Supplementary Material (ESI) for Chemical Communications
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Electronic Supporting Information

Amine-triggered molecular capsules using dynamic boronate esterification

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1. General

NMR spectra were taken with a JEOL Lambda 500 (^{1}H: 500 MHz) spectrometer. Chemical shifts (δ) are reported downfield from the initial standard Me_4Si. Bruker DPX-400 (^{1}H: 400 MHz) spectrometer was employed for DOSY investigation. Electrospray ionization (ESI) mass spectra were recorded on a JEOL JMS-T100CS spectrometer.

2. Assignment of Et_3NH^+@3

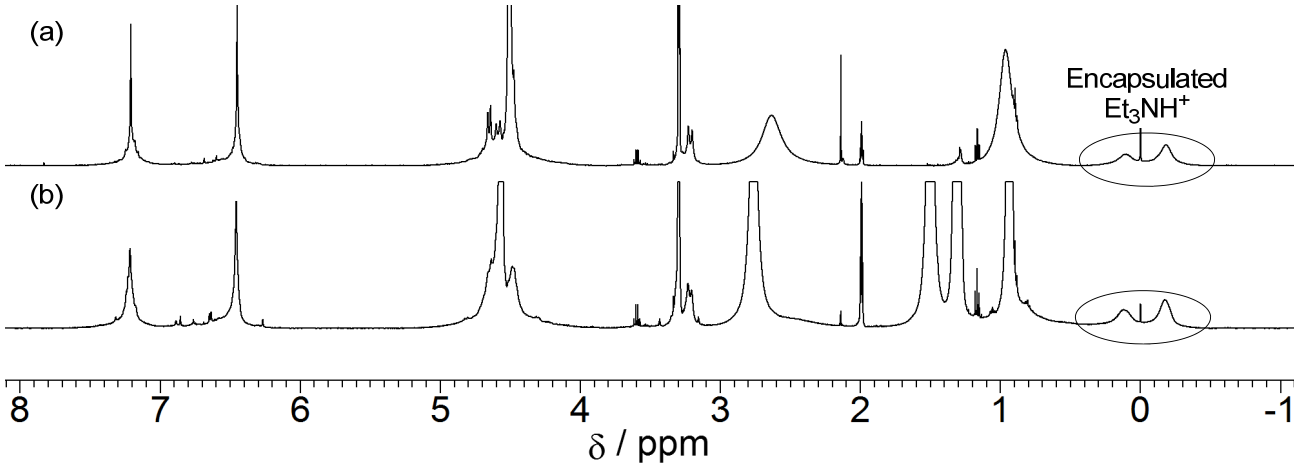

Fig. S1 ^{1}H NMR spectra (500 MHz, CD_3OD−CD_3CN (4:1 v/v), 23 °C); (a) **1** (10 mM) and **2** (10 mM) with Et_3N (30 mM); (b) $^nBu_3N$-triggered **3** with Et_3NHCl (10 mM).

