Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Tri-substituted hexahomotrioxacalix[3]arene derivatives bearing imidazole units: synthesis and extraction properties for cations and chromate anions

Xin-Long Ni,[a,b] Cheng-Cheng Jin,[a] Xue-Kai Jiang,[a] Masashi Takimoto,[a] Shofiur Rahman,[a] Xi Zeng,[b] David L. Hughes,[c] Carl Redshaw[d] and Takehiko Yamato*[a]

[a] *Department of Applied Chemistry, Faculty of Science and Engineering, Saga University, Honjo-machi 1, Saga-shi, Saga 840-8502, Japan. Fax: (internat.) + 81(0)952/28-8548; E-mail: yamatot@cc.saga-u.ac.jp*

[b] *Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, Guizhou, 550025, China*

[c] *Energy Materials Laboratory, School of Chemistry, University of East Anglia, Norwich, NR4 7TJ, UK*

[d] *Department of Chemistry, The University of Hull, UK, HU6 7RX*

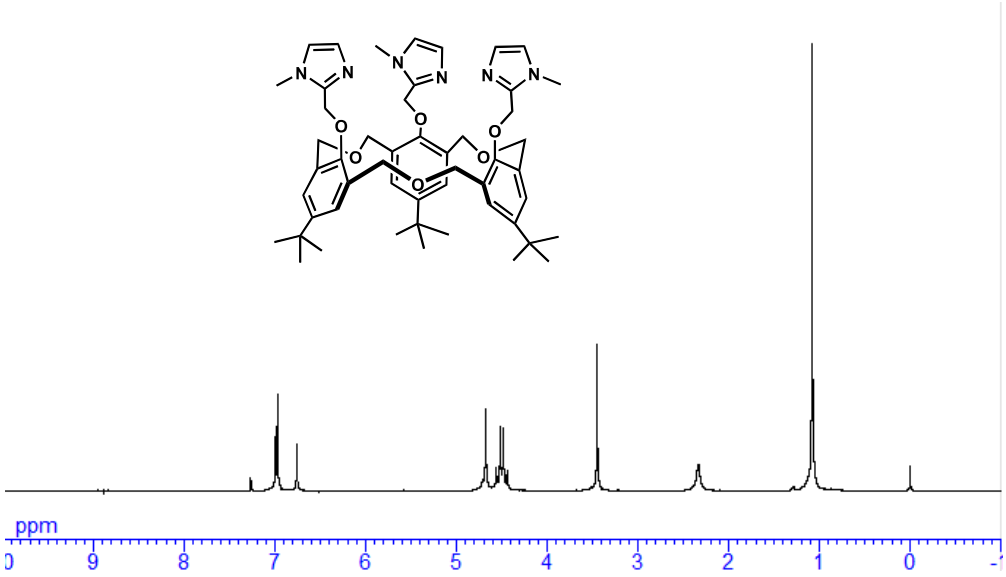

Figure S1. ^{1}H NMR spectrum of *cone*-**2** ($CDCl_3$, 300 MHz).

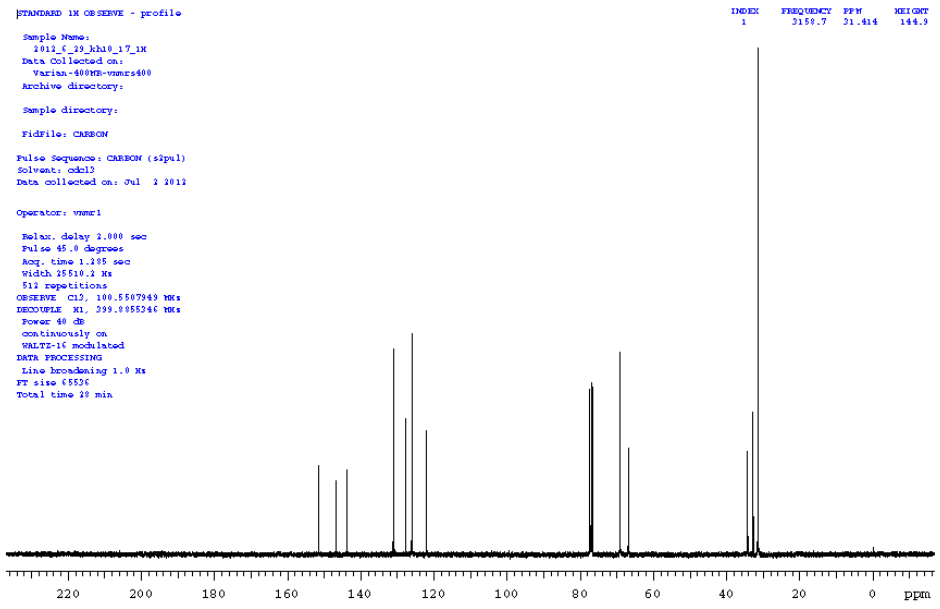

Figure S2. ^{13}C NMR spectrum of *cone*-**2** ($CDCl_3$, 300 MHz).

