Electronic supplementary information

for

Alkali metal complexes of bis-*o*-xylyl-(17-crown-5): from dinuclear monomer and dinuclear polymer to sandwich polymer

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Table S1 Crystallographic data and refinement parameters of **1**, **2** and **3**

	1	**2**	**3**
Formula	$C_{26}H_{46}I_2Na_2O_{12}$	$C_{13}H_{21}F_6KO_5P$	$C_{13}H_{21}Cl_{0.5}Cs_{0.5}O_5$
Formula weight	850.41	441.37	341.48
Temperature	203	203	203
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*-1	*C*2/*c*	$P2_1/c$
Z	1	8	4
a (Å)	8.4111(9)	14.8016(14)	9.6204(4)
b (Å)	10.3053(11)	15.8098(16)	23.8722(11)
c (Å)	11.1643(12)	16.8878(14)	9.3051(4)
α (°)	67.827(2)	90	90
β (°)	85.400(3)	111.541(5)	117.294(2)
γ (°)	79.241(3)	90	90
V (Å^3)	880.34(16)	3675.9(6)	1899.09(15)
D_{calc} (g/cm^3)	1.604	1.595	1.194
$2\theta_{max}$ (°)	52.00	52.00	52.00
R_1, wR_2 [$I > 2\sigma(I)$]	0.0654, 0.2656	0.0623, 0.1662	0.0725, 0.2103
R_1, wR_2 [all data]	0.0671, 0.2666	0.0971, 0.1877	0.0877, 0.2211
No. of reflection used [>2σ(*I*)]	3464 [R_{int} = 0.0348]	3622 [R_{int} = 0.0715]	3730 [R_{int} = 0.0479]

Table S2 Selected bond lengths (Å) and bond angles (°) for **1**

Na1-O1	2.384(9)	Na1-O4	2.437(9)
Na1-O2	2.416(9)	Na1-O5	2.557(9)
Na1-O3	2.479(9)	Na1-O1W	2.244(12)
O1-Na1-O2	69.1(3)	O2-Na1-O3	68.1(3)
O1-Na1-O3	132.0(3)	O2-Na1-O4	114.9(3)
O1-Na1-O4	152.3(3)	O2-Na1-O5	118.1(3)
O1-Na1-O5	84.5(3)	O2-Na1-O1W	69.1(3)
O1-Na1-O1W	95.3(4)	O3-Na1-O4	68.9(3)
O4-Na1-O5	69.3(3)	O3-Na1-O5	135.2(3)
O4-Na1-O1W	97.7(5)	O3-Na1-O1W	101.2(4)
O5-Na1-O1W	99.3(4)		

Table S3 Selected bond lengths (Å) and bond angles (°) for **2**

K1-O1	2.827(3)	K1-O5	2.782(3)
K1-O2	2.970(3)	K1-F1	2.885(2)
K1-O3	2.826(3)	K1-F5	2.702(4)
K1-O4	2.928(3)		
O1-K1-O2	58.94(8)	O2-K1-O3	57.19(8)
O1-K1-O3	116.10(9)	O2-K1-O4	78.41(8)
O1-K1-O4	105.51(8)	O2-K1-O5	95.02(8)
O1-K1-O5	68.41(9)	O2-K1-F1	145.34(8)
O1-K1-F1	136.24(9)	O2-K1-F5	96.35(16)
O1-K1-F5	67.79(16)	O3-K1-O4	59.94(8)
O4-K1-O5	57.39(8)	O3-K1-O5	115.12(9)
O4-K1-F1	114.20(10)	O3-K1-F1	99.67(7)
O4-K1-F5	173.15(15)	O3-K1-F5	113.53(14)
O5-K1-F1	119.20(9)	O5-K1-F5	128.09(13)

