Electronic supplementary information for

First hyperpolarizabilities of Pt(4-ethynylbenzo-15-crown-5)$_2$(bpy) derivatives with the complexation of mono-cations (Li^+, Na^+, K^+) and di-cations (Mg^{2+}, Ca^{2+}): the development as cation detector

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Table S1 NPA charge distribution for the fragments (F1 – F8) of compounds **L** and its metal

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cation derivatives computed atB3LYP/6-31G**/LanL2DZ level

Compound	**L**	**L*(Li$^+$)$_2$**	**L*(Na$^+$)$_2$**	**L*(K$^+$)$_2$**	**L*(Mg^{2+})$_2$**	**L*(Ca^{2+})$_2$**
M$^{+/2+}$	——	1.499	1.535	1.689	3.249	3.425
S1	-0.427	-0.299	-0.316	-0.393	-0.294	-0.375
S2	-0.427	-0.299	-0.316	-0.394	-0.294	-0.375
S3	0.384	0.456	0.455	0.457	0.518	0.513
S4	0.385	0.456	0.454	0.457	0.518	0.513
S5	-0.296	-0.286	-0.285	-0.285	-0.271	-0.280
S6	-0.296	-0.286	-0.285	-0.285	-0.271	-0.271
S7	0.303	0.322	0.322	0.322	0.345	0.344
S8	0.374	0.437	0.436	0.433	0.501	0.498

Table S2 First hyperpolarizability and its corresponding important tensorial component (10^{-30} esu) calculated at the CAM-B3LYP level with the ultrafine integration grid.

	L	**L*(Li$^+$)$_2$**	**L*(Na$^+$)$_2$**	**L*(K$^+$)$_2$**	**L*(Mg^{2+})$_2$**	**L*(Ca^{2+})$_2$**
β_{xxx}	3.3	0.2	-0.6	-0.6	-0.0	0.0
β_{xxy}	17.6	-4.5	-4.2	-4.8	-19.7	-21.9
β_{xyy}	2.3	-0.3	0.1	-0.0	-0.0	-0.0
β_{yyy}	54.1	15.7	16.0	15.2	2.2	1.7
β_{xzz}	0.0	-0.0	-0.0	-0.0	-0.0	0.0
β_{yzz}	1.2	0.6	0.8	0.6	0.3	0.1
β_x	5.7	-0.2	-0.4	-0.6	-0.0	0.0
β_y	72.9	11.8	12.6	11.0	-17.2	-20.1
β_z	-0.5	1.7	0.2	-0.4	2.5	2.3

β_{tot}	73.1	11.9	12.6	11.0	17.4	20.2

Table S3 First hyperpolarizability and its corresponding important tensorial component (10^{-30} esu) calculated at the CAM-B3LYP level with the superfine integration grid.

	L	**L*(Li^+)$_2$**	**L*(Na^+)$_2$**	**L*(K^+)$_2$**	**L*(Mg^{2+})$_2$**	**L*(Ca^{2+})$_2$**
β_{xxx}	3.3	0.2	-0.6	-0.6	-0.0	0.0
β_{xxy}	17.6	-4.5	-4.2	-4.8	-19.7	-21.9
β_{xyy}	2.3	-0.3	0.1	-0.0	-0.0	-0.0
β_{yyy}	54.1	15.7	16.0	15.2	2.2	1.7
β_{xzz}	0.0	-0.0	-0.0	-0.0	-0.0	0.0
β_{yzz}	1.2	0.7	0.8	0.6	0.3	0.1
β_x	5.7	-0.2	-0.4	-0.6	-0.0	0.0
β_y	72.9	11.8	12.6	11.0	-17.2	-20.1
β_z	-0.5	1.7	0.2	-0.4	2.5	2.3
β_{tot}	73.1	11.9	12.6	11.0	17.4	20.2

Table S4 First hyperpolarizability and its corresponding important tensorial component(10^{-30} esu) calculated at the LC-BLYP level.

	L	**L*(Li$^+$)$_2$**	**L*(Na$^+$)$_2$**	**L*(K$^+$)$_2$**	**L*(Mg^{2+})$_2$**	**L*(Ca^{2+})$_2$**
β_{xxx}	1.0	0.2	-0.5	-0.4	-0.0	0.0
β_{xxy}	5.2	-5.3	-5.2	-5.8	-16.4	-17.9
β_{xyy}	1.0	-0.2	0.3	0.3	-0.0	-0.0
β_{yyy}	23.4	7.4	7.5	6.9	-1.5	-1.7
β_{xzz}	-0.0	-0.0	-0.0	-0.0	-0.0	0.0
β_{yzz}	0.8	0.7	0.8	0.7	0.4	0.2
β_{x}	2.1	-0.0	-0.1	-0.2	-0.0	0.0
β_{y}	29.4	2.9	3.1	1.8	-17.5	-19.3
β_{z}	-0.1	1.5	1.2	0.8	2.5	2.4
β_{tot}	29.5	3.3	3.3	2.0	17.7	19.5

Table S5 First hyperpolarizability and its corresponding important tensorial component(10^{-30} esu) calculated at the M06-2X level.

