Electronic Supplementary Information for:

Di-phosphonate cavitands as molecular cups for L-lactic acid

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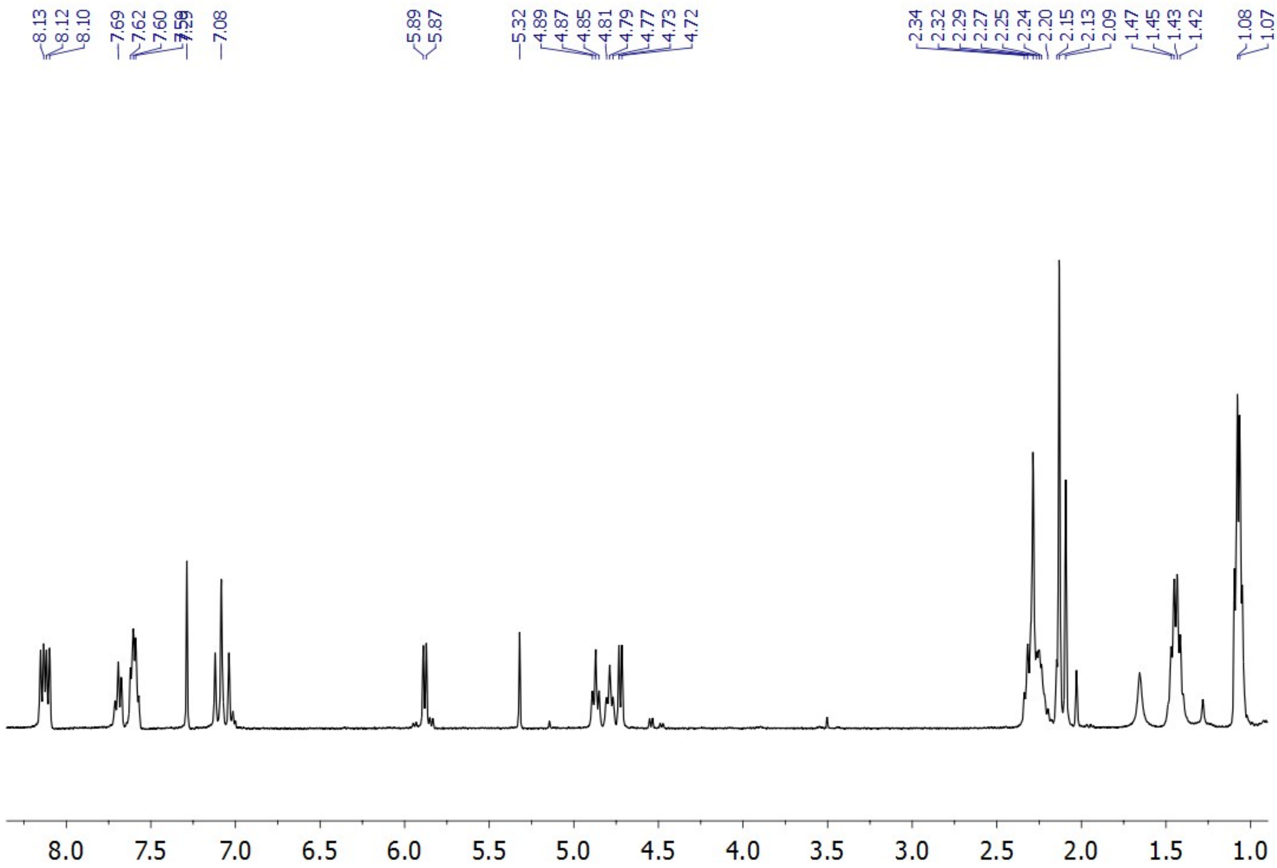


Figure S1. ^{1}H NMR spectrum of **ABii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 400 MHz, 298K).

