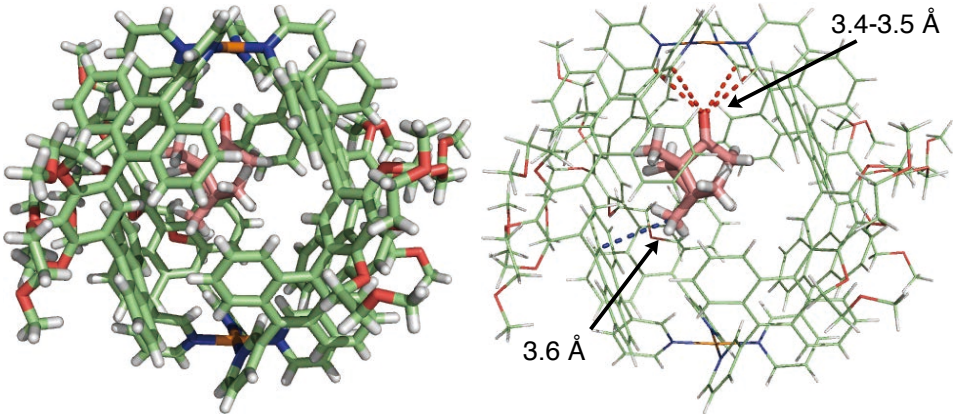


Figure S39b. Crystal structure (stick representation) of **1•CMP** and highlighted host-guest interactions (blue dot lines: CH-π interactions, red dot lines: hydrogen-bonding interactions). The counterions are omitted for clarity.

Theoretical calculations of MTO and its isomers without/within 1

The conformational isomers of **MTO** (20 structures) were initially generated through automatic conformational analysis using Conflex 8, Rev. C program. DFT calculations of **MTO** and its isomers without/within **1** were performed by using the Gaussian 16 program package.[S8] The geometry optimizations and vibrational frequency calculations were optimized with the CAM-B3LYP/ LanL2DZ (for Pt),6-31G(d) (for C, H, N, O) level of theory. No imaginary number was obtained for the optimized structures. Single point calculations were performed at the same levels of theory combined with the PCM continuum solvent method (H_2O).

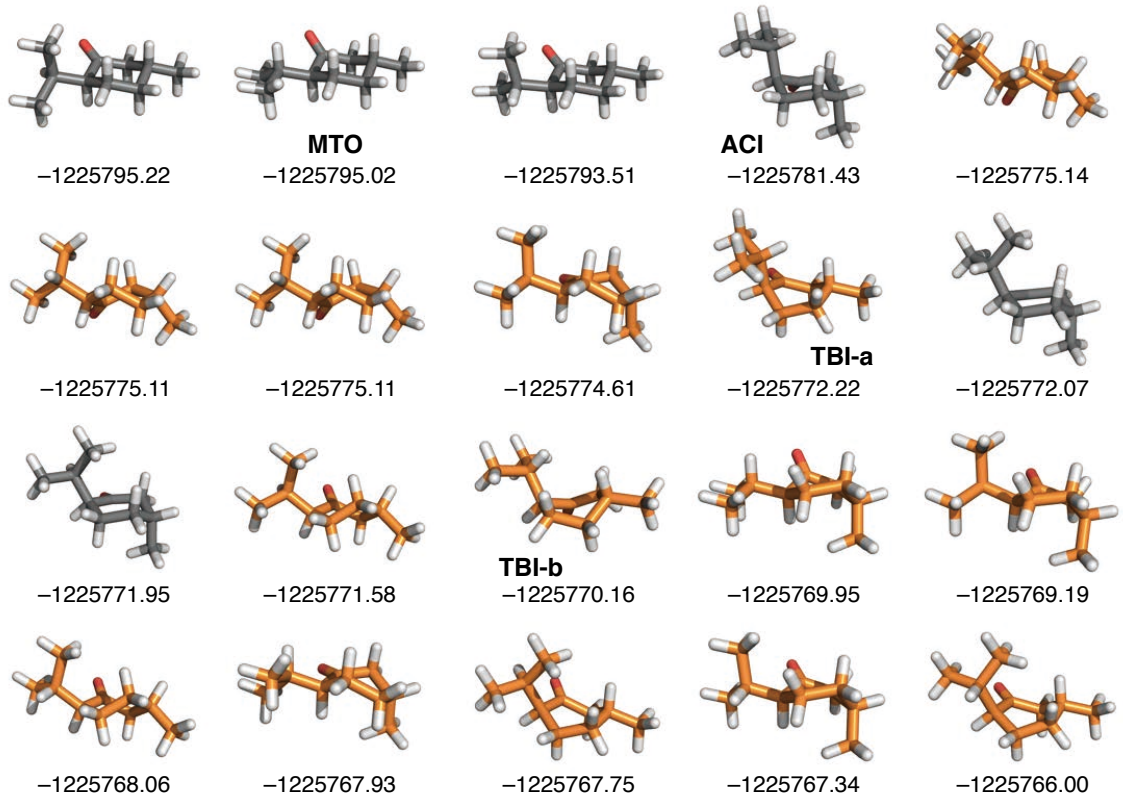


Figure S40a. Optimized structures and energies (kJ/mol) of **MTO** and its isomers (DFT calculation, CAM-B3LYP/ 6-31G(d) level).

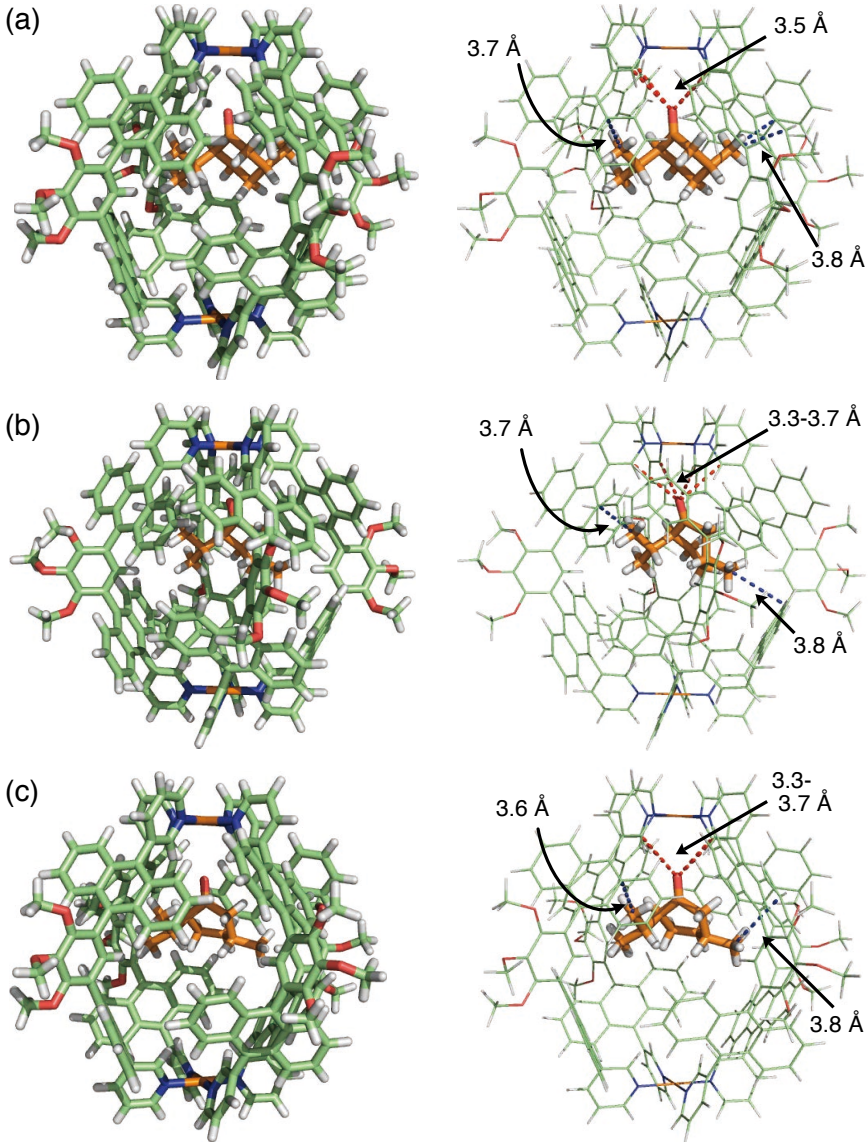
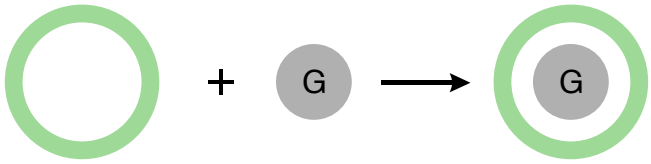
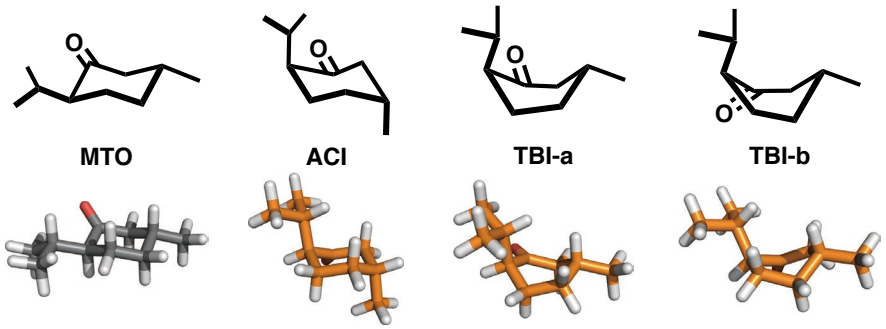


Figure S40b. Optimized structures and their host-guest interactions of (a) **1•ACI**, (b) **1•TBI-a**, and (c) **1•TBI-b** (R = -OCH_3; DFT calculation, B3LYP/LanL2DZ (for Pt) and 6-31G(d) (for C, H, N, O) levels, vacuum).



	1	G	1·G	$\Delta E_{(1\cdot G - (1 + G))}$
MTO	–23155817.23	–1225795.02	–24381634.94	–22.68
ACI	–23155817.23	–1225781.43	–24381629.28	–30.61
		$\Delta E_{(\mathbf{ACI - MTO})}$ = 13.59	$\Delta E_{(\mathbf{1\cdot ACI - 1\cdot MTO})}$ = 5.66	
MTO	–23155817.23	–1225795.02	–24381634.94	–22.68
TBI-a	–23155817.23	–1225772.22	–24381622.14	–32.68
		$\Delta E_{(\mathbf{TBI\text{-}a - MTO})}$ = 22.80	$\Delta E_{(\mathbf{1\cdot TBI\text{-}a - 1\cdot MTO})}$ = 12.80	
MTO	–23155817.23	–1225795.02	–24381634.94	–22.68
TBI-b	–23155817.23	–1225770.16	–24381616.11	–28.72
		$\Delta E_{(\mathbf{TBI\text{-}b - MTO})}$ = 24.86	$\Delta E_{(\mathbf{1\cdot TBI\text{-}b - 1\cdot MTO})}$ = 18.83	

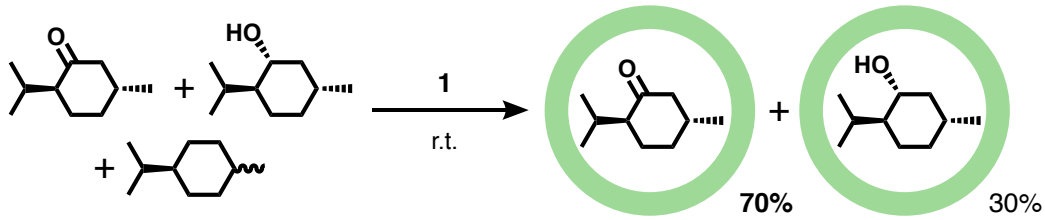
Figure S41. The calculated energies (kJ/mol) of **MTO**, **ACI**, **TBI-a**, and **TBI-b** before and after encapsulation by **1**.



	MTO	ACI	TBI-a	TBI-b
without **1**	1763.32 cm^{-1}	1765.85 cm^{-1}	1762.16 cm^{-1}	1759.06 cm^{-1}
within **1**	1711.14 cm^{-1}	1700.85 cm^{-1}	1696.04 cm^{-1}	1695.51 cm^{-1}

Figure S42. The calculated wavenumbers of the C=O bonds of **MTO** and its isomers without/within **1** (DFT calculation, CAM-B3LYP/6-31G(d) level, scaling factor = 0.953[S9], vacuum).

Competitive binding of MTO, MTA, and MTL by 1 in the solid state RS254



A small open vessel including solid **1** (1.0 mg, 0.26 μmol) was put in a closed glass vessel (50 mL) including **MTO** (4.0 mg, 26 μmol), **MTA** (3.7 mg, 26 μmol), and **MTL** (4.0 mg, 26 μmol), without direct contact between **1** and the CMTs. After standing 14 h at r.t., the small vessel was taken out from the large vessel and then stood for 1 h under vacuum (480 Pa) at r.t. The resultant solid was dissolved in D_2O (0.4 mL) and then the formation of host-guest complexes **1•MTO**, **1•MTA**, and **1•MTL** in a 70:0:30 ratio was confirmed by NMR analysis. Under similar conditions, control binding experiments were examined using β-cyclodextrin (1.0 mg, 0.88 μmol), γ-cyclodextrin (1.0 mg, 0.77 μmol), or cucurbit[6]uril (1.0 mg, 1.0 μmol) as a host compound.

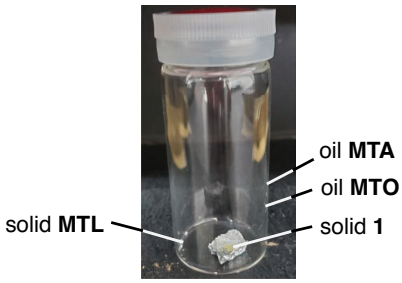


Figure S43a. Experimental setup for the binding of volatilized CMTs by solid **1**.

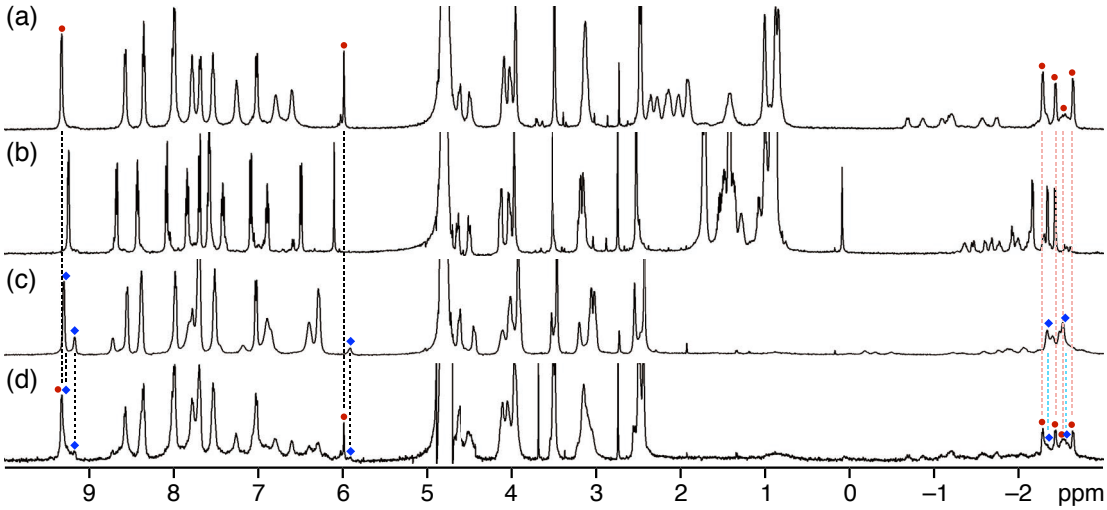


Figure S43b. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO**, (b) **1•MTA**, (c) **1•MTL**, and (d) products after the competitive binding of volatilized **MTO**, **MTA**, and **MTL** by solid **1** at r.t. for 14 h.

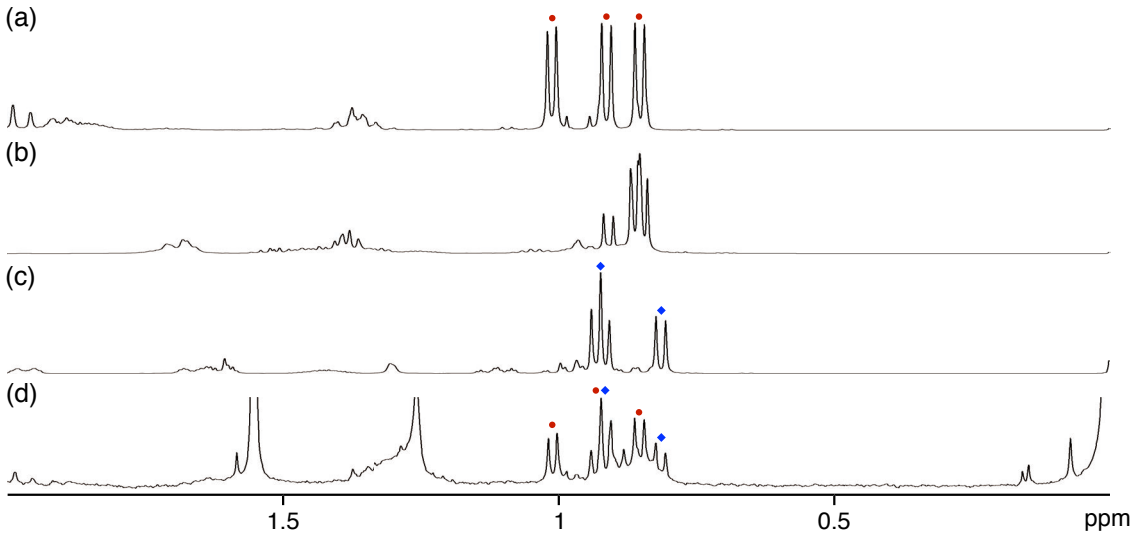


Figure S43c. ^{1}H NMR spectra (400 MHz, $CDCl_3$, r.t.) of (a) **MTO**, (b) **MTA**, (c) **MTL**, and (d) guests extracted from the products obtained from a mixture of solid **1** and volatilized **MTO**, **MTA**, and **MTL**.