Table S4 Selected bond lengths (Å) and bond angles (°) for **3**

Cs1-O1	3.370(5)	Cs1-O4	3.190(5)
Cs1-O2	3.287(6)	Cs1-O5	3.345(5)
Cs1-O3	3.088(5)		
O1-Cs1-O2	51.61(12)	O2-Cs1-O3	50.57(15)
O1-Cs1-O3	98.84(15)	O2-Cs1-O4	90.24(17)
O1-Cs1-O4	108.62(15)	O2-Cs1-O5	89.50(17)
O1-Cs1-O5	69.09(14)	O2-Cs1-O2A	180.0
O1-Cs1-O1A	180.0	O2-Cs1-O3A	129.43(15)
O1-Cs1-O2A	128.39(12)	O2-Cs1-O4A	89.76(17)
O1-Cs1-O3A	81.16(15)	O2-Cs1-O5A	90.50(17)
O1-Cs1-O4A	71.38(15)	O3-Cs1-O4	54.54(16)
O1-Cs1-O5A	110.92(14)	O3-Cs1-O5	90.85(15)
O4-Cs1-O5	50.49(13)	O3-Cs1-O3A	180.0
O4-Cs1-O4A	180.0	O3-Cs1-O4A	125.46(16)
O4-Cs1-O5A	129.51(14)	O3-Cs1-O5A	89.15(15)
O5-Cs1-O5A	180.0		

Symmetry operations: (A) -x,-y+1,-z+1

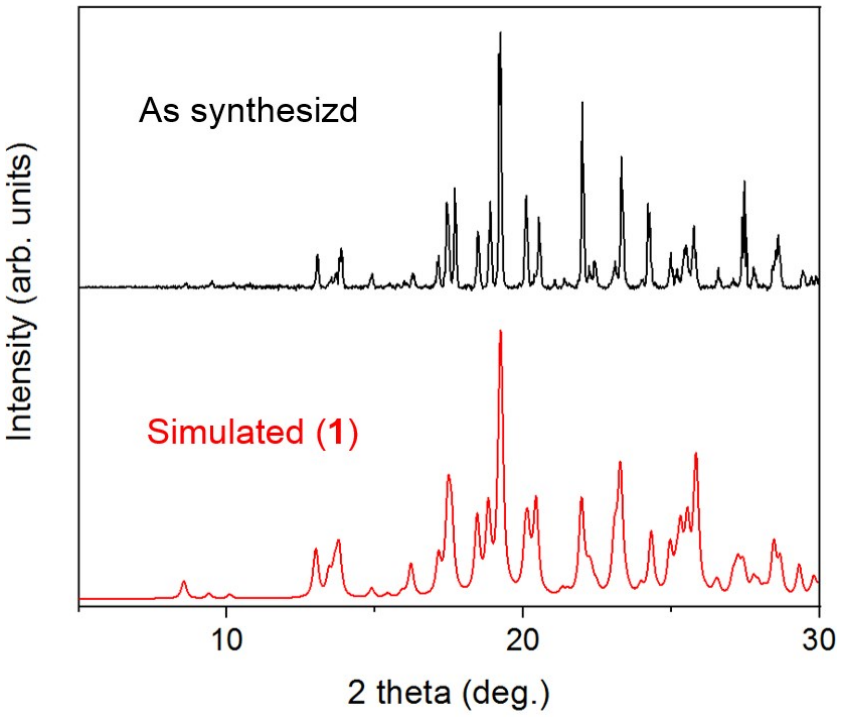

Fig. S1 PXRD patterns of **1**.