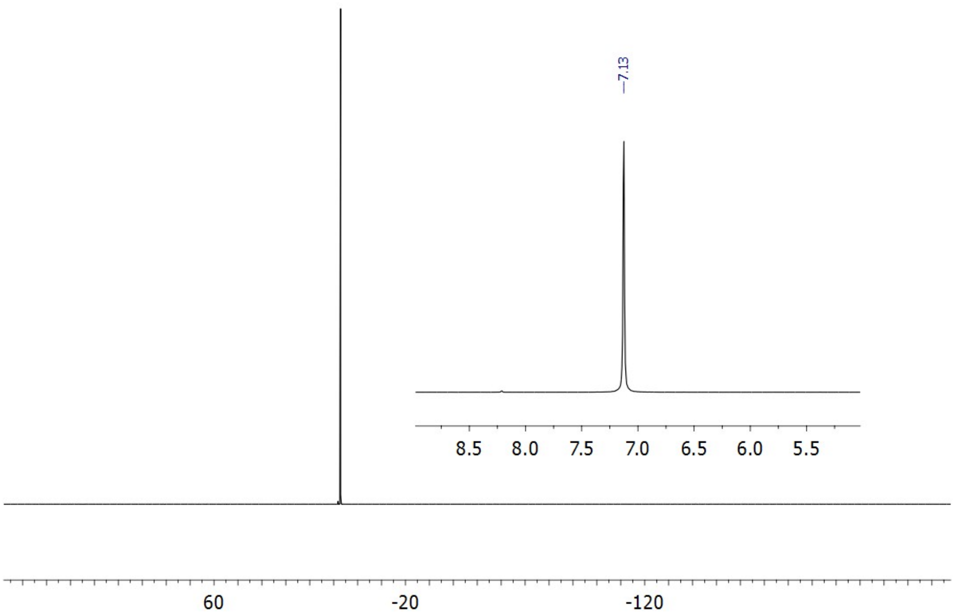


Figure S2. ^{31}P NMR spectrum of **ABii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 162 MHz, 298K).