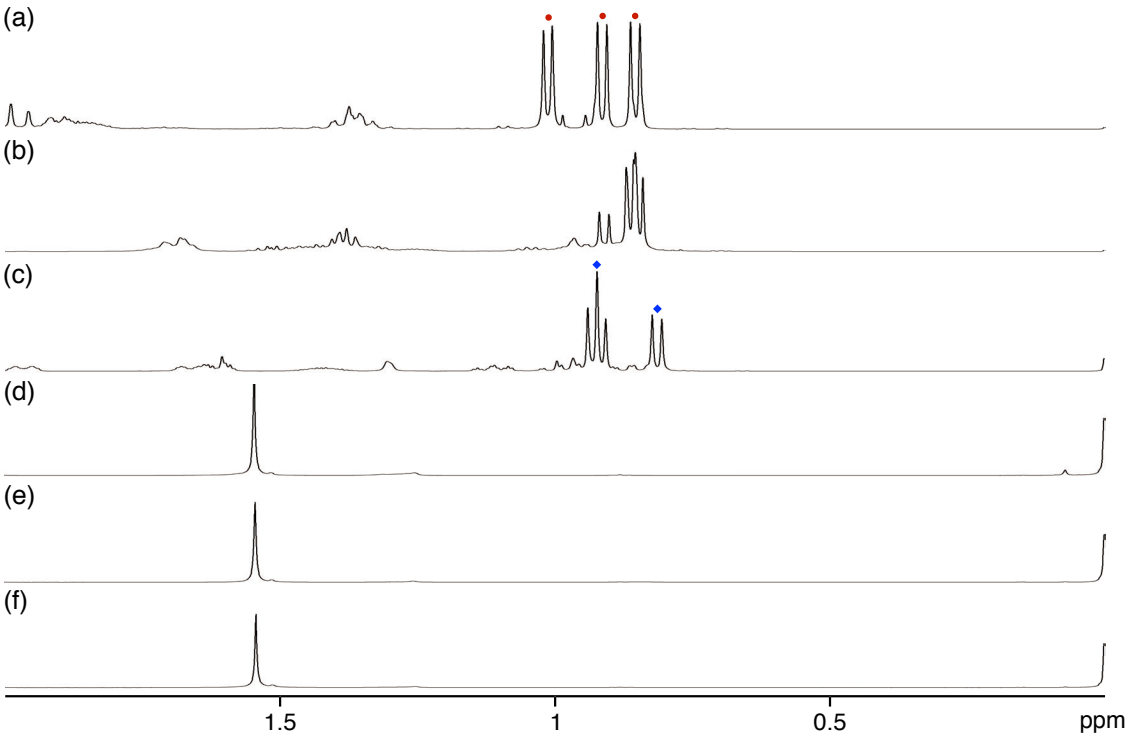
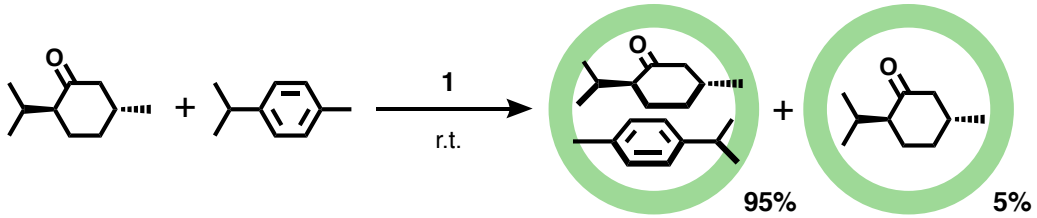


Figure S43d. ^{1}H NMR spectra (400 MHz, $CDCl_3$, r.t.) of (a) **MTO**, (b) **MTA**, (c) **MTL**, and bound guests extracted from (d) β-cyclodextrin, (e) γ-cyclodextrin, and (f) cucurbit[6]uril solids after treatment with a mixture of volatilized **MTO**, **MTA**, and **MTL**.

Pair-selective formation of 1•(MTO•CMN) in the solid state RS231, 249



A small open vessel including solid **1** (0.6 mg, 0.16 μmol) was put in a closed glass vessel (50 mL) including **MTO** (0.5 mg, 3.2 μmol) and **CMN** (2.1 mg, 16 μmol), without direct contact between **1** and the CMTs. After standing for 2 d at r.t., the small vessel was taken out from the large vessel and then stood for 20 min under vacuum (480 Pa) at r.t. The resultant solid of **1** was dissolved in D_2O (0.4 mL) and the formation of host-guest complexes **1**•(**MTO**•**CMN**), **1**•**MTO**, and **1**•(**CMN**)$_n$ in a 95:5:0 ratio was confirmed by NMR analysis. In the same way, host-guest complexes **1**•(**MTO**•**CMN**), **1**•**MTO**, and **1**•(**CMN**)$_n$ in an 82:18:0 ratio were obtained from solid **1** (0.6 mg, 0.16 μmol), **MTO** (2.45 mg, 16 μmol), and **CMN** (2.1 mg, 16 μmol) under the same conditions.

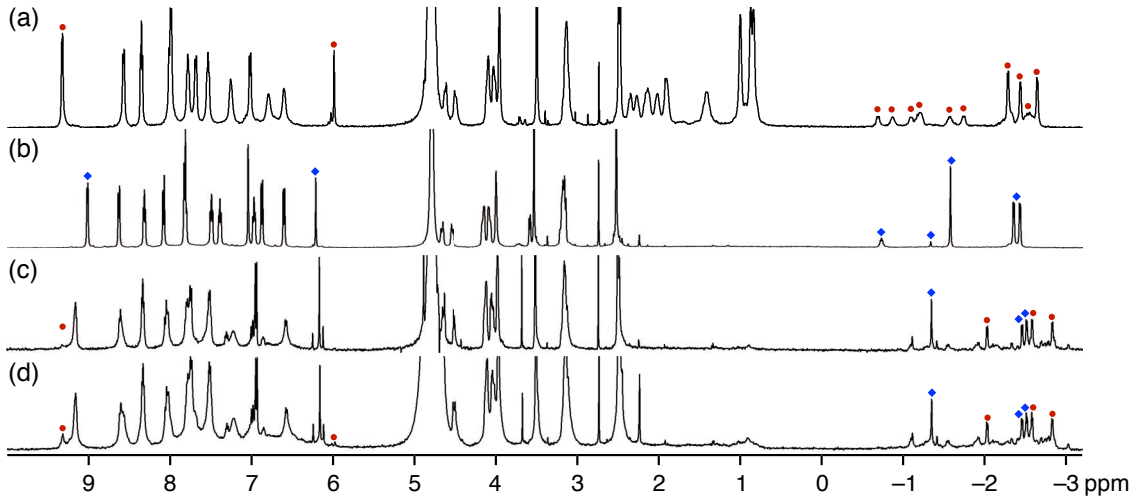
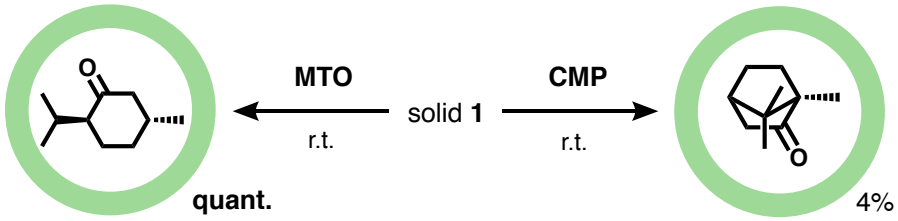


Figure S44. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of (a) **1•MTO**, (b) **1•(CMN)$_2$**, and products obtained from mixtures of solid **1** and volatilized **MTO** and **CMN** in (c) a 1:20:100 ratio and (d) a 1:100:100 ratio at r.t. for 2 d.

Formation of 1•MTO in the solid state RS235, 246



A small open vessel including solid **1** (0.6 mg, 0.16 μmol) was put in a closed glass vessel (50 mL) including **MTO** (4.1 mg, 27 μmol) without direct contact between **1** and **MTO**. After standing for 14 h at r.t., the small vessel was taken out from the large vessel and then stood for 1 h under vacuum (480 Pa) at r.t. The resultant solid was dissolved in D_2O (0.4 mL) and the quantitative formation of host-guest complex **1•MTO** was confirmed by NMR analysis. In the same way, the formation of host-guest complex **1•CMP** (4%) was confirmed by NMR analysis.

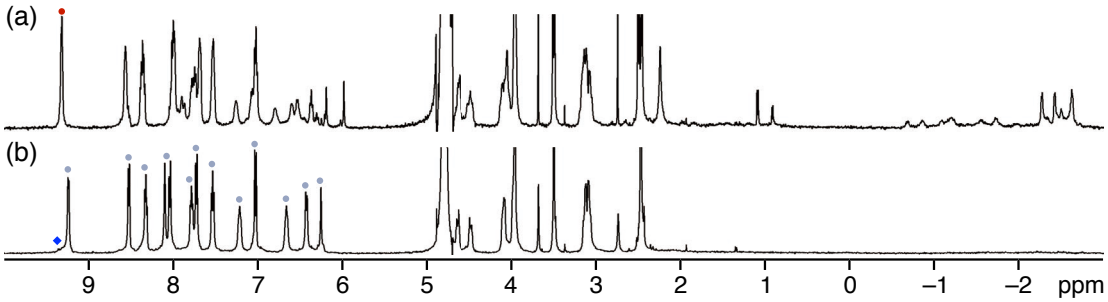


Figure S45. ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of products obtained from mixtures of solid **1** and volatilized (a) **MTO** (165 equiv.) or (b) **CMP** (100 equiv.) at r.t. (gray circle: **1**).

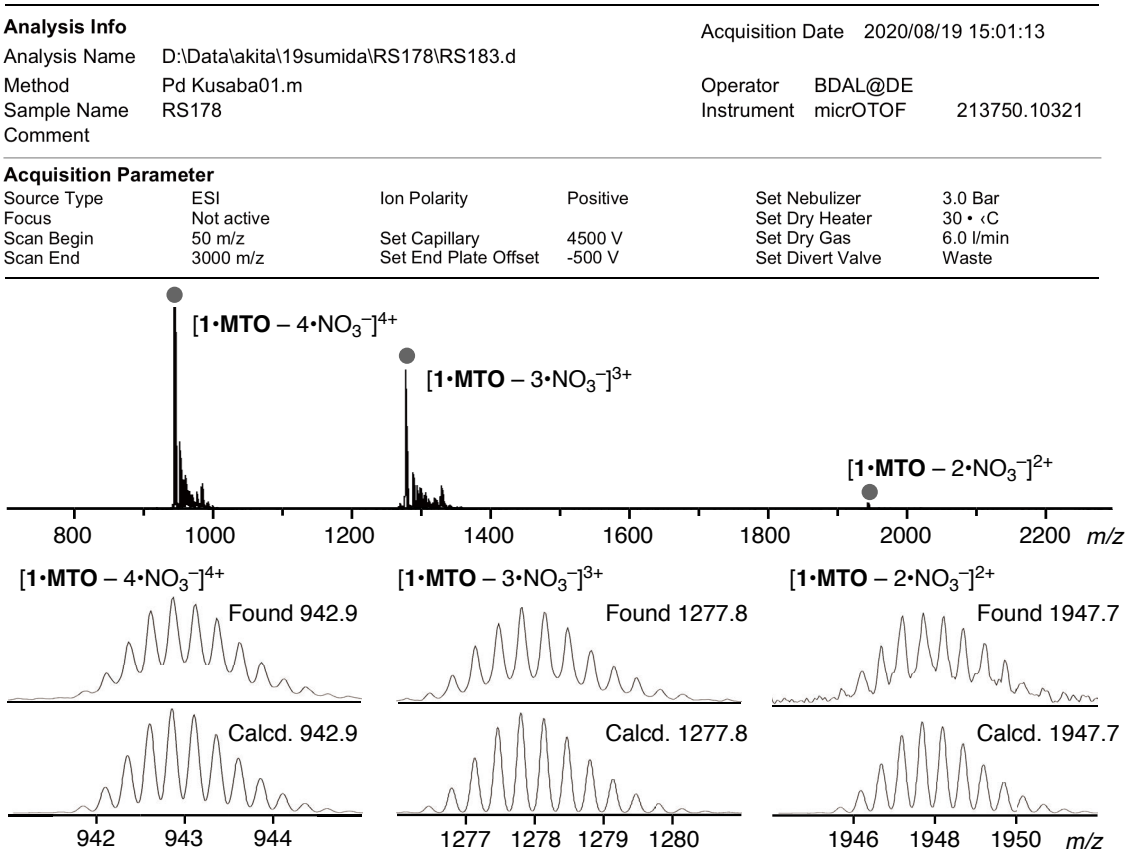
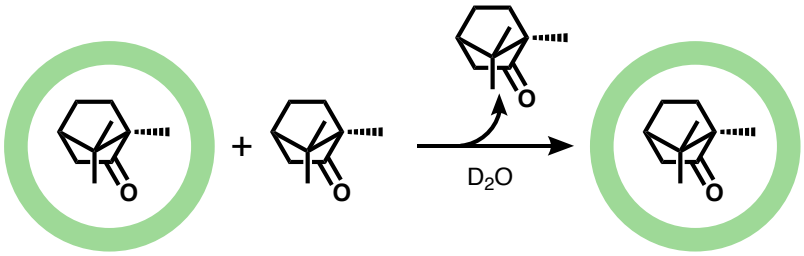


Figure S46. ESI-TOF MS spectrum (H_2O) of products obtained from a mixture of solid **1** and volatilized **MTO** in a 1:165 ratio.

Suppressed volatilities of CMP and MTL by 1 in water RS106, 107



Time-course volatility profiles of **CMP** within/without capsule **1** in water were investigated at 80 ºC by ^{1}H NMR analysis. The NMR sample was prepared using **1** (1.5 mg, 0.39 μmol), **CMP** (0.6 mg, 3.9 μmol), and D_2O (0.5 mL). The stability of **1•CMP** was also confirmed by ESI-TOF MS analysis after heating the sample at 80 ºC for 25 h. The control experiment (without **1**) was examined under the same conditions. Dimethyl sulfone (0.2 mg, 2.0 μmol) was used as an internal standard. In the same way, time-course volatility profiles of **MTL** within/without capsule **1** were investigated at 80 ºC by ^{1}H NMR analysis.

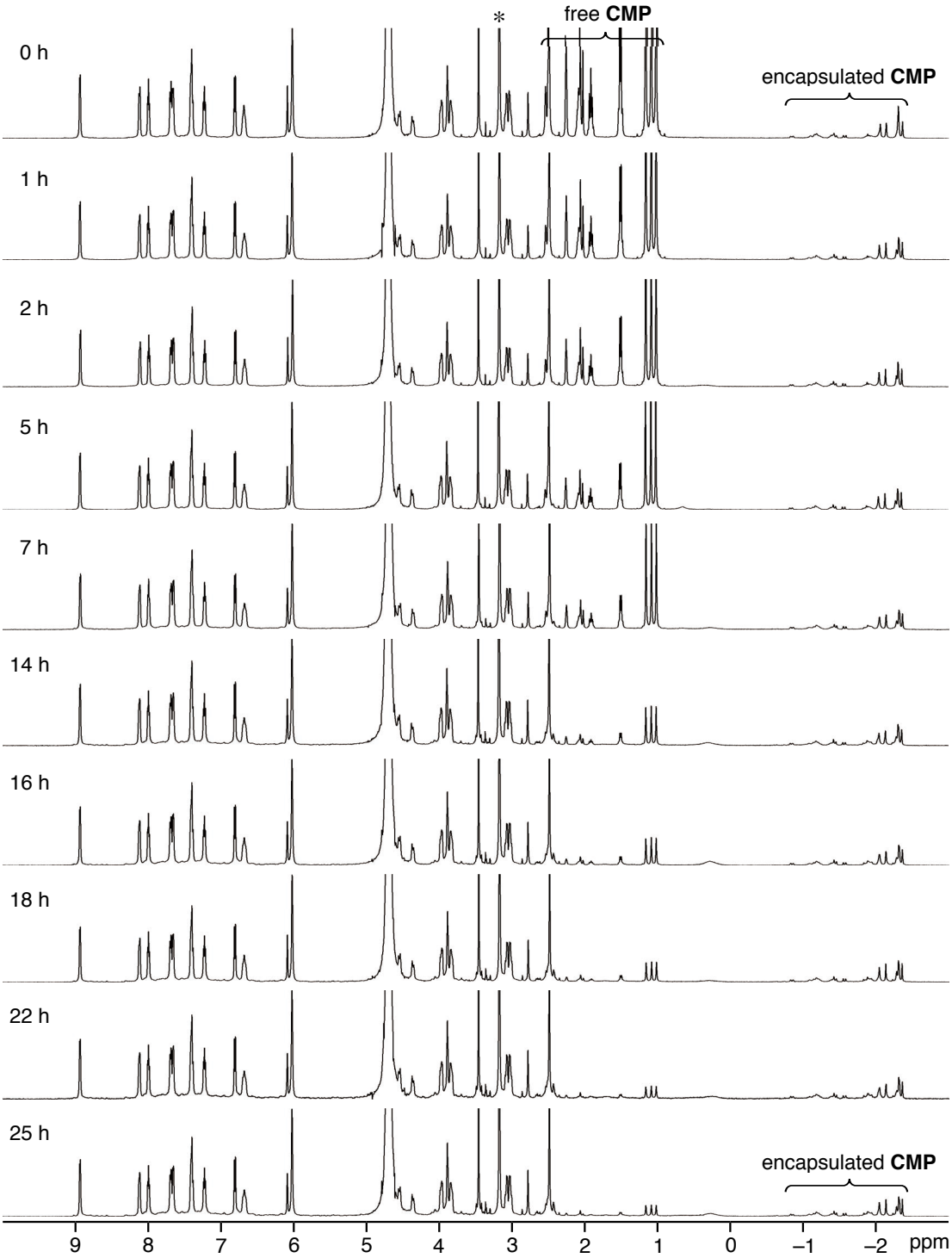


Figure S47a. Time-dependent ^{1}H NMR spectra (500 MHz, r.t.) of a mixture of **1•CMP** and **CMP** in D_2O before/after heating 80 ºC for 25 h (*: dimethyl sulfone as an internal standard).