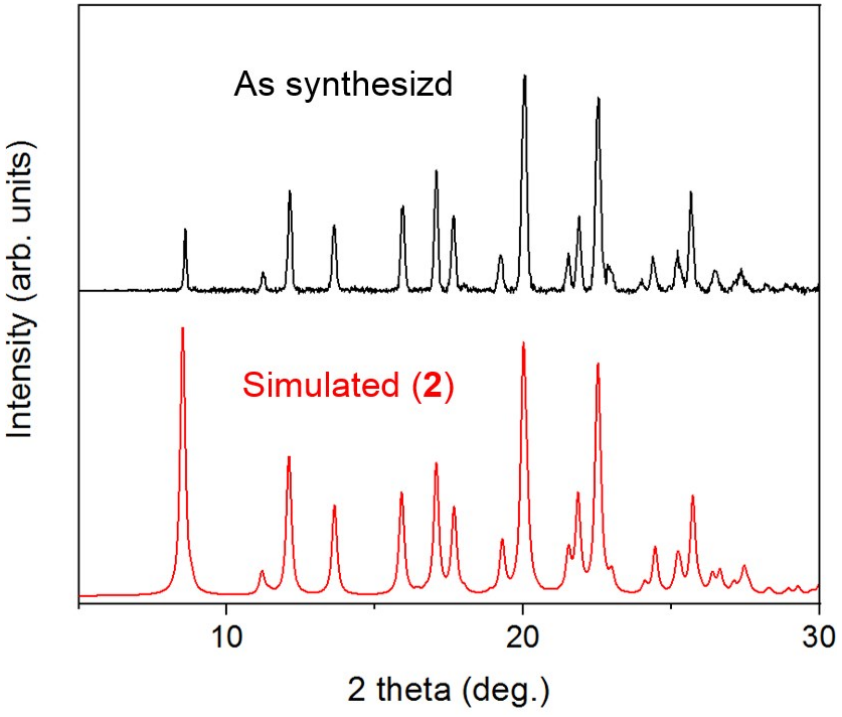

Fig. S2 PXRD patterns of **2**.

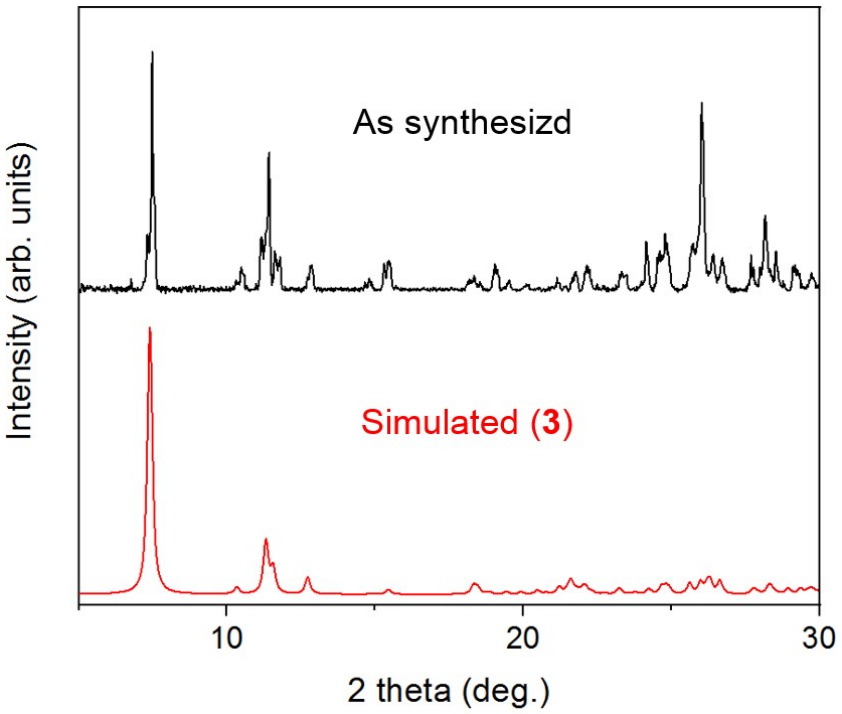

Fig. S3 PXRD patterns of **3**.