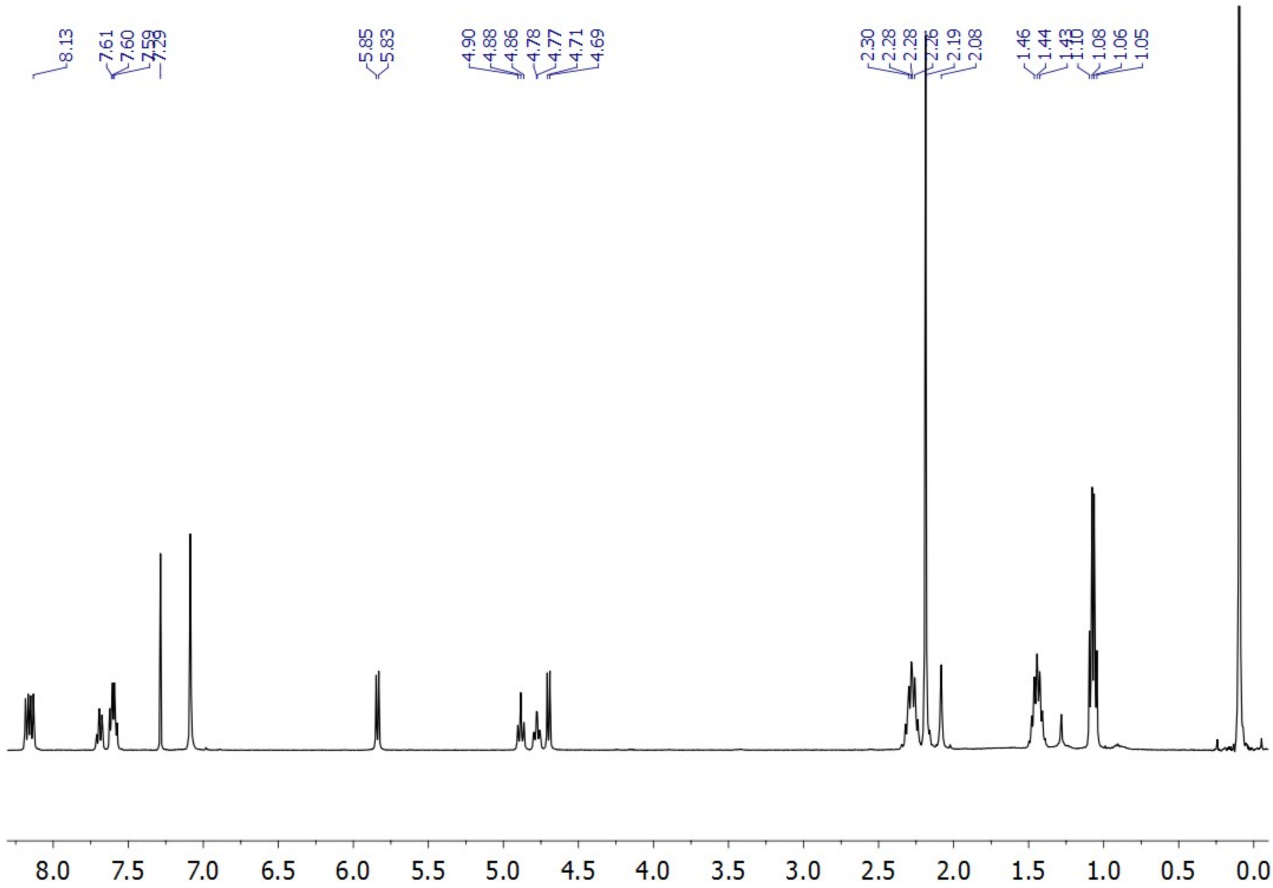


Figure S3. ^{1}H NMR spectrum of **ACii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 400 MHz, 298K).

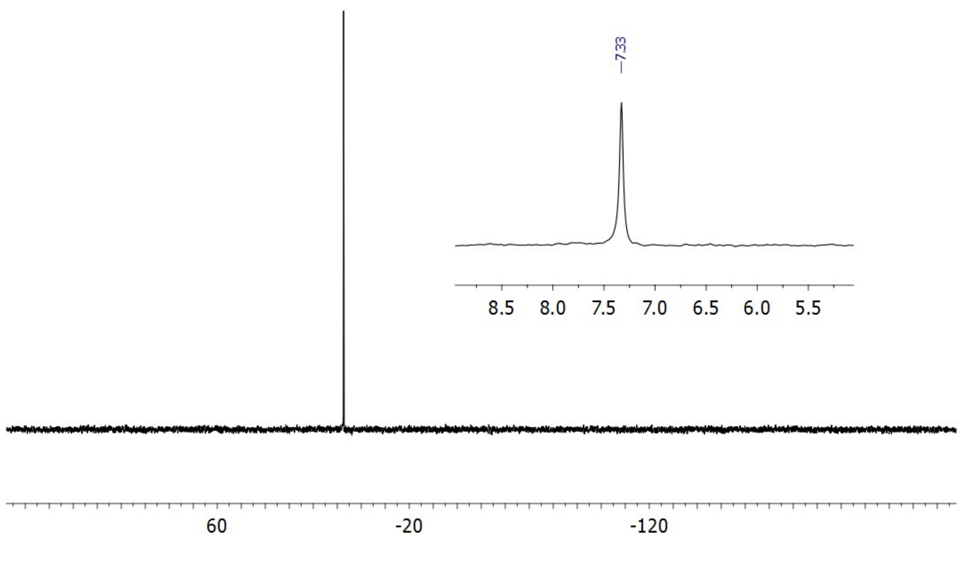


Figure S4. ^{31}P NMR spectrum of **ACii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 162 MHz, 298K).