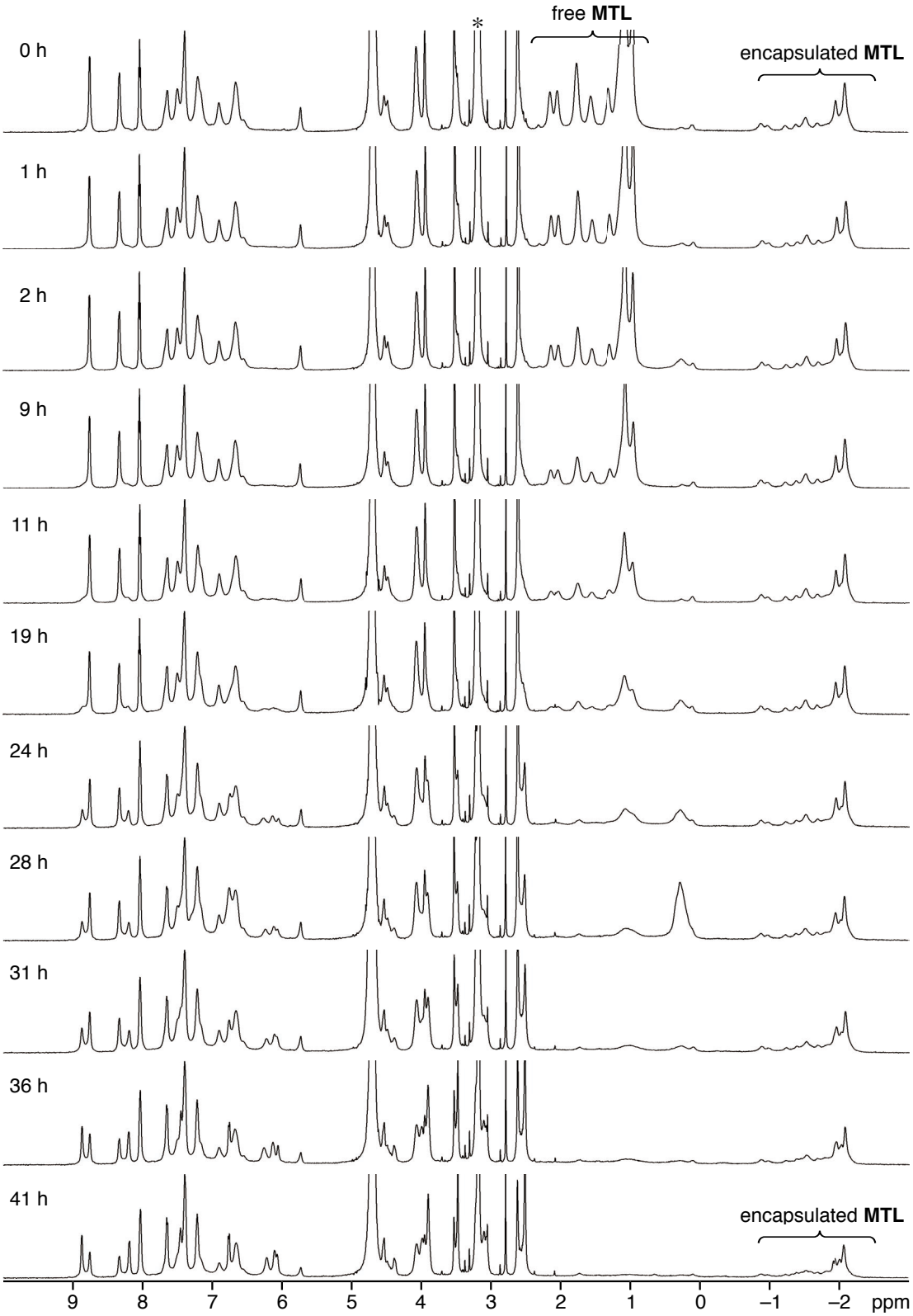


Figure S47b. Time-dependent ^{1}H NMR spectra (500 MHz, r.t.) of a mixture of **1•MTL** and **MTL** in D_2O before/after heating at 80 ºC for 41 h (*: dimethyl sulfone as an internal standard).

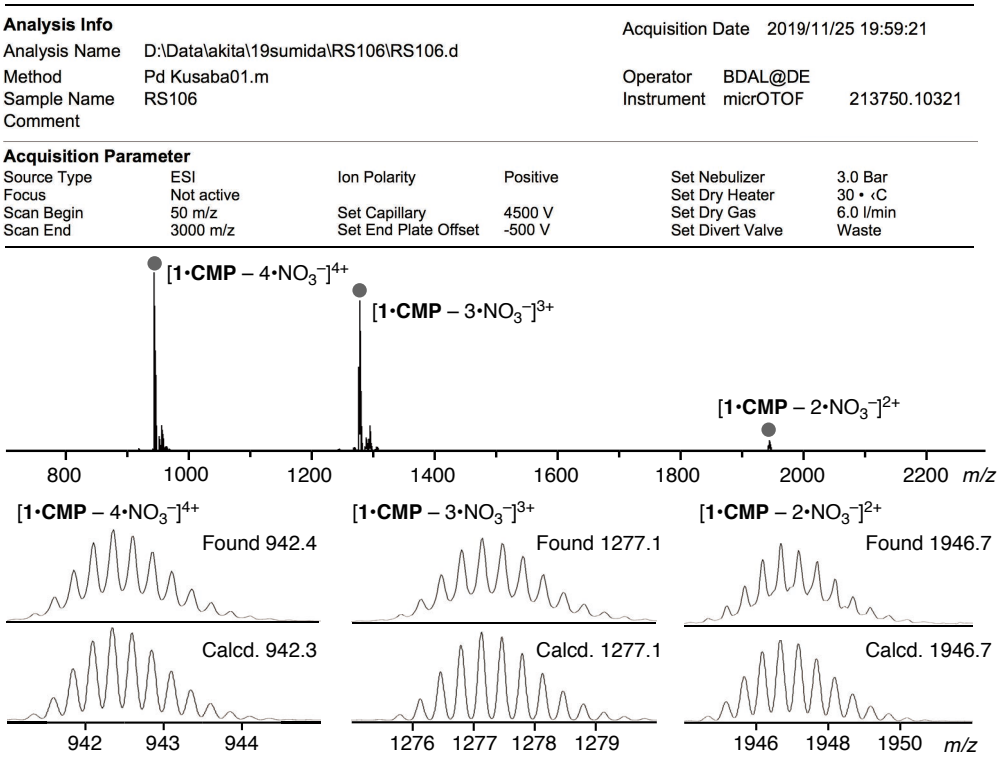


Figure S47c. ESI-TOF MS spectrum of **1•CMP** in D_2O after heating at 80 ºC for 25 h.

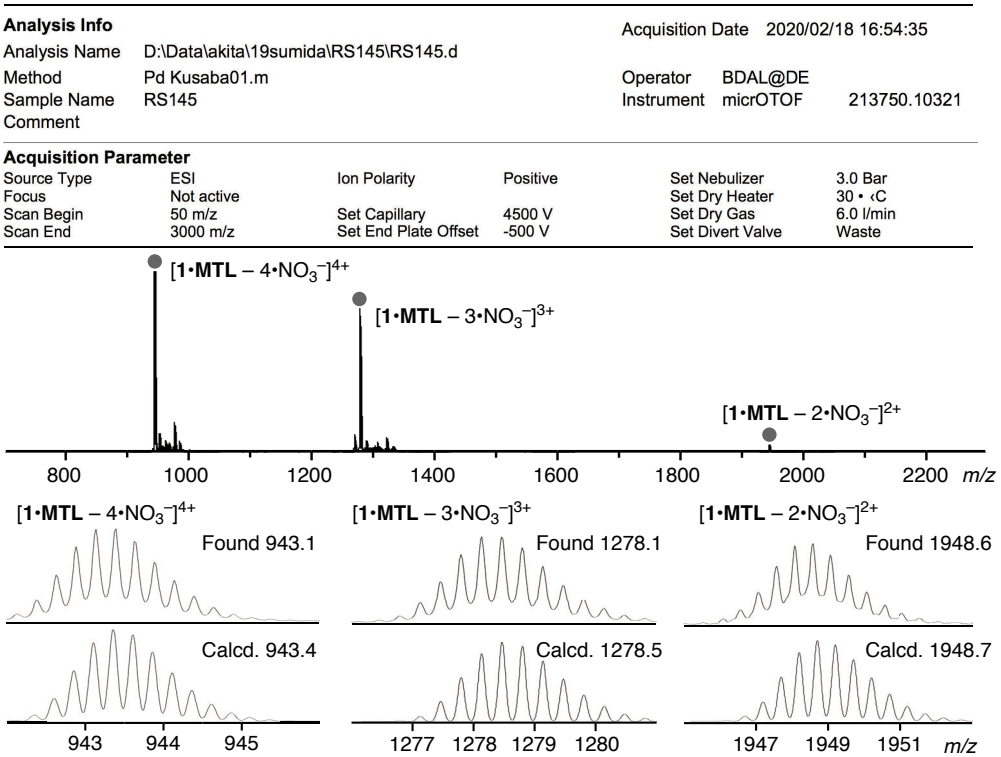


Figure S47d. ESI-TOF MS spectrum of **1•MTL** in D_2O after heating at 80 ºC for 41 h.

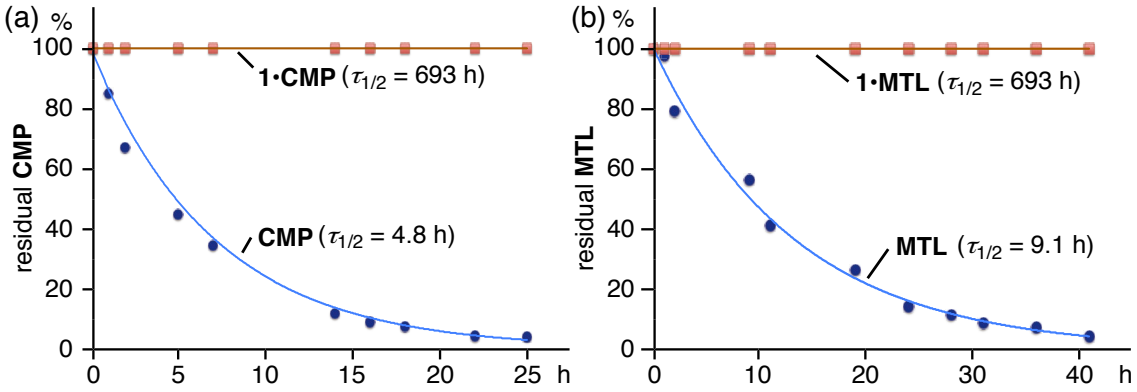
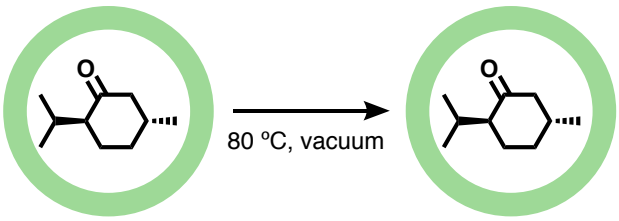


Figure S47e. Time-course volatility profiles (%) of (a) **CMP** and (b) **MTL** within/without **1** in water at 80 ºC and their half-life times.

Suppressed volatilities of MTO and MTL by 1 in the solid state RS229, 232, 234



The volatility of **MTO** from solid **1•MTO** was investigated under vacuum (480 Pa) at 80 ºC for 1 h by ^{1}H NMR analysis. Solid **1•MTO** was prepared using **1** (0.6 mg, 0.16 μmol), **MTO** (3.1 mg, 20 μmol), and D_2O (0.4 mL). The control experiments (**MTO** (neat)) were examined under vacuum (480 Pa) at r.t. and 80 ºC. Coronene (0.2 mg, 0.7 μmol) was used as an internal standard for the control experiments. In the same way, the volatilities of **MTL** from solid **1•MTL** and **MTL** (neat) were investigated under vacuum (480 Pa) at 80 ºC by ^{1}H NMR analysis.

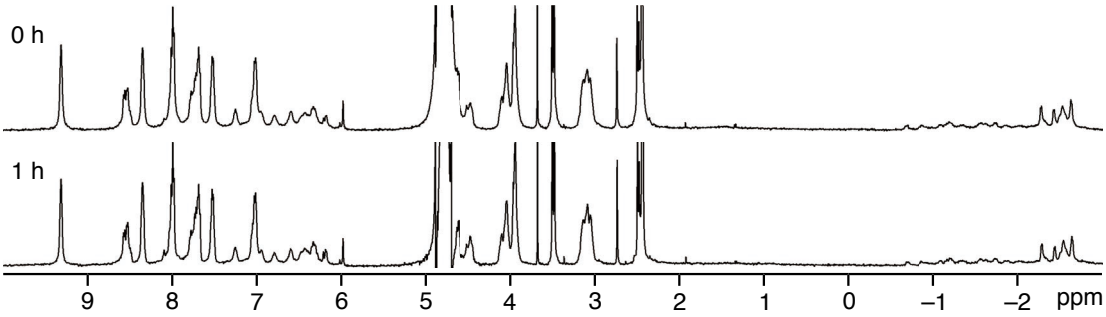


Figure S48a. Time-dependent ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of solid **1•MTO** before/after heating at 80 ºC under vacuum (480 Pa) for 1 h.

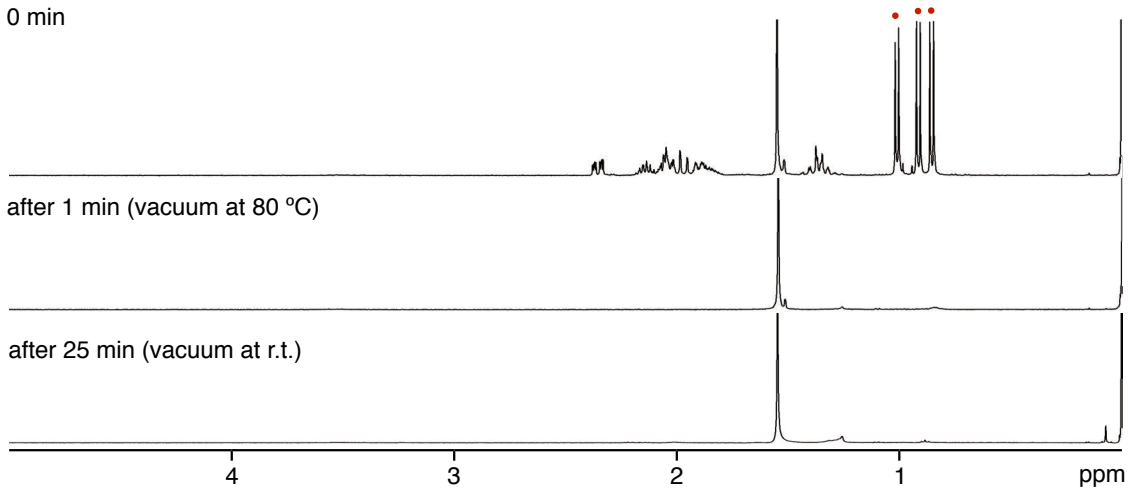


Figure S48b. Time-dependent ^{1}H NMR spectra (400 MHz, $CDCl_3$, r.t., coronene as an internal standard) of **MTO** (neat) before/after heating at 80 ºC under vacuum (480 Pa) for 1 min or standing at r.t. for 25 min.

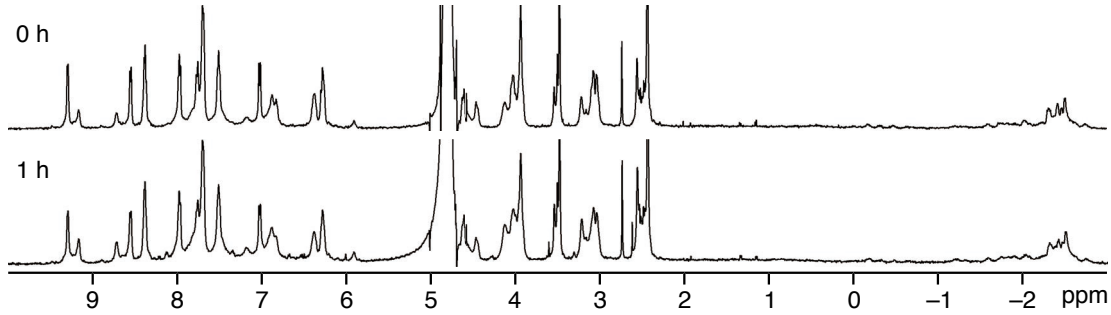


Figure S48c. Time-dependent ^{1}H NMR spectra (500 MHz, D_2O, r.t.) of solid **1•MTL** before/after heating at 80 ºC under vacuum (480 Pa) for 1 h.

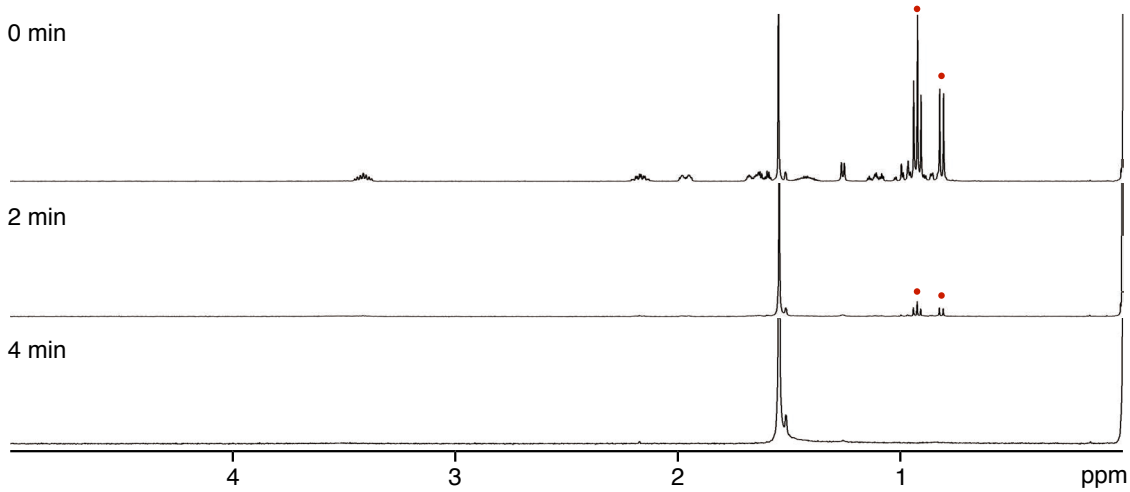


Figure S48d. Time-dependent ^{1}H NMR spectra (400 MHz, $CDCl_3$, r.t., coronene as an internal standard) of **MTL** (solid) before/after heating at 80 ºC under vacuum (480 Pa) for 2 and 4 min.