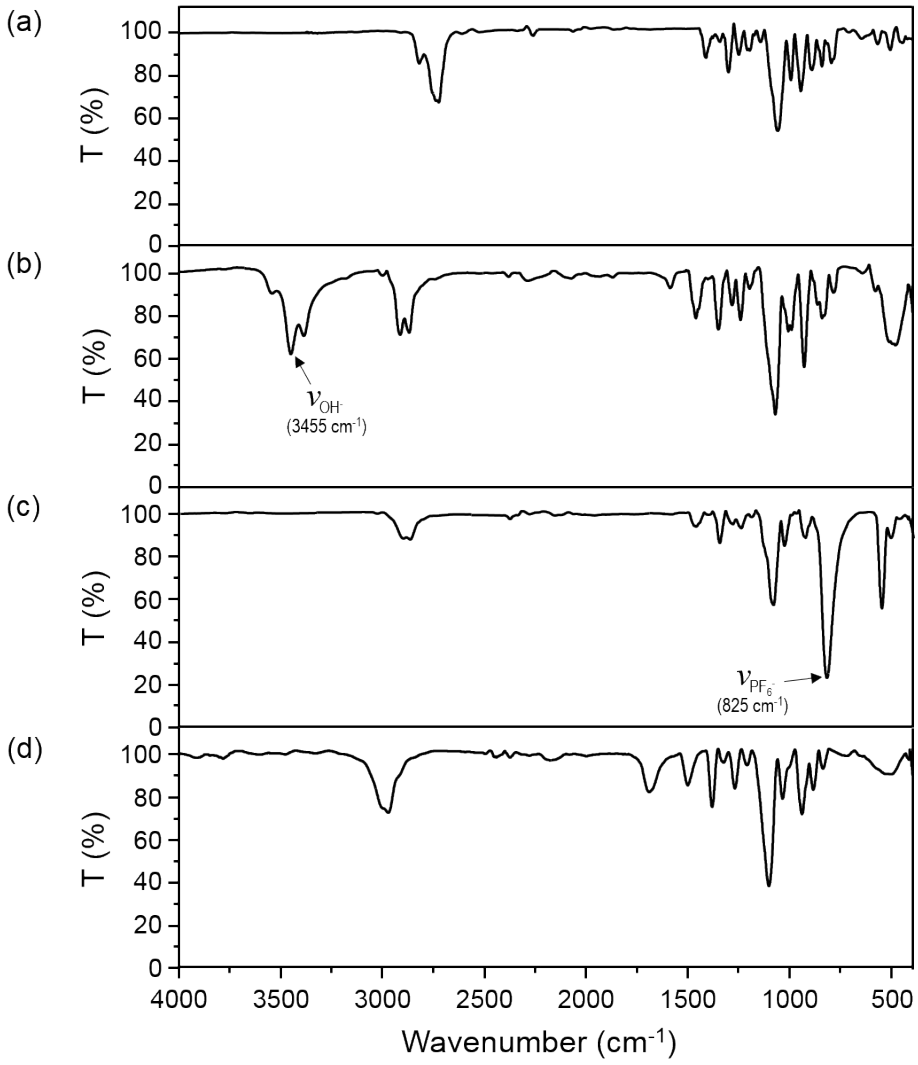

Fig. S4 IR spectra of (a) **L**, (b) **1**, (c) **2** and (d) **3**.