3. DOSY spectra of $^{n}Bu_3N$-triggered 3

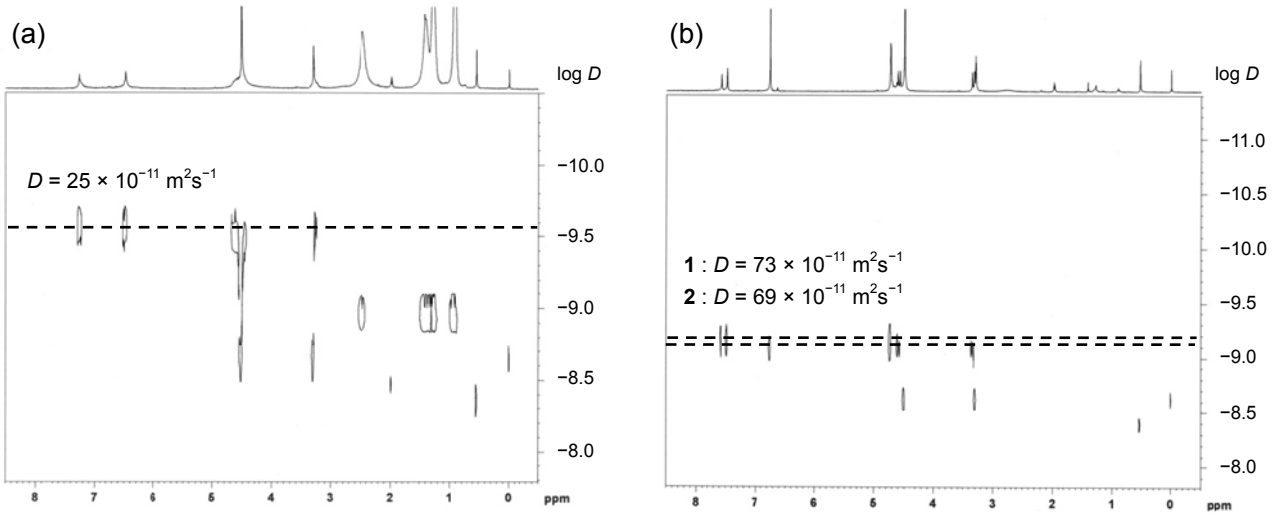

Fig. S2 DOSY spectra (400 MHz) in CD_3OD–CD_3CN (4:1 v/v) at 23 °C: (a) **1**·**2** with $^{n}Bu_3N$, (b) **1** and **2**. [**1**] = [**2**] = 10 mM, [$^{n}Bu_3N$] = 30 mM.

4. pH-Dependency for the formation of 3

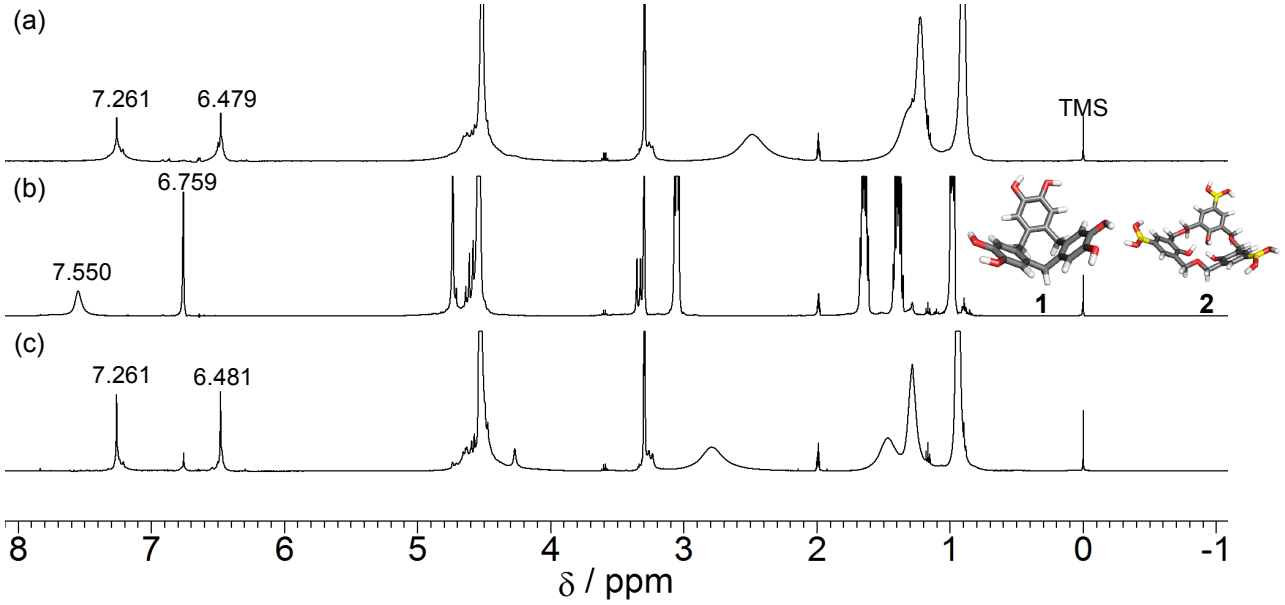

Fig. S3 pH-Dependency for the formation of **3** in CD_3OD−CD_3CN (4:1 v/v). (a) in the presence of $^{n}Bu_3N$ (30 mM), (b) addition of 2.5 μL of 12N HCl, (c) subsequent excess amount of $NaHCO_3$ addition. The data were collected using 500 MHz ^{1}H NMR at 23 °C. [**1**] = [**2**] = 10 mM.