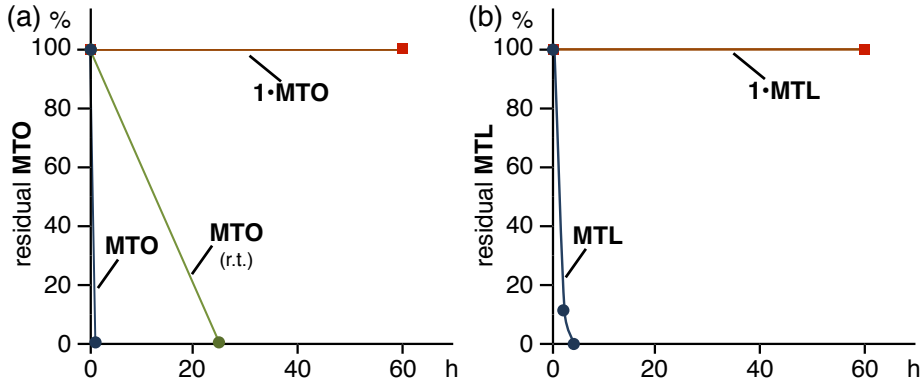


Figure S48e. Time-course volatility profiles (%) of **MTO** or **MTL** from (a) solid **1•MTO** and **MTO** (neat), and (b) solid **1•MTL** and **MTL** (neat) at 80 ºC (or r.t.) under vacuum (480 Pa).

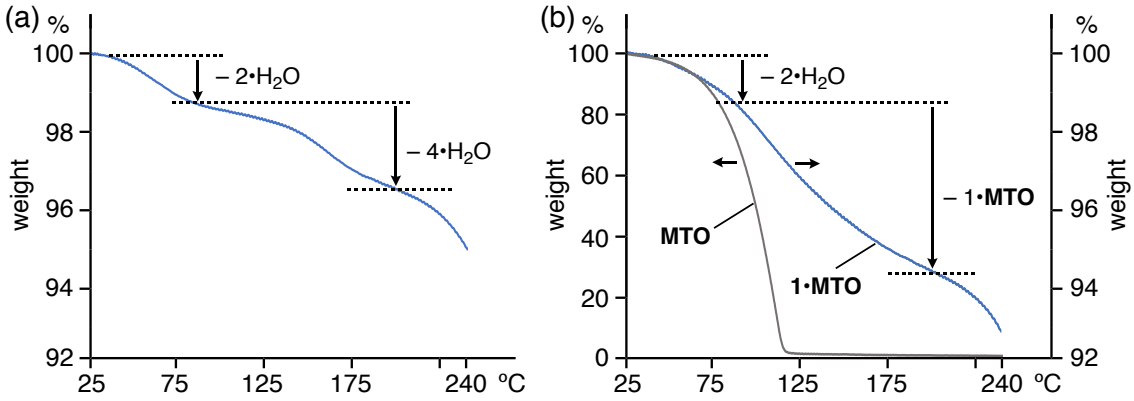


Figure S49. Thermogravimetry (TG) curves (heating rate of 10 ºC/min from 25 ºC to 240 ºC) of (a) **1** and (b) **MTO** and **1•MTO**.

Table S4. Cartesian coordinates of **ACI** (E_{opt} = –466.875425129 hartree, E_{sp} = –466.875425098 hartree).

C	0.24166	-1.29907	-0.82665	H	2.5259	-0.56557	1.6883
C	1.14014	-1.56115	0.38585	H	0.52342	0.76426	1.81952
C	2.02718	-0.35569	0.73429	H	1.75303	1.79688	1.0717
C	1.14931	0.89718	0.92692	H	-1.08916	0.21683	-1.62573
C	0.2341	1.12584	-0.26167	H	3.7814	0.70271	0.00829
C	-0.64982	-0.0503	-0.65766	H	3.72608	-1.0023	-0.46512
C	3.1166	-0.1057	-0.31159	H	2.69897	0.18604	-1.28069
C	-1.81875	-0.22998	0.34595	H	-1.40696	-0.53829	1.31587
C	-2.78969	-1.3189	-0.11639	H	-3.62924	-1.40187	0.58108
C	-2.57559	1.08563	0.55034	H	-2.31928	-2.30363	-0.17956
O	0.21673	2.1764	-0.86761	H	-3.20096	-1.07759	-1.1034
H	0.86611	-1.15821	-1.71632	H	-3.41385	0.94428	1.23975
H	-0.3752	-2.17816	-1.03424	H	-1.93744	1.87559	0.95626
H	0.52166	-1.81368	1.25616	H	-2.97894	1.45174	-0.40031
H	1.76981	-2.43736	0.19294				

Table S5. Cartesian coordinates of **TBI-a** (E_{opt} = –466.871918132 hartree, E_{sp} = –466.871918108 hartree).

C	-0.15962	-0.96539	1.30963	H	-1.26497	-0.23996	-1.49592
C	-1.26995	-1.38537	0.33228	H	-1.83817	1.97174	-0.49554
C	-1.79738	-0.21965	-0.53651	H	-2.01794	1.20759	1.07752
C	-1.49077	1.13329	0.11461	H	1.51231	0.38929	1.508
C	-0.0095	1.3376	0.38961	H	-3.64018	0.4158	-1.51302
C	0.79748	0.08727	0.73209	H	-3.49515	-1.33691	-1.31079
C	-3.2861	-0.37103	-0.8391	H	-3.87735	-0.31567	0.08238
C	1.63686	-0.39018	-0.48656	H	0.963	-0.5244	-1.34342
C	2.31064	-1.73708	-0.21114	H	2.9618	-2.01086	-1.0473
C	2.69438	0.64585	-0.87562	H	1.59095	-2.54903	-0.07606
O	0.49143	2.44179	0.35124	H	2.93399	-1.68406	0.68928
H	-0.61843	-0.53847	2.20961	H	3.23136	0.32239	-1.77327
H	0.39464	-1.84301	1.65276	H	2.25949	1.62837	-1.06452
H	-0.91491	-2.18737	-0.32447	H	3.42952	0.76241	-0.07075
H	-2.09761	-1.81394	0.90984				

Table S6. Cartesian coordinates of **TBI-b** (E_{opt} = –466.871131711 hartree, E_{sp} = –466.871131726 hartree).

C	-0.11237	-1.42369	0.82892	H	-1.42536	-0.8022	-1.38564
C	-1.6105	-1.12539	0.71492	H	-0.98212	1.52442	-1.33293
C	-1.9017	-0.29411	-0.53541	H	-1.96736	1.79624	0.08927
C	-1.25978	1.09226	-0.36238	H	1.40775	-0.02019	1.54436
C	-0.02403	1.107	0.52382	H	-3.57746	0.44603	-1.7136
C	0.79136	-0.17202	0.65205	H	-3.83968	-1.16041	-1.01665
C	-3.39397	-0.17757	-0.83224	H	-3.92293	0.27776	0.0129
C	1.76662	-0.31161	-0.54996	H	1.17111	-0.58072	-1.43439
C	2.77046	-1.43803	-0.2909	H	3.42002	-1.58343	-1.15988
C	2.51966	0.98593	-0.85256	H	2.28415	-2.39376	-0.07671
O	0.31002	2.12282	1.0971	H	3.40933	-1.18863	0.56413
H	0.0987	-1.90125	1.79048	H	3.2427	0.82522	-1.65857

H	0.13902	-2.16302	0.06015	H	1.85328	1.79704	-1.15705
H	-2.16925	-2.06784	0.68988	H	3.06758	1.33245	0.03008
H	-1.96416	-0.57694	1.59971				

Table S7. Cartesian coordinates of **MTO** (E_{opt} = –466.880602588 hartree, E_{sp} = –466.880602555 hartree).

C	-0.08395	-1.37218	-0.34961	H	-2.29605	-0.00452	-1.33635
C	-1.54335	-1.39186	0.10898	H	-1.96943	2.05225	0.00496
C	-2.28801	-0.10183	-0.24133	H	-1.55422	1.06465	1.42157
C	-1.52196	1.10729	0.32366	H	0.65813	-0.27424	1.33051
C	-0.07518	1.08726	-0.12666	H	-4.25732	0.80061	-0.02532
C	0.70201	-0.17661	0.23368	H	-4.28453	-0.96251	-0.1825
C	-3.73285	-0.12047	0.2481	H	-3.77329	-0.21707	1.33935
C	2.17734	-0.09648	-0.19347	H	2.19377	0.24281	-1.23604
C	2.8924	-1.44691	-0.10902	H	3.95491	-1.32523	-0.34228
C	2.92822	0.94032	0.64719	H	2.48688	-2.18234	-0.80913
O	0.39847	1.99116	-0.78261	H	2.82529	-1.86996	0.90106
H	0.40132	-2.30654	-0.05561	H	3.96623	1.03116	0.31129
H	-0.04103	-1.32778	-1.44649	H	2.46422	1.92517	0.57243
H	-2.05972	-2.24994	-0.33689	H	2.94888	0.64247	1.70308
H	-1.57986	-1.53935	1.19803				

Table S8. Cartesian coordinates of **1** (R = -OCH_3; E_{opt} = –8819.08385474 hartree, E_{sp} = –8819.58378719 hartree).

N	7.04754	-2.22227	-0.42899	C	4.47480	0.63499	4.89473
C	6.03963	-2.80509	0.24588	C	3.23221	2.63684	5.61545
H	5.26684	-2.14779	0.62686	C	5.65020	-1.05777	-3.18224
C	5.96308	-4.17696	0.45721	H	4.91640	-1.33949	-2.43623
C	7.00153	-4.96110	-0.04831	C	-4.65793	5.12731	-2.06145
H	6.98287	-6.03589	0.10066	C	3.39571	1.24051	5.62420
C	8.04751	-4.36115	-0.74017	C	6.38094	0.66017	2.06051
H	8.86574	-4.94748	-1.14222	H	5.49317	0.99703	1.53833
C	8.03834	-2.99021	-0.92037	C	3.13316	0.36823	-5.16425
H	8.82560	-2.48064	-1.46268	H	4.06540	0.81911	-4.84305
N	6.77783	-0.47748	-2.72971	C	3.18354	5.12435	-4.00095
N	7.06697	1.85759	-0.99192	C	3.04179	-1.05600	-5.28075
C	8.16635	2.57418	-0.69054	C	4.38131	4.49003	-3.52845
H	9.01668	2.02271	-0.30845	C	-3.49844	5.90704	-2.39159
C	8.20605	3.94564	-0.86087	C	1.33998	-6.27763	3.28964
H	9.11175	4.48895	-0.61710	C	0.16043	-5.53048	3.28078
C	7.07999	4.59998	-1.34458	H	0.13355	-4.60232	2.71849
H	7.08454	5.67613	-1.48451	C	-0.98959	-5.93902	3.94809
C	5.92917	3.87131	-1.65483	C	-0.95672	-7.12717	4.70350
C	5.97814	2.49414	-1.46505	C	0.22021	-7.88767	4.73549
H	5.11870	1.87617	-1.69701	C	1.34658	-7.47965	4.00456
C	-4.92122	3.94450	-2.77380	C	1.67315	-3.02711	-5.85054
N	-7.31513	-1.38137	-0.58869	N	7.33721	0.08140	1.31069
C	-8.41827	-2.14773	-0.49399	C	-2.64014	5.49334	-3.42608
H	-9.15896	-1.84620	0.23669	C	4.84577	-4.89402	2.58079
C	-8.59384	-3.26502	-1.28926	C	5.38417	1.45473	4.20693
H	-9.49856	-3.85398	-1.19168	C	3.73132	4.45939	-6.28110

C	-7.60184	-3.61150	-2.19909	H	3.50016	4.44678	-7.34093
H	-7.71330	-4.48678	-2.83091	C	-4.08950	3.54104	-3.83219
C	-6.45023	-2.82884	-2.30340	C	-4.33721	2.35445	-4.59503
C	-6.35968	-1.71489	-1.47604	H	-5.17617	1.71753	-4.33744
H	-5.49250	-1.06663	-1.52111	C	-3.54641	2.01094	-5.64822
C	4.58007	-0.79327	4.89957	H	-3.76086	1.10888	-6.21121
H	5.37390	-1.27329	4.33787	C	-2.44406	2.82875	-6.01542
C	4.16916	3.45028	4.95047	H	-1.84816	2.56775	-6.88424
C	5.26762	2.85441	4.24622	C	-2.14545	3.94059	-5.28994
C	6.22049	3.71811	3.61543	H	-1.30244	4.56168	-5.56614
H	7.07364	3.28102	3.10771	C	-2.94294	4.33820	-4.16908
C	6.10057	5.07329	3.67956	N	-6.82261	1.86731	1.89217
H	6.85060	5.70974	3.22073	C	-5.67983	2.02147	2.58758
C	5.00235	5.66468	4.36191	H	-4.91604	1.26708	2.43939
H	4.92041	6.74571	4.41037	C	-5.46012	3.08459	3.45597
C	4.06801	4.87724	4.96288	C	-6.49569	4.00870	3.60992
H	3.23128	5.33058	5.47967	H	-6.36672	4.84884	4.28461
N	-7.16292	1.50588	-0.99223	C	-7.67788	3.85005	2.89663
H	-8.49568	4.55421	2.99813	C	-3.60424	1.55317	8.00788
C	-7.80794	2.77275	2.03959	H	-3.47070	1.11829	8.99258
H	-8.70623	2.61340	1.45557	C	-2.58582	2.23528	7.41567
C	-6.12006	3.12585	-2.43325	H	-1.63844	2.34030	7.92825
C	2.54943	-5.79110	2.56287	C	4.92445	3.84306	-5.81477
C	6.49540	0.82846	3.43615	H	5.59646	3.37459	-6.52671
C	4.79592	-4.75160	1.18513	C	0.73310	-0.73706	-6.06206
C	-3.25453	7.10862	-1.65377	H	-0.19372	-1.15716	-6.43041
H	-2.38282	7.69926	-1.90642	C	2.52308	-5.67071	1.15916
C	2.89241	5.07167	-5.40081	C	6.40666	-0.91881	-5.43353
H	1.98555	5.54712	-5.75475	H	6.26038	-1.09274	-6.49468
C	5.23332	3.85360	-4.48805	C	6.04012	-4.67958	4.69312
H	6.15957	3.39958	-4.15227	H	6.93744	-4.42387	5.24751
N	-6.97770	-1.00558	2.26636	C	1.89426	6.63274	-0.81508
C	-7.96252	-1.01687	3.18435	H	1.02816	7.16254	-1.19138
H	-8.78848	-0.33531	3.02036	C	0.85885	0.61068	-5.92507
C	-7.91846	-1.85739	4.28148	H	0.02720	1.26268	-6.16867
H	-8.73281	-1.84564	4.99676	C	-1.38287	6.24642	-3.71439
C	-6.82397	-2.69821	4.44785	C	-0.15111	5.73668	-3.30232
H	-6.76199	-3.36091	5.30502	H	-0.12516	4.79325	-2.76546
C	-5.79111	-2.68800	3.50857	C	1.04799	6.38701	-3.57113
C	-5.92282	-1.82578	2.42617	C	1.02765	7.61273	-4.26049
H	-5.15651	-1.78545	1.66094	C	-0.20360	8.15963	-4.65154
C	1.80405	-1.62913	-5.73178	C	-1.39678	7.46439	-4.39828
C	-4.57243	-3.53633	3.63935	C	-7.28728	3.16666	-3.19944
C	-4.55805	-4.82965	3.09310	H	-7.33617	3.82046	-4.06419
C	-5.69718	-5.38762	2.42768	C	-8.37399	2.37438	-2.85068
H	-6.60832	-4.80259	2.36229	H	-9.29187	2.39220	-3.42695
C	-5.66781	-6.64486	1.90552	C	3.58986	-5.02104	-0.96681
H	-6.54933	-7.05775	1.42562	H	4.44489	-4.63724	-1.51236
C	-4.48413	-7.42790	1.99125	C	2.48334	-5.40824	-1.65810
H	-4.47011	-8.42647	1.56691	H	2.46207	-5.32279	-2.73951
C	-3.37729	-6.92810	2.60728	C	-5.25422	6.76025	-0.35374
H	-2.47519	-7.52459	2.65933	C	-3.11343	3.92881	3.54004
C	-3.36915	-5.62514	3.19894	C	-3.25780	4.50076	2.23526

C	3.71474	-1.56488	5.61250	H	-4.20360	4.40780	1.71339
H	3.82306	-2.64421	5.60658	C	-2.23893	5.17962	1.64131
C	2.07873	1.17383	-5.46573	H	-2.37703	5.60966	0.65512
H	2.17623	2.25023	-5.37422	C	-1.00409	5.35162	2.32102
C	2.76080	-3.86276	-5.53066	H	-0.20051	5.89870	1.84012
C	2.66584	-5.28814	-5.61900	C	-0.82988	4.83788	3.56883
H	1.72913	-5.72411	-5.94140	H	0.10699	4.99122	4.08839
C	3.72003	-6.09442	-5.31593	C	-1.86176	4.09283	4.22623
H	3.62577	-7.17178	-5.39970	C	-4.10035	7.52637	-0.67241
C	4.95457	-5.52815	-4.89743	H	-3.90566	8.45006	-0.13809
H	5.79318	-6.17988	-4.67427	C	3.86423	5.22142	-1.25425
C	5.08876	-4.17758	-4.78634	C	4.68935	4.52979	-2.15750
H	6.03979	-3.75737	-4.47672	C	-4.39589	-4.12746	-2.88639
C	4.00408	-3.29389	-5.09250	C	-4.45848	-4.83821	-1.64461
C	-1.68120	3.54163	5.51061	H	-5.24762	-4.60984	-0.93669
C	3.70337	-5.41237	3.27802	C	-3.55674	-5.81070	-1.33885
C	-2.23619	-5.12108	3.86798	H	-3.63164	-6.33918	-0.39449
C	7.67259	0.38163	4.03962	C	-2.52470	-6.14644	-2.25628
H	7.80318	0.49916	5.11054	H	-1.84038	-6.95499	-2.01966
C	7.57321	-0.32291	-4.96916	C	-2.40745	-5.47266	-3.43232
H	8.36163	-0.02257	-5.64970	H	-1.62512	-5.73268	-4.13433
C	-8.27887	1.55077	-1.74435	C	-3.32178	-4.43048	-3.79051
H	-9.09709	0.91006	-1.43920	H	-6.41847	5.04375	-0.78298
C	2.33617	5.79372	-3.10070	H	-5.93284	7.11274	0.41642
C	-5.26286	-2.49071	-4.48167	O	-2.59766	8.00775	-4.74126
C	-4.16985	-2.77672	-5.36554	O	2.22774	8.20037	-4.44609
C	-4.10757	-2.07887	-6.61281	O	-1.34669	5.01227	7.91792
H	-3.27624	-2.28226	-7.27645	O	3.39021	4.04894	7.98742
C	-5.07155	-1.19135	-6.98328	O	-2.07946	-7.42216	5.39023
H	-5.01845	-0.69602	-7.94740	O	2.49432	-8.21117	4.05693
C	-6.16393	-0.92173	-6.11405	O	-3.36158	-5.12628	-7.38290
H	-6.93801	-0.22825	-6.42719	O	1.33981	-4.45128	-8.28672
C	-6.24884	-1.54144	-4.90414	C	-3.81341	-5.30670	-8.72647
H	-7.09802	-1.34055	-4.25978	H	-3.46804	-6.25382	-9.14155
C	2.23181	6.71795	0.50018	H	-4.90198	-5.30709	-8.66180
H	1.64176	7.32785	1.17691	H	-3.48007	-4.48924	-9.36966
C	8.46546	-0.35011	1.90589	C	1.33352	-3.79096	-9.55609
H	9.20621	-0.81417	1.26611	H	0.49950	-4.13137	-10.17234
C	6.00645	-4.53530	3.33971	H	1.27984	-2.70561	-9.41729
H	6.88326	-4.16543	2.81915	H	2.27843	-4.04972	-10.03347
C	2.52068	0.38847	6.37182	C	-2.85464	8.14779	-6.14223
H	1.73582	0.84781	6.95962	H	-2.86907	7.16406	-6.62422
C	4.90391	-5.17600	5.38837	H	-3.84069	8.60486	-6.22203
H	4.94193	-5.28682	6.46700	H	-2.10806	8.78648	-6.61744
C	2.03516	3.24929	6.26429	C	2.48210	9.05338	-5.56428
C	2.15370	3.99383	7.45215	H	1.99703	8.67654	-6.46752
C	1.00727	4.57677	8.01055	H	2.14595	10.07306	-5.37510
C	-0.23388	4.45314	7.36601	H	3.56501	9.03924	-5.69218
C	-0.36583	3.69160	6.20027	C	-1.38529	6.44219	7.95110
C	0.78280	3.09144	5.68150	H	-1.36164	6.84470	6.93249
H	0.70260	2.50257	4.77301	H	-2.33122	6.70571	8.42385
C	-5.34130	-3.15288	-3.24487	H	-0.55371	6.84476	8.53216
C	3.36855	6.02163	0.99209	C	3.82093	5.15293	8.78585