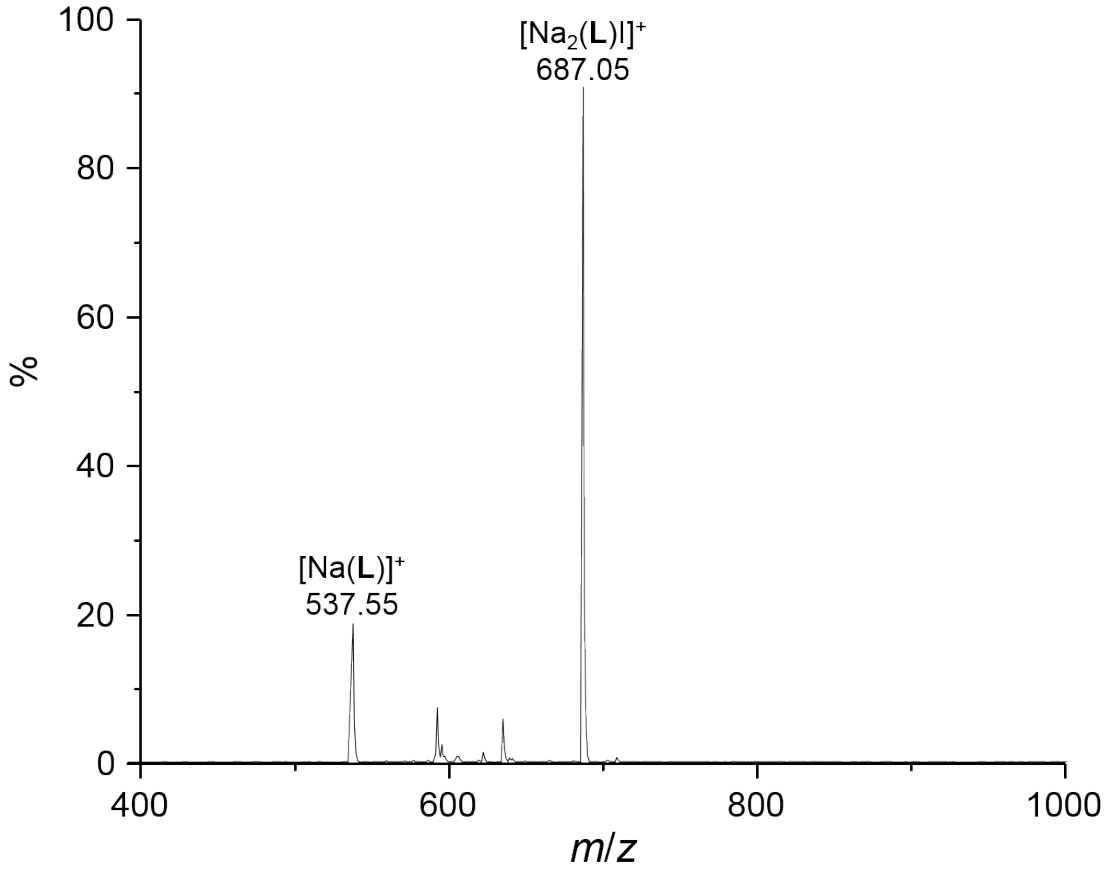

Fig. S5 ESI-mass spectrum of **1**.