5. Guest encapsulation of 3

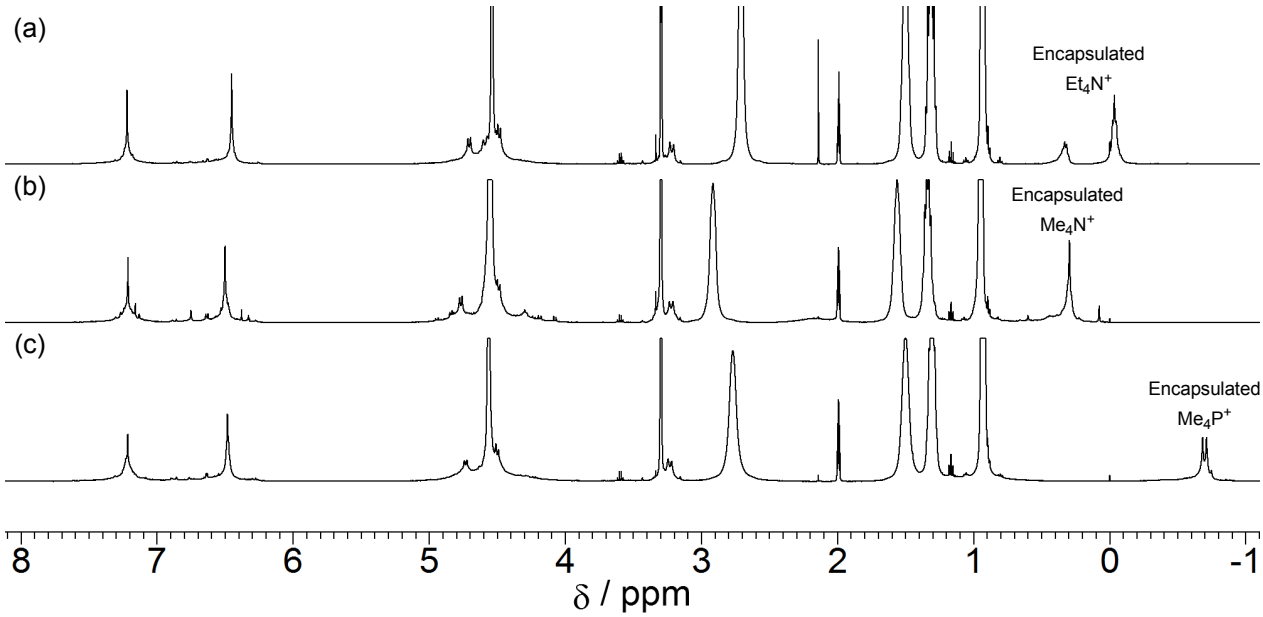

Fig. S4 ^{1}H NMR spectra (500 MHz, CD_3OD–CD_3CN (4:1 v/v), 23 °C) of ^{n}Bu_3N-triggerd **3** by adding 10 mM of (a) Et_4NI, (b) Me_4NI and (c) Me_4PBr. [**1**] = [**2**] = 10 mM, [^{n}Bu_3N] = 30 mM.