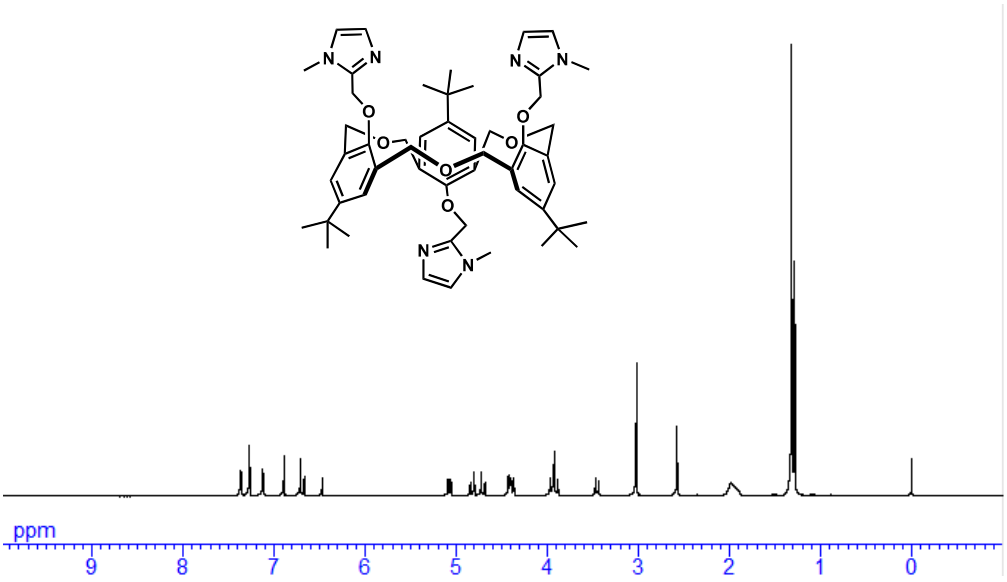

Figure S3. ^{1}H NMR spectrum of *partial-cone*-**2** ($CDCl_3$, 300 MHz).

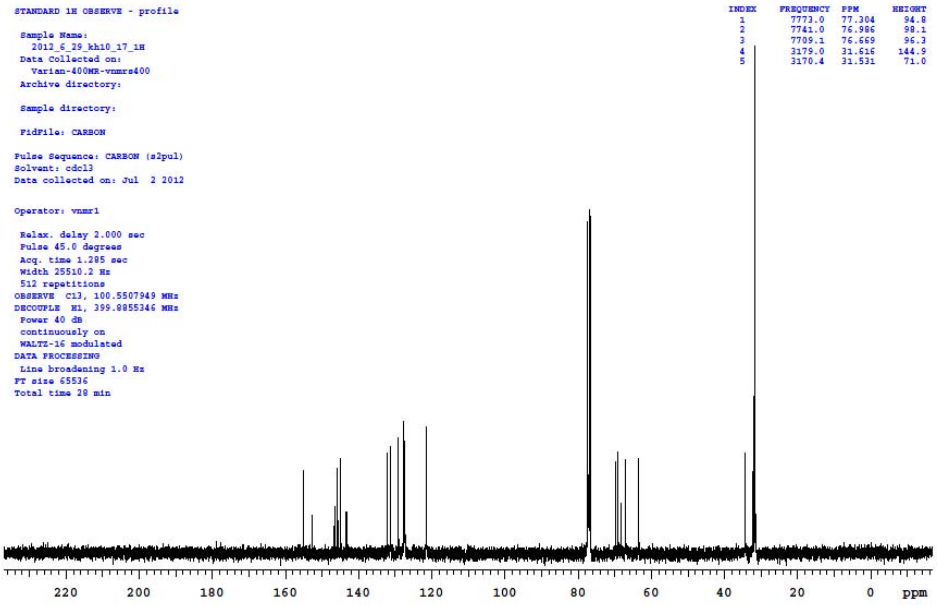

Figure S4. ^{13}C NMR spectrum of *partial-cone*-**2** ($CDCl_3$, 300 MHz).