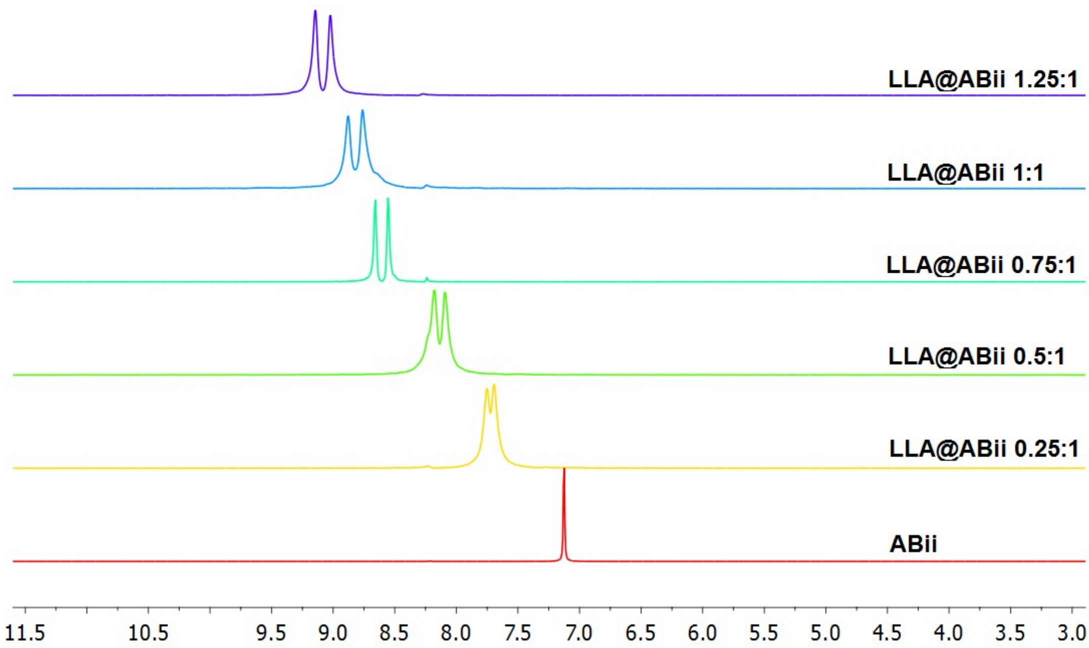


Figure S5. [31]P NMR titration of **ABii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 162 MHz) with LLA.

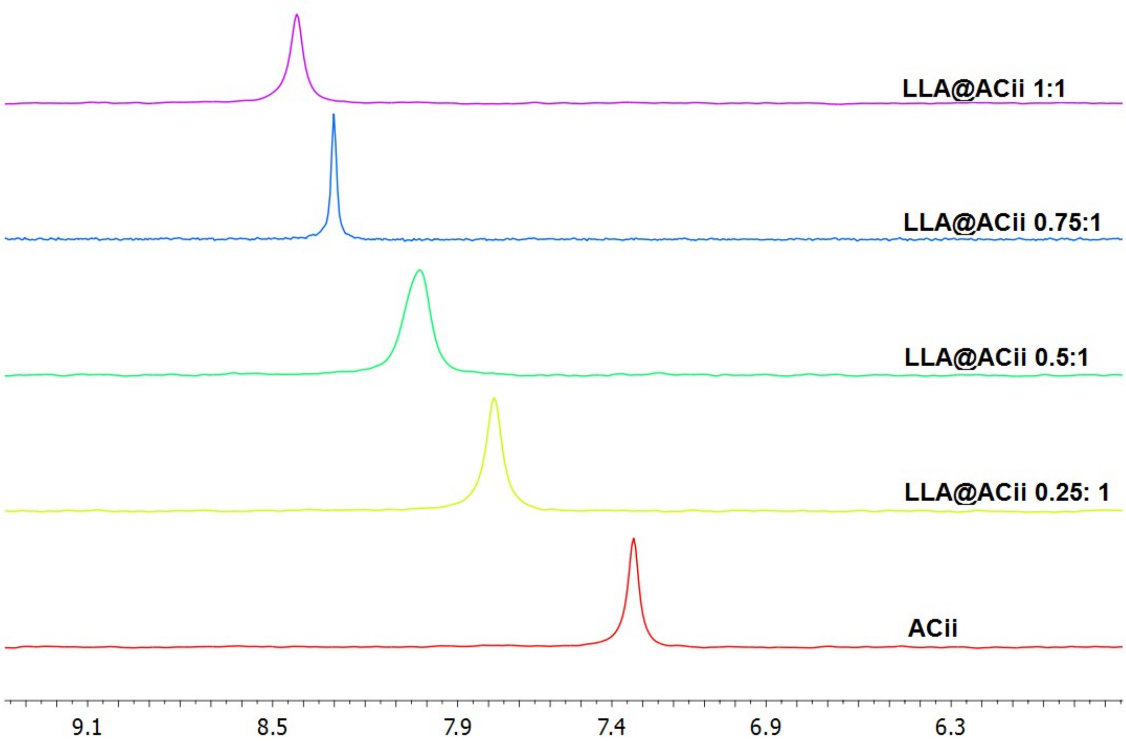


Figure S6. [31]P NMR titration of **ACii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 162 MHz, 298K) with LLA.