H	3.61463	6.06765	2.04742	H	4.91002	5.13179	8.73475
C	-6.11254	2.27823	-1.33024	H	3.44893	6.09937	8.38720
H	-5.23812	2.21220	-0.69356	H	3.49799	5.04813	9.82188
C	5.40936	-1.29360	-4.53080	C	-2.46189	-8.77051	5.66880
C	4.15383	5.30043	0.14614	H	-3.54034	-8.73350	5.82684
H	5.02022	4.78410	0.54442	H	-2.23309	-9.42946	4.82824
C	-3.45179	-3.02245	4.31020	H	-1.96982	-9.14878	6.56509
C	-2.27119	-3.83205	4.43322	C	2.44469	-9.50768	3.45306
C	-1.15799	-3.29078	5.15375	H	1.69140	-10.13579	3.93192
H	-0.27640	-3.90625	5.27779	H	2.23374	-9.41799	2.38189
C	-1.19335	-2.03903	5.68555	H	3.43453	-9.94158	3.59297
H	-0.33353	-1.65095	6.22101	O	-1.08430	-5.50385	-9.08285
C	-2.35656	-1.23489	5.55123	O	-0.24825	9.37046	-5.28448
H	-2.38218	-0.24498	5.99437	O	0.27552	-9.03596	5.47546
C	-3.44638	-1.71378	4.89184	O	1.09325	5.28199	9.17866
H	-4.33605	-1.09721	4.82645	C	-0.68574	10.45718	-4.46396
C	-5.51967	5.60259	-1.02071	H	-0.67632	11.34215	-5.10030
C	-4.15554	3.22588	4.16486	H	-1.69895	10.27969	-4.09368
C	2.68209	5.87638	-1.74075	H	0.00077	10.60400	-3.62285
C	3.65793	-5.13609	0.45899	C	1.01610	-8.92765	6.69389
C	7.72594	-0.10897	-3.61158	H	0.97055	-9.90903	7.16619
H	8.61300	0.36058	-3.20410	H	2.05778	-8.66402	6.49211
C	2.67870	-0.96277	6.37640	H	0.56113	-8.18194	7.35507
H	2.02448	-1.58703	6.97665	C	0.57587	4.60326	10.32629
C	3.77861	-5.51971	4.70335	H	0.71047	5.28260	11.16807
H	2.91816	-5.89616	5.24042	H	-0.48679	4.38056	10.19844
C	-3.19987	-3.73014	-5.00327	H	1.13373	3.67841	10.50967
C	4.12079	-1.89984	-4.97376	C	-0.52453	-6.81954	-9.05173
C	8.66548	-0.20876	3.26661	H	-0.66479	-7.23369	-10.05024
H	9.58984	-0.56017	3.71043	H	0.54206	-6.78138	-8.81483
C	1.36535	-5.94953	-0.96924	H	-1.04947	-7.44328	-8.31989
H	0.49121	-6.26250	-1.53021	Pt	-7.06911	0.25193	0.64070
C	1.39012	-6.08128	0.38491	Pt	7.05698	-0.18406	-0.71183
H	0.54189	-6.51219	0.90108	C	-0.99687	-4.81732	-7.90379
C	0.36965	-3.61018	-6.28505	C	0.23537	-4.27179	-7.50979
C	-0.76735	-3.48286	-5.48536	C	-2.73218	2.83029	6.12213
H	-0.68484	-2.96647	-4.53398	C	-3.98880	2.67455	5.44527
C	-2.01231	-3.96031	-5.87833	C	-5.03447	1.95135	6.10455
C	-2.13365	-4.64527	-7.10116	H	-5.99472	1.84577	5.61099
H	-5.66161	0.88051	7.83020	C	-4.85206	1.41374	7.34229

Table S9. Cartesian coordinates of **1•ACI** (R = -OCH_3; E_{opt} = –9285.98284472 hartree, E_{sp} = –9286.47087292 hartree).

N	-7.11988	0.81483	1.89719	C	2.64002	-0.66669	6.38352
C	-5.99486	1.17655	2.54249	H	2.06906	-1.39329	6.95293
H	-5.0866	0.67372	2.22783	C	3.78666	-1.0887	5.65728
C	-5.98423	2.14676	3.54125	H	4.0645	-2.1375	5.64985
C	-7.19856	2.75951	3.8564	C	4.54454	-0.18135	4.98285
H	-7.22916	3.51782	4.63218	H	5.42494	-0.52256	4.44936
C	-8.35613	2.39531	3.18013	C	5.89378	-3.41538	-4.75475
H	-9.31024	2.85731	3.406	C	5.62783	-4.12201	1.33093
C	-8.28273	1.41678	2.20663	C	-2.49385	-4.50102	-3.95736
H	-9.15799	1.09497	1.65549	C	-3.9512	3.58897	3.81954

N	-7.37896	0.68762	-1.00899	C	-8.56537	0.7638	-1.63908
N	-7.04806	-2.20113	-0.90446	H	-9.33048	0.06631	-1.32035
C	-8.11628	-3.00564	-1.05368	C	-0.85484	-2.23766	5.16294
H	-8.95837	-2.82166	-0.39748	H	-0.06255	-1.70768	5.68112
C	-8.13598	-4.01649	-1.99598	C	-2.81894	1.39053	7.29001
H	-9.01324	-4.64608	-2.08995	H	-1.91495	1.65569	7.82371
C	-7.02381	-4.20019	-2.8082	C	1.63202	5.86052	-2.94826
H	-7.01361	-4.98255	-3.56031	C	-5.41361	3.39848	-2.71579
C	-5.90884	-3.37328	-2.66087	C	-7.60815	-3.40224	3.76688
C	-5.96584	-2.38278	-1.68414	H	-8.43906	-3.6645	4.41156
H	-5.12866	-1.71698	-1.49861	C	-2.40865	5.81719	3.01805
C	4.70677	-1.23724	-4.81024	H	-1.84498	6.69556	2.71957
N	6.94146	2.75231	-0.78792	C	-2.00039	5.06997	4.07987
C	7.91575	3.64881	-0.54568	H	-1.106	5.34291	4.62635
H	8.84576	3.26118	-0.14785	C	-2.10176	6.01422	-3.64881
C	7.73618	4.99721	-0.7943	C	-0.8346	5.58493	-3.25279
H	8.54559	5.69022	-0.59557	H	-0.73582	4.60579	-2.79527
C	6.51482	5.43665	-1.29006	C	0.30815	6.35682	-3.42643
H	6.34567	6.49043	-1.48665	C	0.18726	7.63056	-4.01505
C	5.49068	4.5185	-1.53296	C	-1.07657	8.08256	-4.42111
C	5.76089	3.18017	-1.27363	C	-2.20759	7.26714	-4.25882
H	5.00808	2.4223	-1.45673	C	4.48873	-4.96437	3.33144
C	-3.12239	-2.27083	4.34559	C	5.58947	-4.27071	2.72648
H	-4.08989	-1.79156	4.25171	C	6.61545	-3.74237	3.57493
C	-2.47081	-6.19105	2.80756	H	7.46394	-3.23781	3.1257
C	-3.75872	-5.57636	2.66041	C	6.55988	-3.88704	4.92759
C	-4.78615	-6.30227	1.97481	H	7.35838	-3.4984	5.55149
H	-5.76603	-5.85165	1.86372	C	5.4604	-4.55583	5.53121
C	-4.56123	-7.5472	1.47129	H	5.42602	-4.66459	6.61016
H	-5.35826	-8.08392	0.96698	C	4.46216	-5.0665	4.75887
C	-3.2797	-8.14935	1.59765	H	3.62899	-5.57385	5.22666
H	-3.10758	-9.13657	1.18177	C	-5.72157	-1.50377	-6.48483
C	-2.27475	-7.48825	2.2355	H	-6.57445	-0.93729	-6.84456
H	-1.29617	-7.94489	2.31427	C	-2.51871	3.52956	-5.08802
N	7.1441	0.3814	-2.45748	H	-1.74744	4.22742	-5.3891
C	-2.94015	-3.59349	3.82752	C	-2.74735	3.93195	4.5261
C	-1.43852	-5.52036	3.49331	C	-7.77205	2.5519	-3.00857
C	-6.38636	1.52378	-1.36472	H	-7.92593	3.28766	-3.79137
H	-5.44933	1.40663	-0.83163	C	-4.80593	0.04516	7.06045
C	4.72873	-2.6255	-5.01963	H	-5.43794	-0.74887	7.44472
C	-1.66134	-4.22592	4.00163	C	-1.46006	-5.39989	-3.53816
C	-5.57021	-2.6759	2.09886	H	-0.61194	-5.54862	-4.19472
H	-4.79536	-2.34144	1.41741	C	-2.63721	2.32926	-5.71786
C	-4.55044	1.75411	-4.36505	H	-1.96551	2.07083	-6.5305
H	-5.34218	1.05866	-4.10916	C	1.16337	-3.22679	-6.29975
C	-3.50227	-3.01561	-5.60376	C	-0.01062	-3.26367	-5.54492
C	-4.47952	3.01623	-3.69143	H	-0.0259	-2.77639	-4.575
C	-4.66584	-2.88339	-4.77516	C	-1.17404	-3.87401	-6.00118
C	3.54978	-3.28422	-5.50547	C	-1.16192	-4.53465	-7.24386
C	-1.05541	3.49602	6.32798	C	0.01269	-4.5312	-8.00899
C	0.15743	3.1215	5.74882	C	1.15156	-3.84923	-7.55309
H	0.14662	2.60279	4.79485	C	6.95453	-0.12764	-5.16809
C	1.38257	3.40436	6.34347	H	6.87932	-0.32645	-6.2323
C	1.40838	4.06676	7.5841	C	8.05776	0.54061	-4.65036
C	0.19893	4.4234	8.1979	H	8.86501	0.87507	-5.29176
C	-1.02165	4.15943	7.5573	C	-4.3288	4.38999	2.69337
C	-3.28936	5.15239	-3.38002	H	-5.23129	4.14388	2.14453
N	-6.77069	-2.08096	1.9723	C	-3.58912	5.46627	2.30787
C	2.38609	-2.54036	-5.78763	H	-3.90275	6.05999	1.45561

C	-4.35953	1.78143	5.41024	C	5.89599	-4.76258	-4.95209
C	-3.97161	-4.28539	3.17336	C	4.62139	-4.66493	0.517
C	-4.56221	-1.61976	-7.29967	C	4.643	-4.53953	-0.90965
H	-4.53803	-1.13443	-8.26984	H	5.46596	-4.01783	-1.38586
C	3.5492	-0.48605	-5.06836	C	3.66573	-5.08285	-1.68568
C	3.50291	0.93189	-4.86904	H	3.71082	-4.98461	-2.76515
H	4.3924	1.45001	-4.52791	C	2.59854	-5.80514	-1.08665
C	2.37577	1.65013	-5.12507	H	1.83705	-6.25468	-1.71558
H	2.37025	2.72507	-4.9761	C	2.54039	-5.95017	0.26564
C	1.21335	0.99867	-5.61765	H	1.73682	-6.52008	0.71421
H	0.32159	1.58011	-5.82626	C	3.53292	-5.37789	1.1256
C	1.22059	-0.34416	-5.84202	C	4.72469	-5.42023	-5.41596
H	0.34004	-0.82721	-6.24535	H	4.73652	-6.49476	-5.5641
C	2.37463	-1.14776	-5.56683	C	-3.64358	-4.34726	-3.1091
N	7.57213	-1.25569	-0.10483	C	-4.70284	-3.52611	-3.52575
C	6.61478	-1.99884	0.47899	C	3.12734	5.19895	-1.10244
H	5.71094	-1.47986	0.77575	C	3.31311	5.01723	0.30609
C	6.74646	-3.36443	0.70192	H	4.27696	4.68867	0.67848
C	7.94397	-3.96474	0.30919	C	2.31249	5.26795	1.19366
H	8.08929	-5.02795	0.47107	H	2.48167	5.12736	2.25573
C	8.93855	-3.19772	-0.28679	C	1.05614	5.74779	0.73576
H	9.87764	-3.63917	-0.6001	H	0.26978	5.96098	1.45251
C	8.71975	-1.84708	-0.48651	C	0.8442	5.95663	-0.59243
H	9.46087	-1.21295	-0.95796	H	-0.10417	6.35345	-0.93003
C	5.9299	-0.54354	-4.3153	C	1.85342	5.67279	-1.56962
C	-2.34824	3.18415	5.64801	H	6.79516	-2.92512	-4.40334
C	-5.31769	-3.65619	3.05394	H	6.79352	-5.34097	-4.75813
C	-4.72409	2.5022	4.25936	O	2.29292	-3.85973	-8.2966
C	3.59669	-4.70451	-5.67791	O	-2.30314	-5.16638	-7.58426
H	2.70801	-5.21228	-6.02893	O	3.65357	-7.92314	4.02757
C	-3.48978	-2.3363	-6.86346	O	-1.06172	-7.77845	5.05027
H	-2.60472	-2.41136	-7.4826	O	2.63065	4.2637	8.12095
C	-5.76243	-2.09981	-5.26122	O	-2.1996	4.46776	8.16687
H	-6.65403	-2.00564	-4.65147	O	1.32115	8.35695	-4.09657
N	7.35203	1.10375	1.5903	O	-3.43948	7.72625	-4.6126
C	8.49698	0.89542	2.26674	C	1.53906	9.29294	-5.15462
H	9.34826	0.55576	1.68938	H	1.09724	10.26329	-4.92749
C	8.57988	1.10324	3.63119	H	2.62272	9.3887	-5.23201
H	9.52063	0.93324	4.14205	H	1.13172	8.92493	-6.09895
C	7.44992	1.52483	4.32123	C	-3.66394	7.9215	-6.01287
H	7.4872	1.68922	5.39328	H	-2.96256	8.64883	-6.42563
C	6.25303	1.73902	3.6336	H	-3.57517	6.96886	-6.54619
C	6.26055	1.52032	2.26051	H	-4.68378	8.29448	-6.10375
H	5.36357	1.68022	1.67372	C	2.24043	-3.16032	-9.5439
C	-3.41644	3.91708	-4.04111	H	2.04267	-2.09648	-9.37298
C	5.00667	2.17204	4.32915	H	3.22514	-3.27876	-9.9956
C	4.66188	3.53401	4.36056	H	1.4769	-3.58239	-10.19964
C	5.4735	4.54356	3.74937	C	-2.68718	-5.35442	-8.94783
H	6.39591	4.25294	3.25786	H	-2.44349	-4.47823	-9.55274
C	5.12871	5.86025	3.80407	H	-2.20934	-6.23367	-9.38051
H	5.76861	6.61036	3.35065	H	-3.76795	-5.49691	-8.92092
C	3.93748	6.26455	4.46561	C	3.83157	-9.21711	3.44209
H	3.6756	7.3166	4.50268	H	3.68513	-9.16469	2.35781
C	3.13639	5.33511	5.05574	H	4.86097	-9.50372	3.65599
H	2.22944	5.64317	5.56171	H	3.14384	-9.94378	3.87819
C	3.4652	3.94254	5.03916	C	-1.27722	-9.16797	5.30571
C	-2.11393	-1.60804	4.97468	H	-2.35888	-9.27779	5.39149
H	-2.27979	-0.60878	5.36127	H	-0.90685	-9.78439	4.48357
C	-3.65899	1.41771	-5.33707	H	-0.79875	-9.48251	6.23342