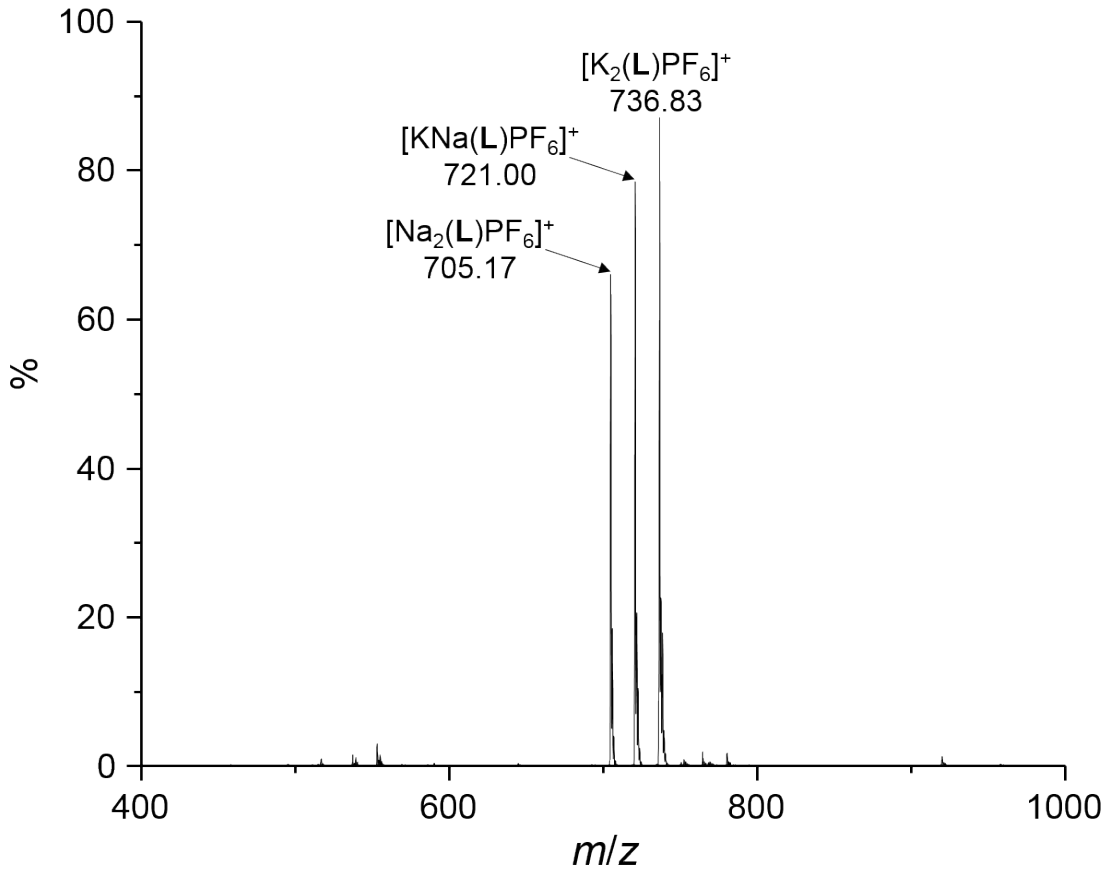

Fig. S6 ESI-mass spectrum of **2**. The sodium ions bound to the ligand **L** are derived from the glass flasks.

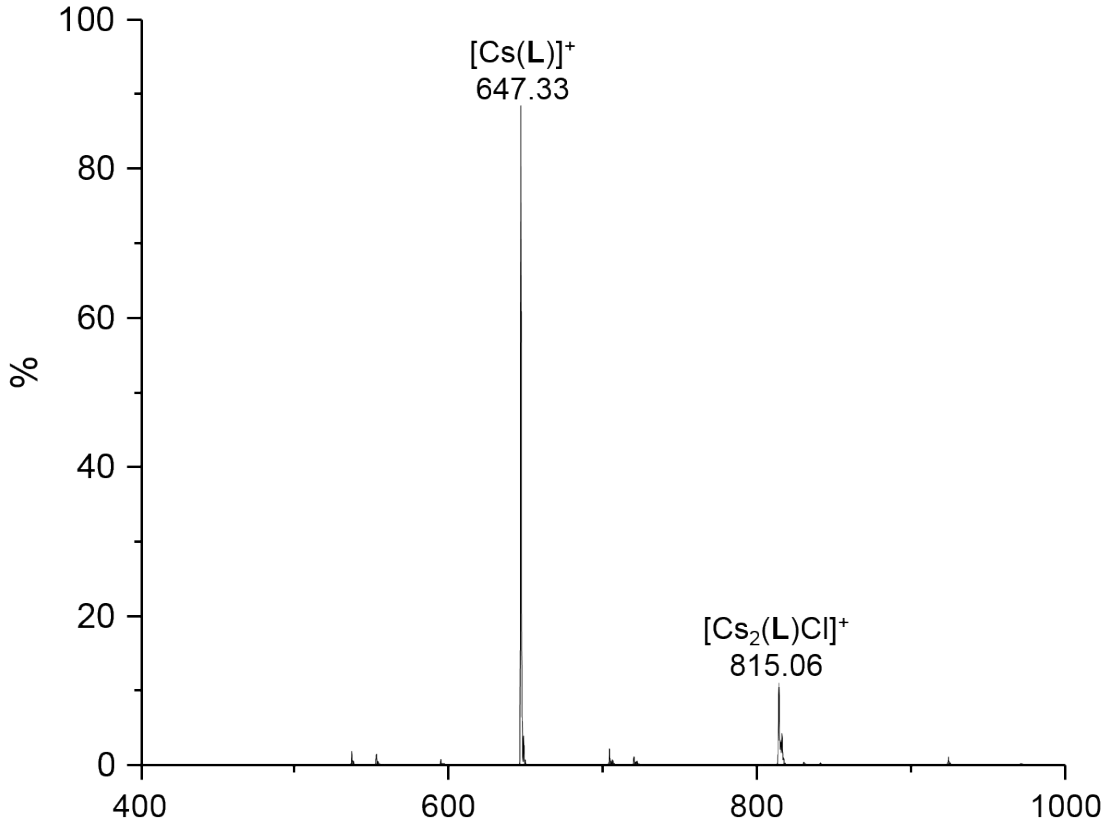

Fig. S7 ESI-mass spectrum of **3**.