6. Competitive titration of THF@3 with CsCl

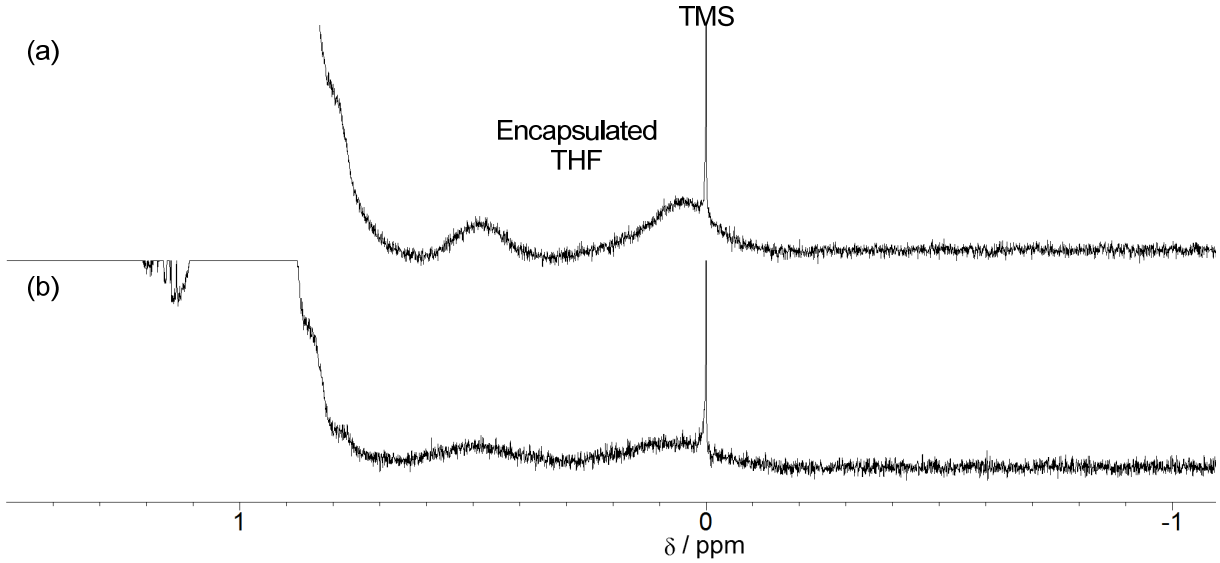

Fig. S5 Up-field region of ^{1}H NMR (500 MHz, 23 °C) of THF@**3** with the addition of 100 mM of CsCl in CD_3OD–CD_3CN (4:1 v/v). [**1**] = [**2**] = 10 mM, [^{n}Bu_3N] = 30 mM, [THF] = 250 mM. (a) 0 and (b) 100 mM of CsCl.

7. ESI MS spectra

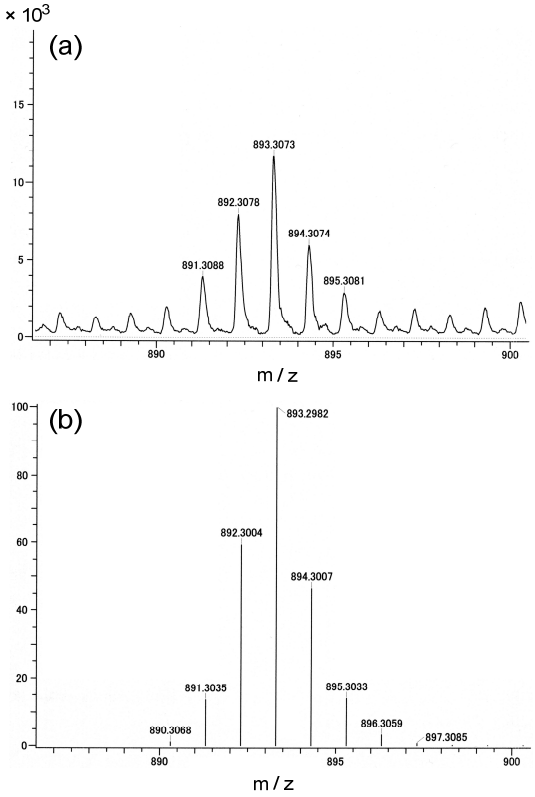

Fig. S6. (a) ESI MS spectra of **1** and **2** in the presence 3 equivalents of $^{n}Bu_3N$ in MeOH, [**1**] = [**2**] = 0.1 mM, negative mode, a spray temperature of 250 ºC; (b) isotope pattern for $C_{48}H_{44}B_3O_{15}^-$.

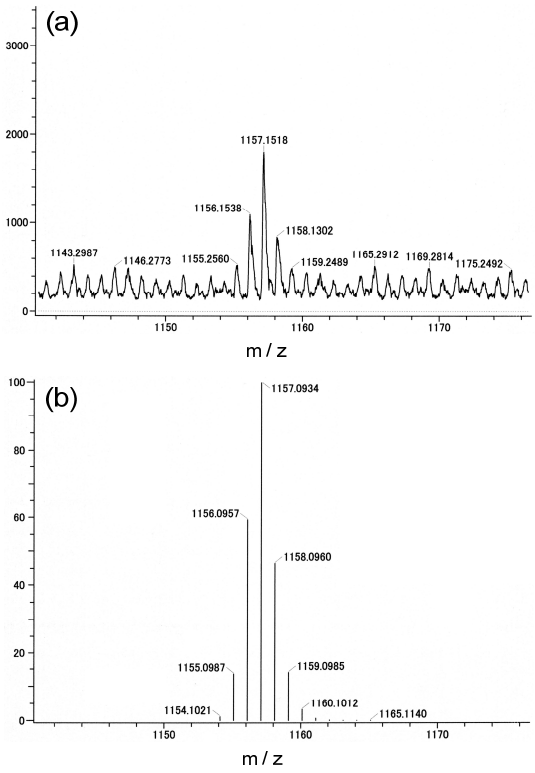

Fig. S7. (a) ESI MS spectra of $^{n}Bu_3N$-triggered capsule **3** upon the addition of $CsClO_4$ (0.3 mM) in MeOH, [**1**] = [**2**] = 0.1 mM, negative mode, a spray temperature of 250 ºC; (b) isotope pattern for $C_{48}H_{42}B_3Cs_2O_{15}^-$.