H	-3.73947	0.45986	-5.83827	C	2.90663	5.3848	8.96348
C	-4.24147	5.53385	-2.41438	H	3.98476	5.53435	8.89523
C	-4.16307	6.78898	-1.73141	H	2.38574	6.27931	8.6144
H	-3.34248	7.45495	-1.96373	H	2.62571	5.18697	9.99805
C	-5.10364	7.16737	-0.82278	C	-2.47759	5.86061	8.34247
H	-5.03636	8.13601	-0.33837	H	-1.70882	6.34184	8.94962
C	-6.1878	6.30125	-0.51404	H	-2.55287	6.35679	7.36864
H	-6.94054	6.61886	0.20048	H	-3.43999	5.91251	8.85106
C	-6.28727	5.08448	-1.11713	O	-1.21381	9.32503	-4.97395
H	-7.12282	4.43629	-0.87769	O	0.05257	-5.18174	-9.21071
C	-5.32628	4.65242	-2.08742	O	0.20256	5.03182	9.42174
C	3.46842	-5.51013	2.52659	O	1.47764	-9.04954	5.30049
C	-3.15686	2.13063	6.11264	C	0.7726	-6.41729	-9.19865
C	2.65423	2.98767	5.6794	H	0.71841	-6.81112	-10.21362
C	-6.3704	-4.01945	3.89636	H	1.81764	-6.25411	-8.92193
H	-6.21132	-4.78254	4.65146	H	0.30694	-7.12666	-8.50572
C	-8.79506	1.68566	-2.6431	C	-0.16337	4.18103	10.51193
H	-9.76404	1.72131	-3.12746	H	-0.12376	4.80039	11.40802
C	8.11957	0.78758	-3.29102	H	-1.17612	3.79215	10.37664
H	8.95296	1.31631	-2.84429	H	0.54719	3.35271	10.60772
C	-2.41809	-3.807	-5.17833	C	2.10705	-8.83283	6.56599
C	3.93478	5.10942	-3.40702	H	2.16691	-9.80895	7.04751
C	2.65389	5.56087	-3.8697	H	3.11289	-8.42519	6.43374
C	2.45131	5.68555	-5.28076	H	1.50562	-8.15654	7.18336
H	1.47869	6.00378	-5.63534	C	-1.7837	10.30765	-4.105
C	3.44172	5.4062	-6.17212	H	-1.83097	11.23215	-4.68056
H	3.2646	5.5105	-7.23724	H	-2.7904	10.01429	-3.79576
C	4.71632	4.97952	-5.7107	H	-1.14856	10.45648	-3.22482
H	5.50321	4.77283	-6.42885	Pt	7.25779	0.74996	-0.43665
C	4.95117	4.83279	-4.37728	Pt	-7.07725	-0.68932	0.48997
H	5.92972	4.50963	-4.03865	C	-1.24154	2.0726	0.23175
C	-1.54154	-6.07804	-2.3613	H	-0.62102	2.61396	0.95475
H	-0.75832	-6.77357	-2.07715	C	-0.32203	1.47466	-0.84453
C	-7.77505	-2.43321	2.79533	H	0.51685	0.96093	-0.35912
H	-8.71896	-1.92009	2.65732	H	0.11775	2.28458	-1.43723
C	-5.16034	0.71237	5.92715	C	-1.057	0.50057	-1.77058
H	-6.0811	0.44939	5.41818	H	-0.36731	0.08686	-2.51123
C	-0.64639	-3.50303	4.7088	H	-1.8176	1.03878	-2.34754
H	0.30574	-3.98674	4.88262	C	-1.74537	-0.64853	-0.99694
C	-3.61475	0.38873	7.7545	H	-2.39875	-1.20676	-1.67799
H	-3.34749	-0.14782	8.65851	C	-2.63462	-0.02894	0.06196
C	-0.10184	-6.16521	3.65237	C	-1.96345	0.94239	1.00161
C	0.04749	-7.33354	4.42567	H	-2.70229	1.3501	1.69687
C	1.31373	-7.92352	4.54274	H	-1.22881	0.37798	1.59073
C	2.41997	-7.36395	3.88566	O	-3.83314	-0.28283	0.13891
C	2.29278	-6.17676	3.15767	C	-1.48706	-2.66236	0.53633
C	1.02325	-5.60616	3.0558	C	-0.75489	-1.66616	-0.36517
H	0.90777	-4.69184	2.48201	H	-2.25259	-3.20875	-0.02584
C	4.15038	4.94321	-2.02915	H	-1.96877	-2.17687	1.39104
C	-2.6633	-5.9003	-1.50678	H	-0.79056	-3.40334	0.93926
H	-2.71907	-6.44562	-0.57067	C	-2.24331	3.07053	-0.3487
C	6.08053	-0.2721	-2.96055	H	-2.88233	3.48484	0.43534
H	5.32344	-0.58513	-2.25107	H	-2.89202	2.62098	-1.10836
C	-6.53578	2.48024	-2.36445	H	-1.72034	3.90787	-0.81879
C	-3.67625	-5.06626	-1.87046	C	0.03102	-2.41418	-1.44398
H	-4.53764	-4.96313	-1.21967	H	0.63637	-1.74519	-2.06252
C	4.21378	1.21239	4.97977	H	-0.64579	-2.96987	-2.1017
C	3.02907	1.63248	5.67557	H	0.70898	-3.14162	-0.98638
C	2.2722	0.64348	6.38265	H	-0.03732	-1.11432	0.25448

H	1.40311	0.96561	6.94253				

Table S10. Cartesian coordinates of **1•TBI-a** (R = -OCH_3; E_{opt} = – 9285.9803323 hartree, E_{sp} = –9286.46815435 hartree).

N	7.38832	-1.21029	0.8266	C	-1.19132	0.96315	5.4595
C	6.34807	-1.52722	1.61949	H	-0.38693	1.67209	5.62247
H	5.41133	-1.0258	1.3978	C	-2.43768	1.42148	4.95608
C	6.45313	-2.45256	2.65427	H	-2.58166	2.47683	4.75185
C	7.69086	-3.06876	2.84594	C	-3.46017	0.54438	4.76562
H	7.8095	-3.7948	3.64382	H	-4.41814	0.91995	4.42423
C	8.76093	-2.74701	2.0201	C	-6.26899	3.76007	-3.8601
H	9.73156	-3.21208	2.14798	C	-4.84165	4.50796	2.00733
C	8.57672	-1.8109	1.02004	C	2.04024	3.94826	-4.53899
H	9.38029	-1.52501	0.35213	C	4.34	-3.7085	3.15525
N	7.05334	-1.32235	-2.05052	C	8.10166	-1.58611	-2.85131
N	6.94448	1.57621	-2.16852	H	8.97607	-0.95848	-2.72963
C	8.01237	2.2633	-2.61226	C	2.40772	2.67472	5.41437
H	8.95334	2.07666	-2.10903	H	1.816	2.32028	6.25236
C	7.91288	3.16137	-3.65837	C	3.95489	-1.62293	6.85406
H	8.79374	3.69803	-3.99131	H	3.10196	-1.8042	7.49461
C	6.67765	3.35317	-4.26353	C	-2.67226	-5.93281	-2.33113
H	6.57076	4.04785	-5.09042	C	4.55725	-3.90488	-3.16485
C	5.55998	2.65019	-3.80841	C	8.51765	3.0917	2.19931
C	5.74409	1.7691	-2.7469	H	9.47783	3.34379	2.63437
H	4.91752	1.20444	-2.3283	C	2.47111	-5.71333	2.47483
C	-5.43733	1.46397	-4.30902	H	1.77915	-6.5082	2.2153
N	-7.31229	-2.19533	0.23616	C	2.31484	-5.02234	3.63684
C	-8.36567	-2.93862	0.62347	H	1.49802	-5.26193	4.30627
H	-9.18744	-2.41121	1.0928	C	0.93602	-6.25322	-3.48309
C	-8.39418	-4.30787	0.4326	C	-0.23904	-5.79372	-2.88613
H	-9.26188	-4.87421	0.75084	H	-0.2249	-4.83837	-2.37044
C	-7.30211	-4.93206	-0.15886	C	-1.43604	-6.49935	-2.94623
H	-7.29618	-6.00647	-0.31176	C	-1.46071	-7.75229	-3.58838
C	-6.19953	-4.17339	-0.5567	C	-0.28922	-8.24072	-4.18288
C	-6.26019	-2.80105	-0.34421	C	0.88813	-7.47708	-4.15895
H	-5.43771	-2.16253	-0.64476	C	-3.35739	5.2063	3.8322
C	4.34422	2.40407	4.00068	C	-4.56681	4.57512	3.38353
H	5.23444	1.84821	3.72811	C	-5.45872	4.03807	4.36702
C	3.37659	6.07652	2.0646	H	-6.3897	3.58491	4.04349
C	4.57415	5.37562	1.69714	C	-5.17436	4.11221	5.69692
C	5.42434	5.95785	0.70222	H	-5.87183	3.71301	6.42622
H	6.33736	5.44389	0.42295	C	-3.97039	4.72187	6.14139
C	5.12153	7.15138	0.12035	H	-3.75672	4.77458	7.20348
H	5.78958	7.58271	-0.61806	C	-3.09644	5.24572	5.23882
C	3.92935	7.84038	0.47459	H	-2.18383	5.71665	5.58106
H	3.69714	8.78813	0.00032	C	4.55686	0.59939	-7.41078
C	3.08678	7.31292	1.40502	H	5.28039	-0.07102	-7.86304
H	2.17562	7.83604	1.66822	C	1.18039	-3.65072	-4.76349
N	-7.51736	0.14817	-1.4725	H	0.29099	-4.25449	-4.8896
C	4.04365	3.62753	3.31794	C	3.22825	-3.98784	4.02203
C	2.52819	5.55552	3.05985	C	6.90911	-3.37219	-3.8933
C	5.93441	-2.0631	-2.15657	H	6.8506	-4.17943	-4.61625

H	5.11935	-1.80019	-1.49009	C	6.043	-0.49955	6.41258
C	-5.30716	2.85806	-4.41955	H	6.81048	0.195	6.73853
C	2.86119	4.34929	3.70219	C	1.14418	4.91234	-3.97396
C	6.14196	2.38729	1.05198	H	0.2084	5.10467	-4.48319
H	5.22977	2.05355	0.57036	C	1.24865	-2.41686	-5.33256
C	3.49173	-2.10915	-4.5062	H	0.40807	-2.03175	-5.90042
H	4.394	-1.51104	-4.44584	C	-2.01591	3.11613	-6.37045
C	2.66027	2.35802	-6.27646	C	-0.75697	2.96586	-5.78628
C	3.45972	-3.39502	-3.8762	H	-0.67611	2.43186	-4.84439
C	3.92855	2.15	-5.63834	C	0.40148	3.45771	-6.37698
C	-4.18142	3.40788	-5.11955	C	0.3059	4.16208	-7.59192
C	1.85491	-3.48358	6.06293	C	-0.95205	4.34579	-8.18284
C	0.60882	-3.06062	5.59774	C	-2.09927	3.80038	-7.58625
H	0.54206	-2.6312	4.60269	C	-7.78306	0.51872	-4.19988
C	-0.55194	-3.17159	6.35701	H	-7.88632	0.66368	-5.27041
C	-0.46614	-3.70858	7.65696	C	-8.82171	-0.03049	-3.45746
C	0.77478	-4.14413	8.14189	H	-9.75485	-0.32268	-3.92521
C	1.92033	-4.05573	7.33678	C	4.45443	-4.45019	1.93491
C	2.19537	-5.45741	-3.3939	H	5.29117	-4.25584	1.27286
N	7.25908	1.71267	0.72198	C	3.55323	-5.41533	1.60277
C	-3.22641	2.55372	-5.70294	H	3.67021	-5.97342	0.68027
C	5.17467	-2.07474	4.76785	C	-6.13195	5.10905	-3.98638
C	4.88007	4.15222	2.31872	C	-3.96475	5.0747	1.06822
C	3.29678	0.79643	-8.03762	C	-4.22059	5.0325	-0.34056
H	3.0684	0.27131	-8.959	H	-5.11278	4.53648	-0.70671
C	-4.50382	0.60136	-4.9057	C	-3.37638	5.61845	-1.23326
C	-4.62187	-0.82407	-4.83193	H	-3.59771	5.57757	-2.29448
H	-5.45046	-1.26319	-4.28702	C	-2.2152	6.29935	-0.77888
C	-3.72784	-1.64317	-5.45028	H	-1.56898	6.79352	-1.49701
H	-3.84521	-2.71976	-5.38661	C	-1.9229	6.3463	0.54919
C	-2.65023	-1.09306	-6.19524	H	-1.04133	6.87272	0.8922
H	-1.9672	-1.75555	-6.71738	C	-2.76851	5.7264	1.52519
C	-2.48708	0.2557	-6.27218	C	-5.01056	5.65572	-4.66832
H	-1.66991	0.6718	-6.84775	H	-4.91585	6.73201	-4.76689
C	-3.39156	1.15788	-5.62434	C	3.30058	3.72889	-3.88399
N	-7.27435	1.87344	0.86813	C	4.223	2.832	-4.44475
C	-6.16763	2.49259	1.32205	C	-3.91679	-5.16376	-0.34674
H	-5.30721	1.864	1.52005	C	-3.95196	-4.99448	1.0751
C	-6.10182	3.86556	1.53283	H	-4.83201	-4.56142	1.53788
C	-7.25488	4.60877	1.26998	C	-2.91537	-5.38926	1.86358
H	-7.24601	5.68238	1.42786	H	-2.97079	-5.26124	2.93925
C	-8.40019	3.97194	0.80857	C	-1.76944	-5.99757	1.28405
H	-9.30777	4.5265	0.59966	H	-0.95934	-6.33136	1.92421
C	-8.37576	2.60367	0.61166	C	-1.69519	-6.1799	-0.06259
H	-9.24088	2.06602	0.24317	H	-0.83043	-6.6654	-0.49603
C	-6.59446	0.88714	-3.56638	C	-2.74964	-5.75914	-0.93624
C	3.07417	-3.27826	5.22721	H	-7.13778	3.35625	-3.35145
C	6.14216	3.43718	1.96512	H	-6.88472	5.77454	-3.57603
C	5.28644	-2.74476	3.53708	O	-3.32529	4.00491	-8.14326
C	-4.06915	4.83185	-5.20562	O	1.46103	4.66	-8.0791
H	-3.22009	5.25192	-5.72924	O	-2.29922	8.18285	4.3898
C	2.3834	1.6401	-7.48304	O	2.5253	7.90732	4.51002
H	1.42069	1.78324	-7.95832	O	-1.60774	-3.71455	8.37619

C	4.85609	1.24577	-6.24995	O	3.13151	-4.43947	7.8259
H	5.82191	1.08545	-5.78388	O	-2.63261	-8.41844	-3.5393
N	-7.05789	-0.49937	2.56599	O	2.02716	-7.96537	-4.72336
C	-8.0579	-0.23574	3.42733	C	-3.03342	-9.31799	-4.57472
H	-8.96628	0.17834	3.00664	H	-2.60908	-10.31142	-4.42794
C	-7.92906	-0.48332	4.78182	H	-4.12068	-9.36631	-4.50451
H	-8.75756	-0.26643	5.44625	H	-2.74196	-8.94482	-5.55906
C	-6.73215	-0.99805	5.26522	C	2.01901	-8.09846	-6.14807
H	-6.60243	-1.19076	6.32531	H	1.23167	-8.78006	-6.47497
C	-5.68121	-1.26177	4.38389	H	1.88695	-7.11808	-6.61857
C	-5.90236	-1.00501	3.03591	H	2.99514	-8.50159	-6.41692
H	-5.12735	-1.2048	2.30518	C	-3.55901	3.37538	-9.4072
C	2.2671	-4.18736	-3.99938	H	-3.49406	2.28661	-9.305
C	-4.35879	-1.76664	4.85053	H	-4.57209	3.65274	-9.69762
C	-4.18268	-3.13371	5.12012	H	-2.84742	3.72407	-10.1577
C	-5.23082	-4.08979	4.92374	C	1.68152	4.80363	-9.4839
H	-6.19908	-3.74692	4.57529	H	1.23943	3.97406	-10.04038
C	-5.03934	-5.41397	5.17726	H	1.27575	5.74351	-9.85859
H	-5.85043	-6.12016	5.03233	H	2.76529	4.79374	-9.60516
C	-3.77556	-5.88098	5.62991	C	-2.54083	9.46811	3.80795
H	-3.63073	-6.93988	5.81597	H	-2.59625	9.38457	2.71708
C	-2.75342	-5.00311	5.82649	H	-3.50468	9.79641	4.19622
H	-1.78834	-5.36526	6.15818	H	-1.76318	10.18005	4.08983
C	-2.91244	-3.59946	5.59734	C	2.81917	9.29834	4.65775
C	3.55547	1.94071	5.00878	H	3.89938	9.37633	4.52998
H	3.81391	1.02116	5.52155	H	2.31202	9.89292	3.89457
C	2.42358	-1.62983	-5.19991	H	2.53603	9.6644	5.64477
H	2.47574	-0.65603	-5.674	C	-1.88061	-4.73155	9.34274
C	3.30169	-5.95645	-2.67771	H	-2.96782	-4.76573	9.42261
C	3.26984	-7.23514	-2.03522	H	-1.50333	-5.70243	9.01386
H	2.36299	-7.82231	-2.09547	H	-1.44567	-4.48797	10.31223
C	4.34899	-7.72741	-1.36721	C	3.29824	-5.8392	8.07476
H	4.30398	-8.70698	-0.90311	H	2.57248	-6.19743	8.80708
C	5.54275	-6.9613	-1.2767	H	3.20016	-6.40329	7.14094
H	6.40002	-7.36494	-0.74767	H	4.30912	-5.95589	8.46458
C	5.61023	-5.72712	-1.84778	O	-0.2892	-9.46232	-4.79652
H	6.52564	-5.15192	-1.76686	O	-1.06665	5.05336	-9.34683
C	4.50242	-5.17733	-2.57101	O	0.87513	-4.65215	9.40683
C	-2.46441	5.7667	2.89915	O	0.11169	9.27192	5.19989
C	4.04781	-2.33744	5.61707	C	-1.59312	6.37405	-9.19358
C	-1.86065	-2.68936	5.82399	H	-1.62627	6.80664	-10.19357
C	7.36506	3.7882	2.54073	H	-2.60142	6.34265	-8.77202
H	7.40569	4.60375	3.25562	H	-0.93789	6.97718	-8.55551
C	8.06298	-2.60696	-3.78234	C	1.46678	-3.7674	10.36208
H	8.92657	-2.79424	-4.40995	H	1.4805	-4.30698	11.30911
C	-8.65542	-0.2091	-2.09651	H	2.48829	-3.50928	10.07036
H	-9.4326	-0.64424	-1.47993	H	0.86476	-2.85818	10.46751
C	1.72772	3.25422	-5.72142	C	-0.27688	9.1214	6.56813
C	-4.92947	-4.97036	-2.56251	H	-0.22	10.11543	7.01177
C	-3.75041	-5.5392	-3.14833	H	-1.30003	8.74305	6.64094
C	-3.71044	-5.68778	-4.57106	H	0.41072	8.44742	7.0907
H	-2.81281	-6.09051	-5.02309	C	0.36416	-10.50108	-4.06198
C	-4.7667	-5.33996	-5.35696	H	0.28448	-11.40125	-4.67155