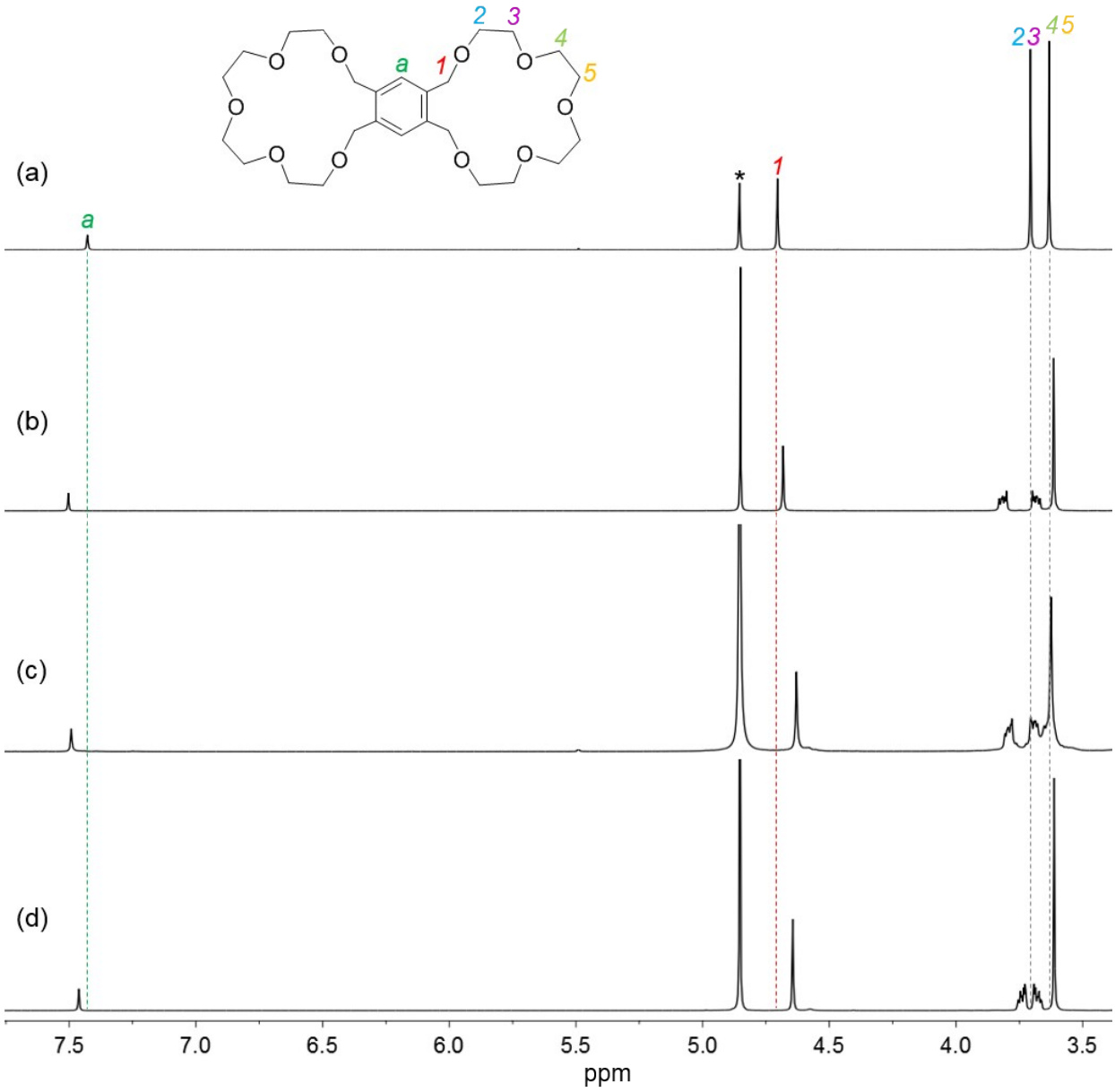

Fig. S8 ^{1}H-NMR spectra of (a) **L**, (b) **1**, (c) **2** and (d) **3** in CH_3OD.