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Electronic supplementary information for

Variational first hyperpolarizabilities of 2,3-naphtho-15-crown-5 ether derivatives with cation-complexing: a potential and selective cation detector

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Table S1. Calculated bond length of M-O and O-O bonds at the B3LYP/6-31G(d,p)/LanL2DZ level.

complex	M-O_1	M-O_2	M-O_3	M-O_4	M-O_5	O_1-O_2	O_2-O_3	O_3-O_4	O_4-O_5	O_5-O_1
N15C5	-	-	-	-	-	2.823	2.889	2.889	2.823	2.569
N15C5*Li^+	2.208	2.202	2.192	2.202	2.208	2.602	2.616	2.616	2.602	2.533
N15C5*Na^+	2.297	2.311	2.308	2.311	2.297	2.741	2.764	2.764	2.741	2.614
N15C5*K^+	2.651	2.684	2.699	2.684	2.651	2.766	2.785	2.785	2.766	2.682
N15C5*Be^{2+}	1.846	1.714	1.707	1.882	1.705	2.470	2.568	2.483	2.434	2.433
N15C5*Mg^{2+}	2.134	2.135	2.138	2.135	2.134	2.515	2.507	2.507	2.515	2.513
N15C5*Ca^{2+}	2.315	2.315	2.350	2.315	2.315	2.679	2.681	2.681	2.679	2.668
N15C5*Co^{2+}	2.483	2.069	2.055	2.069	2.483	2.633	2.639	2.639	2.633	2.521
N15C5*Ni^{2+}	2.542	1.991	1.954	1.991	2.542	2.607	2.585	2.585	2.607	2.487
N15C5*Cu^{2+}	2.441	2.133	2.159	2.133	2.441	2.681	2.693	2.693	2.681	2.541

Table S2. Dipole moments (Debye), individual components of first hyperpolarizabilities (a.u.), total first hyperpolarizabilities (a.u.), and projection of β on dipole moment (a.u.) computed at the BHandLYP /6-311+G(d,p)/LanL2DZ level.

complex	μ_y	β_x	β_y	β_z	β_{tot}	β_{vec}
N15C5	-2.56	177.3	-813.1	0.0	832.2	826.4
N15C5*Li^+	-8.1	42.4	-301.5	0.0	304.4	301.8
N15C5*Na^+	-7.6	62.9	-299.7	0.0	306.2	298.2
N15C5*K^+	-7.7	12.0	-267.5	0.0	267.8	264.7
N15C5*Be^{2+}	-11.1	18.4	205.3	16.1	206.7	-205.1
N15C5*Mg^{2+}	-12.5	-16.0	163.6	0.0	164.4	-163.9
N15C5*Ca^{2+}	-12.0	-55.7	282.1	0.0	287.6	-285.3
N15C5*Co^{2+}	-15.3	999.3	207877.6	-0.5	207880.0	-207725.4
N15C5*Ni^{2+}	-15.4	397.3	42057.3	0.0	42059.2	-41985.2
N15C5*Cu^{2+}	-6.8	3798.0	33944.9	0.0	34156.7	-34141.9

Table S3. Energies, oscillator strengths and major contributions for N15C5, N15C5*Li^+, N15C5*Be^{2+} and N15C5*Co^{2+} at the CAM-B3LYP/6−311+G(d,p)/LanL2DZ level.

complex	ΔE	f_{os}	MO transition
N15C5	5.70	1.4087	HOMO→L+4 (56%), HOMO-1→LUMO (28%)
N15C5*Li^+	5.78	1.1175	HOMO→L+5 (45%), HOMO-1→LUMO (33%)
N15C5*Be^{2+}	5.67	0.9488	HOMO-1→LUMO (42%), HOMO→L+3 (29%)
N15C5*Ni^{2+}	0.98	0.0880	HOMO-1→LUMO (83%), HOMO-11→LUMO (15%)

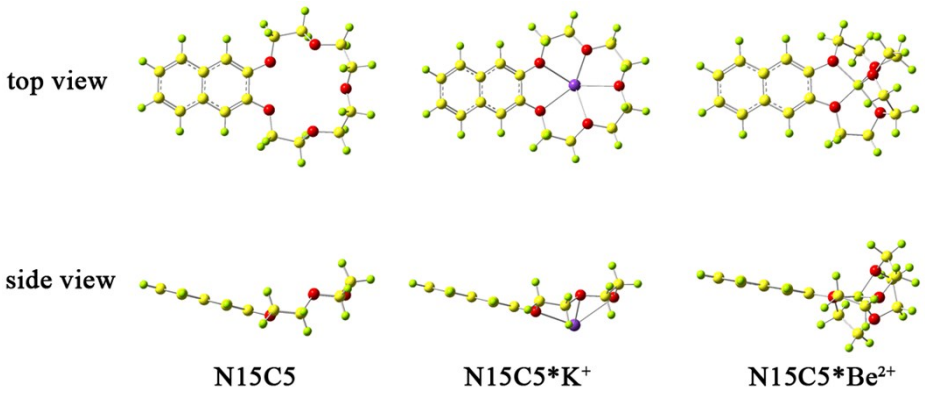

Fig. S1 Optimized structures of N15C5, N15C5*K^+, N15C5*Be^{2+}.

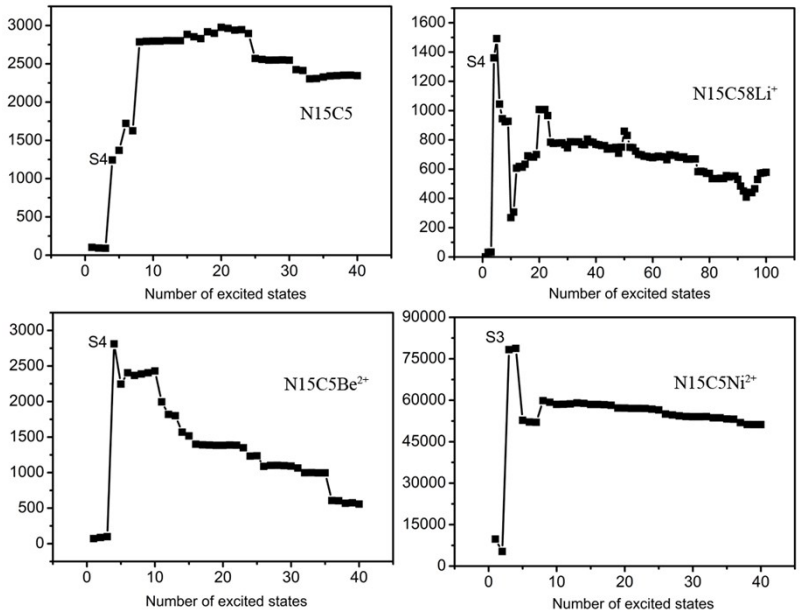

Fig. S2 Convergent behavior of β_{tot} values of N15C5, N15C5*Li^+, N15C5*Be^{2+} and N15C5*Ni^{2+} dependent on the first 40 states.