H	-4.71762	-5.47818	-6.43202	H	1.41756	-10.25759	-3.90014
C	-5.94329	-4.79756	-4.77141	H	-0.13565	-10.6645	-3.10091
H	-6.7853	-4.53693	-5.40458	Pt	-7.29125	-0.16219	0.55011
C	-6.01497	-4.60957	-3.42464	Pt	7.16179	0.19097	-0.66257
H	-6.92011	-4.19943	-2.98984	O	3.91973	0.18763	-0.09273
C	1.45642	5.59435	-2.83874	C	1.18399	0.33108	2.16524
H	0.76734	6.33045	-2.43786	C	0.16006	1.25465	1.48103
C	8.42996	2.05551	1.28806	H	-0.03491	2.10317	2.1469
H	9.29931	1.47961	0.99472	H	-0.79947	0.73875	1.36329
C	6.15606	-1.12943	5.21073	C	0.61904	1.77621	0.10068
H	7.01887	-0.93196	4.58483	H	0.25032	1.08716	-0.66856
C	2.07186	3.83029	4.77924	C	2.1478	1.78092	0.00087
H	1.20754	4.39703	5.10185	H	2.55958	2.48968	0.73724
C	4.91996	-0.74717	7.2478	H	2.49281	2.12822	-0.9784
H	4.83801	-0.23639	8.20142	C	2.7856	0.44269	0.30318
C	1.26566	6.26704	3.42285	C	1.99785	-0.51774	1.1731
C	1.3015	7.47604	4.14277	C	1.15291	-1.51973	0.33323
C	0.09729	8.11532	4.47164	H	2.73523	-1.11685	1.72244
C	-1.12847	7.57657	4.04941	C	0.04011	3.15317	-0.21207
C	-1.17406	6.36793	3.34921	C	2.02053	-2.30986	-0.64799
C	0.03435	5.7316	3.06219	H	0.41608	-0.95533	-0.24976
H	0.01271	4.79199	2.51948	H	-1.04876	3.15871	-0.09814
C	-4.98578	-4.78137	-1.17213	H	0.27253	3.46723	-1.23382
C	2.69342	5.36154	-2.17882	H	0.44809	3.91128	0.46556
H	2.93539	5.91558	-1.27852	H	1.40948	-3.02427	-1.2072
C	-6.51622	0.6873	-2.19283	H	2.78957	-2.88208	-0.11679
H	-5.62182	0.96504	-1.64763	H	2.51399	-1.66483	-1.37977
C	5.81231	-3.10515	-3.07148	C	0.38759	-2.47906	1.24858
C	3.58245	4.46506	-2.68736	H	1.07468	-3.03765	1.89343
H	4.53446	4.32201	-2.18808	H	-0.16711	-3.21161	0.6539
C	-3.30853	-0.85388	5.03696	H	-0.33474	-1.96105	1.88615
C	-2.0455	-1.32168	5.53908	H	0.68595	-0.30919	2.89718
C	-1.0111	-0.35349	5.75392	H	1.88896	0.93783	2.74456
H	-0.06936	-0.68764	6.16895				

Table S11. Cartesian coordinates of **1•TBI-b** (R = -OCH_3; E_{opt} = –9285.97919968 hartree, E_{sp} = –9286.46585631 hartree).

C	-2.01017	-0.78570	-1.03666	C	-7.92138	-1.54829	3.24891
C	-1.26428	-0.02097	-2.16897	C	-7.81964	-2.48457	4.26078
C	-1.03755	1.46919	-1.87725	C	-6.63922	-3.20426	4.39523
C	-0.67896	1.71196	-0.41034	C	-5.57916	-2.97725	3.51512
C	-1.89881	1.32991	0.44707	C	-5.76530	-2.02178	2.52017
C	-2.71573	0.19211	-0.12533	C	-4.29393	-3.72381	3.63424
C	-0.24684	3.14952	-0.13916	C	-4.21192	-5.04464	3.16052
O	-3.90540	0.07578	0.15655	C	-2.98069	-5.76837	3.29624
C	-1.07784	-1.70729	-0.19313	C	-1.87291	-5.17064	3.92901
C	-0.49457	-2.82991	-1.05395	C	-1.96913	-3.85135	4.41106
C	-1.81389	-2.31656	1.00192	C	-3.19169	-3.11232	4.25205
H	-0.29379	-0.49480	-2.33755	C	-2.91990	-7.09878	2.77258
H	-1.82041	-0.12344	-3.10475	C	-4.00065	-7.69035	2.19305
H	-1.94137	2.04573	-2.11618	C	-5.22583	-6.97862	2.07705
H	-0.25080	1.84802	-2.53847	C	-5.32092	-5.69873	2.53223

H	0.15785	1.05045	-0.15022	C	-0.87742	-3.20858	5.08010
H	-2.56900	2.18940	0.56603	C	-0.96792	-1.92575	5.52341
H	-1.59676	1.04230	1.46359	C	-2.17242	-1.19195	5.35439
H	-2.78354	-1.43133	-1.46673	C	-3.24647	-1.77102	4.75179
H	-0.24789	-1.09731	0.18659	C	-0.59071	-5.92398	4.06291
H	0.66650	3.39766	-0.68896	C	0.54787	-5.50114	3.38531
H	-0.05534	3.32211	0.92450	C	1.76329	-6.18417	3.45543
H	-1.02704	3.85468	-0.44739	C	1.82024	-7.33909	4.24204
H	-2.17337	-1.56426	1.71081	C	0.70342	-7.75987	4.97994
H	-1.15382	-2.98822	1.55743	C	-0.50925	-7.06275	4.88792
H	-2.67243	-2.90987	0.66597	C	2.95835	-5.67372	2.72218
H	-1.29090	-3.46952	-1.44690	C	2.95545	-5.63862	1.31381
H	0.16903	-3.46294	-0.45658	C	4.07078	-5.07808	0.60269
H	0.08805	-2.45694	-1.90092	C	5.16980	-4.58681	1.32466
C	-4.27097	3.31670	-3.49442	C	5.19788	-4.64374	2.72730
C	-5.09349	3.85436	-2.49138	C	4.07198	-5.18448	3.43398
C	-4.82171	5.11921	-1.94170	C	1.86694	-6.16711	0.54688
C	-3.66824	5.85122	-2.38427	C	1.86328	-6.11998	-0.81363
C	-2.82560	5.31142	-3.37416	C	2.95789	-5.54585	-1.51460
C	-3.13195	4.06516	-3.95086	C	4.02323	-5.04905	-0.82853
C	-5.66281	5.71362	-0.94612	C	6.31987	-4.17474	3.48427
C	-5.39317	6.94639	-0.43410	C	6.33132	-4.23459	4.84444
C	-4.24828	7.66920	-0.86739	C	5.20913	-4.75094	5.54784
C	-3.41468	7.13321	-1.80073	C	4.12063	-5.20005	4.86440
C	-2.35188	3.52314	-5.02316	C	6.32338	-3.99690	0.58741
C	-2.65708	2.32347	-5.58863	C	6.33842	-2.63835	0.29312
C	-3.75888	1.56401	-5.10910	N	7.33526	-2.04770	-0.39102
C	-4.53729	2.04686	-4.10206	C	8.37696	-2.79257	-0.80623
C	-1.58626	6.03308	-3.79058	C	8.44866	-4.14774	-0.54091
C	-1.63670	7.19935	-4.55893	C	7.41316	-4.75683	0.15838
C	-0.45971	7.87677	-4.91483	O	-1.62326	-7.37420	5.58107
C	0.79123	7.36105	-4.54564	C	-1.94939	-8.72511	5.91460
C	0.85090	6.18010	-3.78295	O	0.80368	-8.85680	5.78965
C	-0.33265	5.55119	-3.41224	C	1.51091	-8.63443	7.01236
C	2.16357	5.61862	-3.34365	O	3.00392	-8.00298	4.35557
C	3.01480	4.98698	-4.26942	C	3.03282	-9.33685	3.83728
C	4.25490	4.41022	-3.83316	H	5.65037	1.21884	1.35910
C	4.59988	4.46272	-2.47191	H	8.05514	1.16755	4.90267
C	3.76222	5.09781	-1.54040	H	9.87880	0.10726	3.55215
C	2.53603	5.69788	-1.98930	H	9.46560	-0.37463	1.14723
C	5.10605	3.80838	-4.81538	H	8.78993	0.21989	-3.37525
C	4.75587	3.77272	-6.13125	H	8.49171	-0.38675	-5.77043
C	3.52009	4.32707	-6.56147	H	6.34221	-1.45366	-6.48736
C	2.68267	4.90842	-5.65911	H	5.05117	-1.27295	-2.40847
C	1.73316	6.39511	-1.02961	H	-8.81833	-0.95788	3.10662
C	2.09307	6.46673	0.28036	H	-8.65531	-2.64142	4.93296
C	3.28235	5.83409	0.73187	H	-6.53081	-3.94329	5.18254
C	4.08745	5.17803	-0.14780	H	-4.98141	-1.79352	1.80560
C	5.89497	3.88451	-2.00906	H	5.00045	4.71919	0.21540
C	6.01110	2.52978	-1.71738	H	6.06020	3.39604	-4.50471
N	7.15182	1.97237	-1.26679	H	5.42397	3.32680	-6.86097
C	8.23805	2.74883	-1.09542	H	3.25230	4.28909	-7.61195
C	8.21276	4.10237	-1.37637	H	1.74083	5.33071	-5.98748

C	7.03294	4.67570	-1.83383	H	5.52421	-1.99866	0.61302
Pt	7.24303	-0.03804	-0.82490	H	5.16443	1.86522	-1.84432
N	6.93518	-0.50707	-2.80367	H	4.86244	-4.64030	-1.38071
C	7.88276	-0.25708	-3.72617	H	0.81601	2.80296	4.59835
C	7.70420	-0.59499	-5.05531	H	3.62269	-7.28109	-5.39703
C	6.51079	-1.18862	-5.44857	H	-5.21855	-4.54457	-0.76947
C	5.51324	-1.43890	-4.50357	H	-3.56666	-6.22273	-0.14985
C	5.78300	-1.08834	-3.18617	H	-1.75371	-6.85853	-1.74162
C	4.19435	-2.02534	-4.87522	H	-1.56674	-5.73144	-3.91032
C	4.05923	-3.41467	-5.02763	H	-5.28503	1.87728	-0.58447
C	2.79151	-3.95991	-5.41958	H	-7.66080	4.10577	-3.38347
C	1.70044	-3.10724	-5.67946	H	-9.65294	2.81167	-2.59253
C	1.84330	-1.71563	-5.50735	H	-9.33961	1.10557	-0.80802
C	3.10476	-1.16669	-5.09104	H	-3.31674	-2.46835	-7.21820
C	5.14761	-4.31591	-4.79418	H	1.71411	-5.80125	-5.79906
C	4.99542	-5.66202	-4.93270	H	6.11440	-3.91324	-4.51165
C	3.73482	-6.20636	-5.30060	H	-8.89582	2.02320	2.22266
C	2.67581	-5.38196	-5.53069	H	-8.71448	3.79675	3.96028
C	3.21307	0.25244	-4.93096	H	-6.46590	4.28420	4.94937
C	2.15170	1.07596	-5.14703	H	-4.83341	1.26710	2.36500
C	0.90651	0.53715	-5.56693	H	-5.63130	1.42903	5.86576
C	0.76618	-0.80367	-5.75479	H	-5.00169	0.47780	8.02253
C	0.39412	-3.67326	-6.12897	H	-2.76432	0.95837	9.00939
C	-0.74431	-3.54500	-5.33960	H	-1.18016	2.40051	7.82173
C	-1.99008	-4.03562	-5.73263	H	3.55609	5.88512	1.78023
C	-2.07996	-4.69413	-6.96208	H	2.95123	-5.52313	-2.59929
C	-0.95750	-4.80769	-7.79614	H	3.27073	-5.59208	5.40711
C	0.28433	-4.30487	-7.38372	H	5.22881	-4.79249	6.63179
O	1.97637	7.94308	-4.82271	H	7.20038	-3.89460	5.39854
C	2.17538	8.71679	-6.00777	H	7.18625	-3.78776	2.95887
O	-0.53946	9.04141	-5.62597	H	6.98459	5.73691	-2.05560
C	-0.94857	10.18043	-4.86356	H	9.30613	-4.71511	-0.88407
O	-2.85267	7.71781	-4.88593	H	-9.30956	-1.81506	0.14109
C	-3.17343	7.75026	-6.28026	H	-1.98479	-7.63990	2.84498
C	-6.30605	3.10451	-2.04802	H	-3.93257	-8.70589	1.81713
C	-6.22810	2.13298	-1.05453	H	-6.08431	-7.46006	1.61993
N	-7.30385	1.44444	-0.62893	H	-6.25959	-5.16570	2.43084
C	-8.50627	1.68900	-1.18028	H	0.07043	1.20297	-5.75113
C	-8.66915	2.63814	-2.17204	H	9.13156	2.26049	-0.72601
C	-7.56065	3.35299	-2.60817	H	7.20080	3.72391	2.82869
Pt	-7.10970	0.05780	0.88105	H	0.83131	6.88530	-1.37331
N	-6.87391	1.57542	2.25075	H	4.97873	7.16966	4.06338
C	-7.94355	2.27200	2.67515	H	-0.27761	4.64626	-2.81539
C	-7.83190	3.25467	3.64093	H	2.26291	2.14819	-5.02736
C	-6.58255	3.52272	4.18498	H	-5.42126	-1.27232	-1.15607
C	-5.46308	2.81094	3.74834	H	4.16718	0.68619	-4.65386
C	-5.65998	1.84319	2.76770	H	-0.13047	5.38455	4.00076
C	-4.11058	3.07268	4.32035	H	-0.77546	6.39901	1.86768
C	-3.76567	2.50898	5.56146	H	-2.98586	5.87053	0.84305
C	-2.48234	2.79643	6.13539	H	-4.52834	4.35132	1.95476
C	-1.58399	3.65062	5.46811	H	9.15376	-2.27798	-1.35890
C	-1.94473	4.22228	4.23492	H	1.48165	7.02175	0.98441
C	-3.22270	3.92590	3.64759	H	3.33649	5.74626	5.18914

C	-2.15417	2.19824	7.39334	H	9.10916	4.69508	-1.23477
C	-3.03232	1.39304	8.05227	H	2.24588	-1.17765	6.77815
C	-4.30676	1.11704	7.48783	H	1.90636	1.24716	6.72072
C	-4.65514	1.64901	6.28343	H	0.48561	-4.61030	2.76781
C	-1.08159	5.13584	3.54744	H	-6.54321	5.17686	-0.61070
C	-1.44250	5.70248	2.36453	H	-6.05442	7.38546	0.30589
C	-2.70125	5.40003	1.77794	H	-4.04657	8.65149	-0.45354
C	-3.55890	4.54566	2.40024	H	-2.54566	7.68770	-2.13139
C	-0.24485	3.93953	6.06287	H	5.83613	-6.32668	-4.76225
C	0.90883	3.42038	5.48665	H	1.03929	-6.62394	1.07421
C	2.17908	3.64701	6.01996	H	7.44274	-5.82016	0.37327
C	2.27847	4.43679	7.16860	H	6.92044	6.14909	2.88061
C	1.13515	5.01094	7.74552	H	-0.17685	-1.20146	-6.10565
C	-0.13312	4.75161	7.20750	H	1.02845	-6.53346	-1.37012
C	3.38255	3.05337	5.36710	H	-0.66136	-3.04300	-4.38049
C	4.30442	3.87295	4.68830	H	-7.81264	-4.32814	-3.00493
C	5.41442	3.28561	3.99359	H	-9.68192	-3.67375	-1.47174
C	5.56262	1.88893	3.98507	H	5.62366	-0.83135	4.17969
C	4.66717	1.06293	4.68324	H	4.08935	-2.21782	5.45560
C	3.57136	1.65856	5.39571	H	-5.39153	1.46751	-3.76965
C	4.17382	5.29785	4.67036	H	-3.99175	0.60742	-5.56375
C	5.08546	6.09018	4.04196	H	-2.07454	1.95070	-6.42524
C	6.19121	5.50730	3.36461	H	-1.51831	4.10458	-5.39701
C	6.34329	4.15437	3.33464	H	-5.09632	-0.95917	-7.94670
C	2.70859	0.79816	6.14878	H	-4.17028	-1.21005	4.66655
C	2.89492	-0.54958	6.17617	H	-2.24193	-0.17755	5.73101
C	3.95368	-1.14165	5.43631	H	-0.12291	-1.45982	6.01942
C	4.80821	-0.36189	4.71908	H	0.03415	-3.77063	5.23617
O	-1.28565	5.26888	7.68024	H	-7.12658	-1.45772	-4.21113
C	-1.47326	5.53340	9.07220	H	-7.01393	-0.45758	-6.43417
O	1.26405	5.82095	8.83909	H	-1.45776	-9.03912	6.83558
C	1.75876	7.13243	8.55602	H	-3.03131	-8.73179	6.05167
O	3.51334	4.71273	7.67267	H	-1.67429	-9.40961	5.10906
C	3.79158	4.20186	8.98044	H	2.30641	-9.97238	4.34675
C	6.69664	1.27165	3.23942	H	2.83437	-9.32813	2.76003
C	6.56743	0.98237	1.88574	H	4.04199	-9.70652	4.01753
N	7.54462	0.40380	1.16313	H	-3.29196	-7.05541	-6.57372
C	8.70895	0.09469	1.76422	H	-4.45324	-6.72041	-7.88553
C	8.92573	0.36239	3.10329	H	-2.72254	-6.94212	-8.26933
C	7.91179	0.95246	3.84867	H	1.33868	-6.36264	-8.62290
C	-3.18493	-3.80233	-4.86986	H	1.20573	-5.25190	-10.00576
C	-4.18125	-2.89291	-5.27492	H	2.76159	-5.41949	-9.14737
C	-5.27630	-2.58956	-4.39836	H	-3.20501	6.73257	-6.68458
C	-5.33182	-3.18584	-3.12689	H	-4.16408	8.19899	-6.34973
C	-4.36286	-4.11983	-2.72789	H	-2.45194	8.35176	-6.83606
C	-3.28728	-4.44563	-3.62306	H	3.25147	8.69615	-6.18369
C	-4.14430	-2.25329	-6.55502	H	1.65200	8.27733	-6.85989
C	-5.13358	-1.41073	-6.96088	H	1.84247	9.74628	-5.87440
C	-6.22567	-1.12317	-6.09743	H	-2.55312	5.51350	9.22342
C	-6.28524	-1.68168	-4.85712	H	-0.99928	4.76571	9.68804
C	-2.35471	-5.45572	-3.22040	H	-1.07854	6.51075	9.35045
C	-2.45782	-6.07906	-2.01495	H	3.09139	4.60188	9.71590
C	-3.49701	-5.72575	-1.11143	H	3.74737	3.10730	8.97594

C	-4.41552	-4.78235	-1.45860	H	4.80537	4.52305	9.21842
C	-6.46500	-2.85082	-2.21645	H	-1.75119	-5.20425	-10.92149
C	-6.34586	-1.82779	-1.28002	H	-2.74267	-4.34803	-9.70889
N	-7.35767	-1.47619	-0.46537	H	-1.14889	-3.68702	-10.19910
C	-8.52928	-2.13374	-0.53949	H	1.80780	7.65250	9.51276
C	-8.72526	-3.16541	-1.43800	H	2.75671	7.08259	8.11216
C	-7.68458	-3.52602	-2.28517	H	1.07538	7.66428	7.88497
O	1.40237	-4.33023	-8.13902	H	-0.97058	11.01989	-5.55854
C	1.67670	-5.40930	-9.03530	H	-1.94455	10.02584	-4.44018
O	-1.08175	-5.40404	-9.01978	H	-0.22848	10.38604	-4.06393
C	-1.72377	-4.60105	-10.01396	H	1.50796	-9.58636	7.54345
O	-3.29569	-5.13849	-7.38368	H	2.54111	-8.32684	6.81358
C	-3.43390	-6.55490	-7.53768	H	1.00248	-7.87602	7.61775
N	-6.90934	-1.32454	2.39135				

Table S12. Cartesian coordinates of **1•MTO** (R = -OCH_3; E_{opt} = –9285.98180862 hartree, E_{sp} = –9286.47302965 hartree).