	L	**L*(Li$^+$)$_2$**	**L*(Na$^+$)$_2$**	**L*(K$^+$)$_2$**	**L*(Mg^{2+})$_2$**	**L*(Ca^{2+})$_2$**
β_{xxx}	2.9	0.2	-0.6	-0.6	-0.0	0.0
β_{xxy}	15.5	-5.0	-4.7	-5.3	-18.8	-20.9
β_{xyy}	2.1	-0.3	0.1	-0.0	-0.0	-0.0
β_{yyy}	47.7	11.7	12.2	11.4	-0.4	-0.8
β_{xzz}	0.0	-0.0	-0.0	-0.0	-0.0	0.0
β_{yzz}	1.3	0.6	0.8	0.6	0.2	0.0

β_x	5.1	-0.1	-0.5	-0.6	-0.0	0.0
β_y	64.5	7.3	8.3	6.7	-19.0	-21.6
β_z	-0.5	1.6	0.5	-0.1	2.2	2.1
β_{tot}	64.7	7.5	8.3	6.7	19.2	21.7

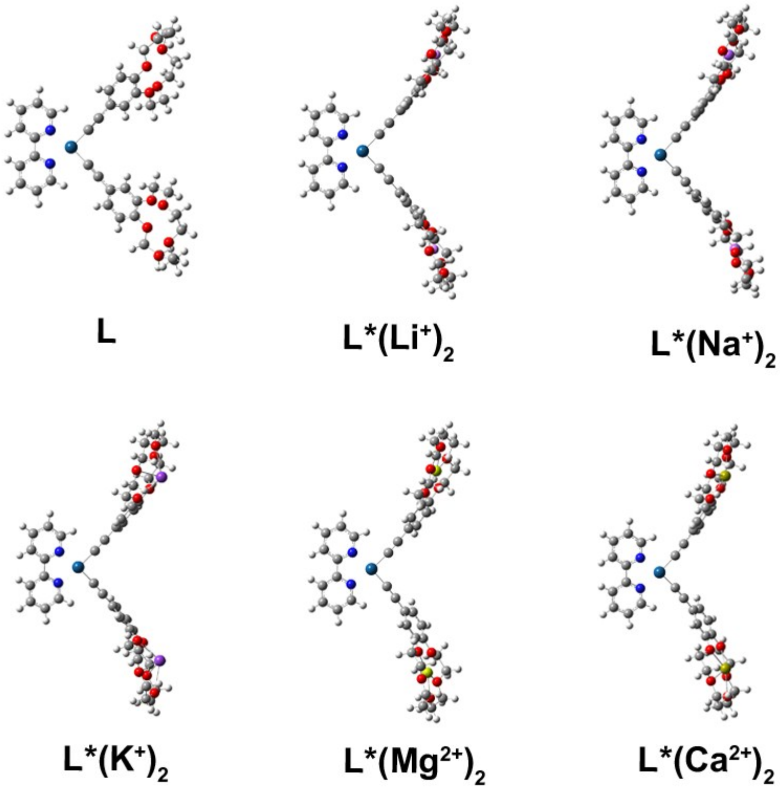

Fig. S1 Geometrical structures of **L** and its cation derivatives

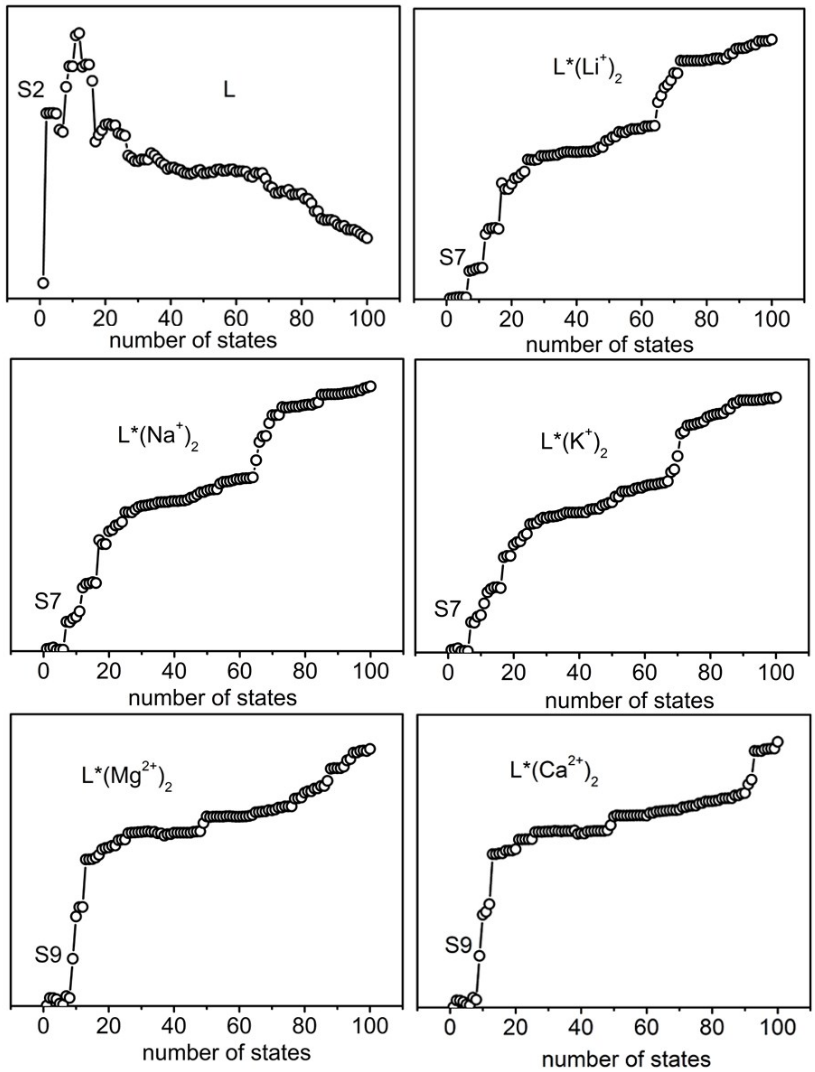

Fig.S2 First hyperpolarizabilies obtained by SOS method with 100 states.