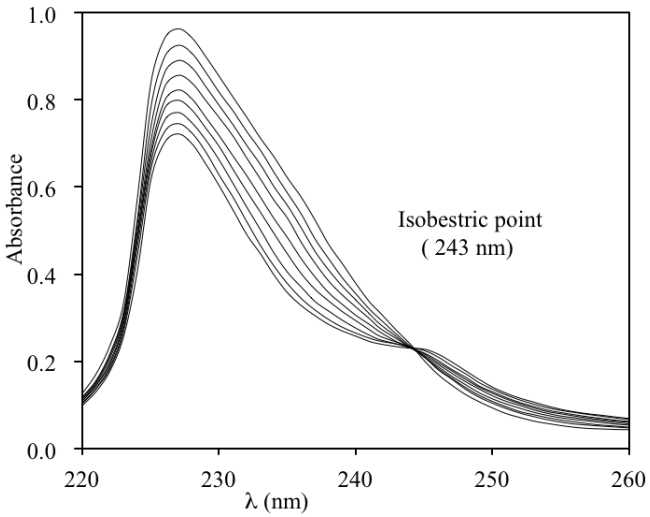

Figure S5. UV-vis spectral changes of *cone*-**2** on addition of $Zn(ClO_4)_2$ (THF:CH_2Cl_2 = 1:50), [*cone*-**2**] = 1×10^{-5} M; [$Zn(ClO_4)_2$] = 0.1–2.5 equiv.

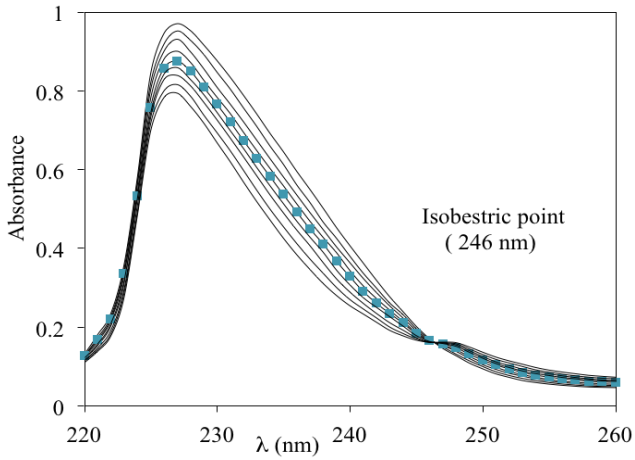

Figure S6. UV-vis spectral changes of *cone*-**2** on addition of $Cu(ClO_4)_2$ (THF:CH_2Cl_2=1:50), [*cone*-**2**] = 1×10^{-5} M; [$Cu(ClO_4)_2$] = 0.1–2.5 equiv.

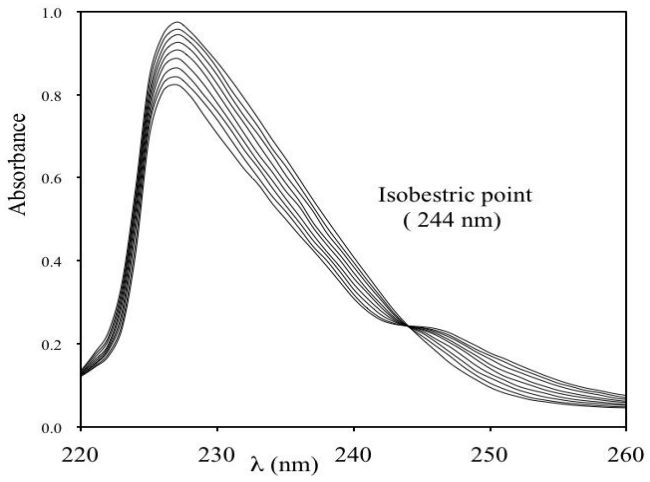

Figure S7. UV-vis spectral changes of *cone*-**2** on addition of $Hg(ClO_4)_2$ (THF:CH_2Cl_2 = 1:50), [*cone*-**2**] = 1×10^{-5} M; [$Hg(ClO_4)_2$] = 0.1–2.5 equiv.

Table S1. Extraction percentages of metal picrates with ligands[a]

Ligand	Extracted metal cations										
	Li^+	Na^+	K^+	Cs^+	Co^{2+}	Ni^{2+}	Cu^{2+}	Zn^{2+}	Cd^{2+}	Ag^+	Hg^{2+}
cone-**2**	2	2	3	4	74	78	98	88	81	93	85
p-cone-**2**	1	1	2	3	61	63	75	76	69	84	75

[a] Aqueous phase: [metal nitrate] = 1×10^{-2} M; [picric acid] = 2.5×10^{-2} M; organic phase: CH_2Cl_2, [ligand] =1×10^{-2} M; at 25 °C, for 12 h.