C	-1.49133	-2.29496	0.40701	C	3.73847	-5.61301	-2.33790
C	-0.74777	-2.74866	-0.86774	C	4.67421	-4.91135	-1.64121
C	0.02075	-1.57848	-1.48513	C	2.61639	-6.45867	2.60595
C	-0.85411	-0.34642	-1.70972	C	1.35748	-5.86895	2.59395
C	-1.50798	0.13222	-0.39165	C	0.27405	-6.39258	3.30063
C	-2.29873	-1.04890	0.14602	C	0.48136	-7.57309	4.02305
C	0.17044	-3.92628	-0.56652	C	1.72437	-8.22633	3.99924
C	-2.32830	1.42405	-0.50079	C	2.80644	-7.66291	3.30739
C	-2.72394	1.93477	0.88701	C	-1.04783	-5.69750	3.30203
O	-3.51402	-1.02113	0.29792	C	-1.16454	-4.41170	3.86937
C	-1.57961	2.53015	-1.24401	C	-2.43536	-3.73968	3.87987
C	-5.65295	1.12448	3.20792	C	-3.56087	-4.37561	3.33075
N	-6.80203	0.84280	2.56697	C	-3.45179	-5.64899	2.74728
C	-7.90386	1.56356	2.84835	C	-2.17747	-6.31103	2.72459
C	-7.88531	2.58235	3.78239	C	-0.04796	-3.73964	4.46541
C	-6.69502	2.87851	4.43485	C	-0.16310	-2.49116	4.99528
C	-5.54176	2.14593	4.14686	C	-1.41942	-1.82858	5.00114
Pt	-6.89397	-0.65537	1.15257	C	-2.51532	-2.43909	4.47401
N	-7.33367	0.74127	-0.30104	C	-4.57715	-6.31452	2.16177
C	-6.39567	1.62027	-0.70221	C	-4.45599	-7.54589	1.59365
C	-6.63100	2.57622	-1.68639	C	-3.19248	-8.19666	1.55668
C	-7.90286	2.60420	-2.26197	C	-2.09769	-7.59584	2.09849
C	-8.87135	1.69753	-1.84886	C	-4.89222	-3.70602	3.41117
C	-8.55368	0.77669	-0.86787	C	-5.24824	-2.70832	2.50809
C	-4.23441	2.44995	4.79697	N	-6.43177	-2.06819	2.57123
C	-3.76729	1.64127	5.84748	C	-7.31300	-2.39099	3.53578
C	-2.50686	1.94347	6.46479	C	-7.03835	-3.37853	4.46300
C	-1.75313	3.04650	6.02728	C	-5.81907	-4.04246	4.39931
C	-2.24909	3.87651	5.00751	O	4.03886	-8.20231	3.21740
C	-3.50102	3.57158	4.37264	C	4.57565	-9.04703	4.23731
C	-4.51585	0.52749	6.34837	O	1.87674	-9.40792	4.67002
C	-4.05234	-0.23326	7.37882	C	1.27668	-10.53949	4.03361
C	-2.79873	0.05827	7.98173	O	-0.56568	-8.13094	4.69204
C	-2.05563	1.10776	7.53521	C	-0.44712	-8.18720	6.11674
C	-3.95135	4.43191	3.31928	H	-5.24692	-1.65066	-1.13253

C	-3.24184	5.53344	2.95045	H	-7.38368	-4.93297	-2.89003
C	-2.02593	5.85925	3.60970	H	-9.13373	-4.63029	-1.12278
C	-1.54436	5.05213	4.59321	H	-8.84190	-2.81314	0.55081
C	-5.56145	3.53106	-2.10398	H	-8.80479	1.30510	2.30578
C	-5.38999	4.73549	-1.39965	H	-8.79457	3.13408	3.99135
C	-4.35647	5.64845	-1.79999	H	-6.65155	3.67783	5.16760
C	-3.53934	5.34990	-2.90674	H	-4.79689	0.51331	2.94970
C	-3.76230	4.17368	-3.64355	H	9.15536	-1.11772	-2.02799
C	-4.77056	3.23858	-3.22717	H	9.62140	-3.56013	-1.97659
C	-6.22222	5.09552	-0.29063	H	8.01870	-5.07188	-0.78468
C	-6.05214	6.27389	0.37073	H	5.71803	-1.60349	0.22749
C	-5.01757	7.17032	-0.01409	H	-5.67359	1.30497	-3.67605
C	-4.19541	6.85833	-1.05348	H	-7.02320	4.42698	0.00554
C	-3.01166	3.88043	-4.82708	H	-6.71269	6.53956	1.19001
C	-3.21696	2.73456	-5.53215	H	-4.89501	8.10802	0.51826
C	-4.17917	1.78586	-5.09105	H	-3.40688	7.54171	-1.34347
C	-4.92999	2.03224	-3.98282	H	-4.57477	-2.39153	1.71647
C	-2.38643	6.23491	-3.25383	H	-5.42809	1.54275	-0.22018
C	-2.57762	7.49661	-3.84518	H	-3.47408	-1.93619	4.52366
C	-1.45900	8.29388	-4.13126	H	-0.60439	-2.54013	-4.66763
C	-0.16972	7.85751	-3.78446	H	-2.44418	-0.55371	8.80424
C	0.02929	6.59748	-3.21237	H	5.73768	-0.78649	4.08554
C	-1.09384	5.80470	-2.97750	H	4.46638	-2.37634	5.40503
C	-0.40875	3.32404	6.61719	H	2.64596	-1.59609	6.92739
C	0.74078	2.97570	5.91805	H	2.04808	0.78003	7.00757
C	2.01973	3.21287	6.42318	H	4.78019	2.53886	-1.77711
C	2.13215	3.84556	7.66338	H	6.15620	6.58050	-1.43942
C	0.98769	4.24008	8.37436	H	8.37625	5.67975	-0.70801
C	-0.28941	3.95884	7.86661	H	8.66812	3.21664	-0.52300
O	-3.85454	7.82035	-4.13297	H	2.88201	5.45297	5.63582
C	-4.30001	9.17756	-4.17512	H	-1.10313	1.33588	7.99843
O	-1.61846	9.50884	-4.73793	H	-5.48572	0.30673	5.91578
C	-1.25054	9.53922	-6.11959	H	8.46662	1.58606	-3.53217
O	0.91573	8.62717	-4.07497	H	8.10903	1.35189	-5.98415
C	1.02231	9.86612	-3.36680	H	6.05183	0.17825	-6.79862
C	1.38609	6.10837	-2.82599	H	4.96642	-0.46485	-2.70659
C	2.34130	5.78955	-3.81048	H	6.20450	-2.58666	-5.19848
C	3.63341	5.29130	-3.42943	H	6.18410	-4.96175	-5.76707
C	3.93123	5.11530	-2.06829	H	4.05705	-6.07987	-6.43268
C	2.98410	5.41873	-1.07714	H	1.97489	-4.79779	-6.54100
C	1.69622	5.92596	-1.46326	H	-4.32501	0.86769	-5.64909
C	4.57822	4.98831	-4.46216	H	-1.50969	-0.84577	5.45123
C	4.26591	5.15242	-5.77753	H	-1.13831	-8.09564	2.06575
C	2.98209	5.62827	-6.15721	H	-3.10758	-9.17679	1.09934
C	2.05849	5.93551	-5.20586	H	-5.32438	-8.03779	1.16737
C	0.76142	6.24373	-0.42503	H	-5.54598	-5.82798	2.18258
C	1.05891	6.04826	0.88838	H	-8.12593	3.33742	-3.03039
C	2.32871	5.53686	1.26666	H	-7.77198	-3.61900	5.22377
C	3.25816	5.24143	0.31730	H	9.33983	0.25891	0.87078
C	5.28080	4.62962	-1.65781	H	4.04924	-5.75925	4.56846
C	5.54585	3.26942	-1.54357	H	5.87936	-4.72261	5.82264
N	6.73825	2.78629	-1.14434	H	7.66462	-3.46349	4.62193
C	7.72843	3.64832	-0.84525	H	7.60263	-3.24699	2.19080

C	7.55339	5.01597	-0.94723	H	-1.49144	6.76295	3.33416
C	6.32104	5.51120	-1.35536	H	-9.27341	0.04676	-0.51753
Pt	7.06878	0.75767	-1.00945	H	-7.18192	-1.85006	-3.96010
N	6.73305	0.56739	-3.02961	H	-2.28607	4.60820	-5.16840
C	7.59876	1.07244	-3.92801	H	-5.53358	-0.71268	-7.74398
C	7.38709	0.94007	-5.28835	H	-0.95459	4.82549	-2.53371
C	6.24517	0.28632	-5.73622	H	-3.60785	6.16738	2.14992
C	5.33275	-0.23046	-4.81387	H	5.45783	1.61615	1.34958
C	5.63195	-0.07186	-3.46617	H	-4.87887	4.20654	2.80518
C	4.07003	-0.90612	-5.22745	H	-0.42477	-0.44480	-6.16741
C	4.08017	-2.27155	-5.55458	H	-0.41955	1.91475	-5.53495
C	2.86072	-2.90631	-5.96392	H	1.69767	3.01352	-4.79585
C	1.66997	-2.15962	-6.06588	H	3.76463	1.74043	-4.67529
C	1.66986	-0.79161	-5.72537	H	-8.24565	-1.84003	3.54686
C	2.88506	-0.15621	-5.29406	H	-2.66019	2.54868	-6.44532
C	2.89746	-4.30600	-6.25902	H	-3.52433	-2.03144	-7.30222
C	4.05347	-5.02222	-6.19035	H	-9.86608	1.70062	-2.27939
C	5.26517	-4.38556	-5.80532	H	-1.01856	-6.73663	-2.47473
C	5.27347	-3.06103	-5.48952	H	-1.12214	-5.35153	-4.49236
C	0.48821	0.01447	-5.81172	H	1.22165	-4.94904	2.03578
C	0.49310	1.33184	-5.46830	H	5.56694	4.63734	-4.18608
C	1.69517	1.95600	-5.03933	H	5.00059	4.92810	-6.54420
C	2.84868	1.23765	-4.96525	H	2.74624	5.75348	-7.20846
C	0.41089	-2.81695	-6.52736	H	1.08380	6.30424	-5.49850
C	-0.68445	-2.93093	-5.67754	H	-4.64582	-1.06064	7.75425
C	-1.88264	-3.52977	-6.06973	H	0.90677	-4.24843	4.49235
C	-1.96588	-4.04387	-7.36658	H	-5.57795	-4.82027	5.11676
C	-0.89298	-3.90736	-8.26062	H	-7.37220	-0.62381	-6.06291
C	0.30086	-3.30056	-7.84638	H	-0.61978	5.30097	5.09893
C	-3.03770	-3.56255	-5.12541	H	0.70294	-2.00052	5.42695
C	-4.17094	-2.76112	-5.36467	H	0.63794	2.48909	4.95280
C	-5.22387	-2.69750	-4.39147	H	7.93522	1.20871	4.81954
C	-5.10704	-3.42585	-3.19601	H	9.77792	0.43003	3.31330
C	-4.00894	-4.27055	-2.97266	H	-4.66404	-5.02187	-1.03457
C	-2.96853	-4.34892	-3.96030	H	-2.78933	-6.54317	-0.72561
C	-4.31650	-1.99681	-6.56617	H	4.23052	4.87564	0.62804
C	-5.43387	-1.25897	-6.81179	H	2.56501	5.39874	2.31647
C	-6.48108	-1.20617	-5.85170	H	0.32776	6.28650	1.65363
C	-6.37140	-1.88938	-4.67924	H	-0.20143	6.65095	-0.70469
C	-1.88975	-5.26383	-3.73344	H	4.25451	7.10267	4.44951
C	-1.83353	-6.03341	-2.61236	H	5.39397	-4.30884	-2.18434
C	-2.84497	-5.92908	-1.61863	H	3.71747	-5.55773	-3.42137
C	-3.89097	-5.07508	-1.79316	H	2.07940	-7.01156	-2.22212
O	1.36498	-3.08998	-8.64879	H	2.08077	-7.10343	0.22761
C	1.71073	-4.00349	-9.69223	H	6.73338	3.98614	2.87549
O	-1.01893	-4.36476	-9.54247	H	6.18932	6.35742	3.06865
C	-1.82054	-3.54293	-10.39536	H	4.22753	-10.07471	4.13063
O	-3.13952	-4.59371	-7.78322	H	5.65632	-9.00738	4.09722
C	-3.10658	-5.98801	-8.10582	H	4.31622	-8.68075	5.23299
C	-6.17647	-3.30967	-2.16317	H	0.42135	-8.77647	6.41634
C	-6.09595	-2.32209	-1.18512	H	-0.37562	-7.17530	6.53036
N	-7.04358	-2.15825	-0.24502	H	-1.36017	-8.66232	6.47498
C	-8.11003	-2.98063	-0.23018	H	3.80821	2.40986	9.19283

C	-8.26134	-3.98835	-1.16338	H	4.77261	3.86288	9.56798
C	-7.28696	-4.15342	-2.14115	H	3.09263	3.73630	10.16216
C	3.22300	2.78429	5.64990	H	-1.00615	3.56831	10.36996
C	3.99454	3.72694	4.94719	H	-1.22972	5.33088	10.27096
C	5.10029	3.29573	4.13957	H	-2.63455	4.24628	10.08808
C	5.39807	1.92502	4.05112	H	1.10931	9.68001	-2.29073
C	4.65236	0.97748	4.77258	H	1.93451	10.34041	-3.72823
C	3.55925	1.41962	5.59286	H	0.16344	10.50901	-3.56696
C	3.71253	5.12776	5.02176	H	-5.37890	9.12652	-4.02513
C	4.47453	6.04394	4.36355	H	-3.84218	9.76958	-3.37954
C	5.57591	5.61731	3.57258	H	-4.08263	9.64074	-5.13784
C	5.87404	4.29279	3.46217	H	2.77922	-3.85876	-9.85648
C	2.84864	0.44225	6.36132	H	1.51898	-5.03670	-9.39415
C	3.17716	-0.87760	6.31113	H	1.16272	-3.78788	-10.60962
C	4.22646	-1.32009	5.46120	H	-2.40014	-6.18801	-8.91344
C	4.93591	-0.42541	4.72025	H	-2.84101	-6.57457	-7.21969
C	6.53829	1.46823	3.20592	H	-4.11687	-6.24625	-8.42210
C	6.39525	1.35675	1.82713	H	1.57622	6.65172	10.46949
N	7.38457	0.93078	1.01875	H	2.46663	6.36741	8.94824
C	8.57410	0.60083	1.55632	H	0.73539	6.83327	8.90549
C	8.80450	0.69442	2.91645	H	-1.82774	-4.03143	-11.36979
C	7.77988	1.12902	3.74846	H	-2.84211	-3.46850	-10.01317
O	-1.44958	4.29992	8.46382	H	-1.38072	-2.54401	-10.48982
C	-1.56995	4.36920	9.88633	H	-1.42771	10.55966	-6.45949
O	1.12512	4.89523	9.56624	H	-0.19419	9.28688	-6.24500
C	1.50070	6.27037	9.45113	H	-1.87263	8.84759	-6.69826
O	3.37459	4.14764	8.13306	H	1.47650	-11.39385	4.68041
C	3.77197	3.49451	9.34294	H	0.19741	-10.39919	3.93078
N	7.42043	-1.26887	-0.90316	H	1.72826	-10.71155	3.05039
C	8.49536	-1.80476	-1.51240	H	-1.50625	-3.07790	-1.58972
C	8.74141	-3.16495	-1.48223	H	0.85517	-1.30967	-0.82073
C	7.85079	-4.00021	-0.81787	H	0.47056	-1.89423	-2.43353
C	6.72938	-3.45839	-0.18685	H	-1.63914	-0.56787	-2.44541
C	6.56478	-2.07893	-0.25340	H	-0.25250	0.46110	-2.13301
C	5.72239	-4.29272	0.52731	H	-0.68580	0.30418	0.32092
C	5.77128	-4.39463	1.92782	H	-2.14857	-3.08669	0.77553
C	4.75814	-5.14164	2.61596	H	-0.75553	-2.07338	1.19266
C	3.74162	-5.78904	1.88836	H	0.63622	-4.30708	-1.47910
C	3.74915	-5.74610	0.48263	H	-0.37639	-4.75191	-0.10148
C	4.73779	-4.96892	-0.21159	H	0.97467	-3.62486	0.11518
C	4.82197	-5.21172	4.04355	H	-3.23950	1.19075	-1.06587
C	5.83481	-4.62875	4.74242	H	-2.14920	3.46087	-1.18327
C	6.85001	-3.90629	4.05760	H	-1.43600	2.30268	-2.30341
C	6.81079	-3.78424	2.70171	H	-0.59708	2.71560	-0.79213
C	2.79675	-6.48076	-0.29394	H	-3.24783	1.17073	1.46452
C	2.79547	-6.42687	-1.65368	H	-3.36935	2.81564	0.81193
H	-1.83833	2.23920	1.45662				