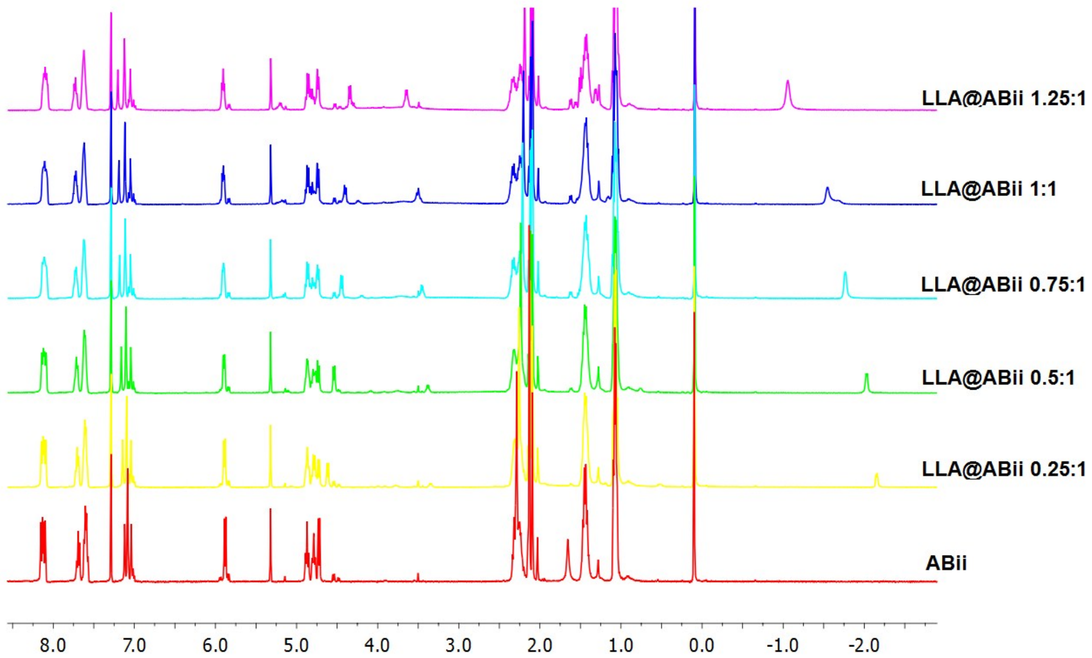


Figure S7. ^{1}H NMR titration of **ABii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 400 MHz) with LLA.

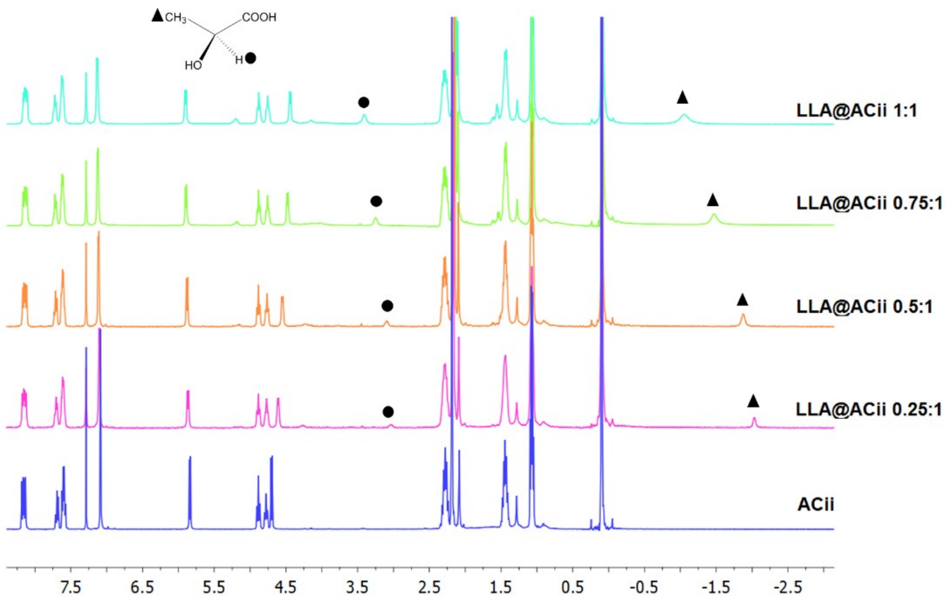


Figure S8. ^{1}H NMR titration of **ACii[C_3H_7, CH_3, Ph]** ($CDCl_3$, 400 MHz, 298K) with LLA.

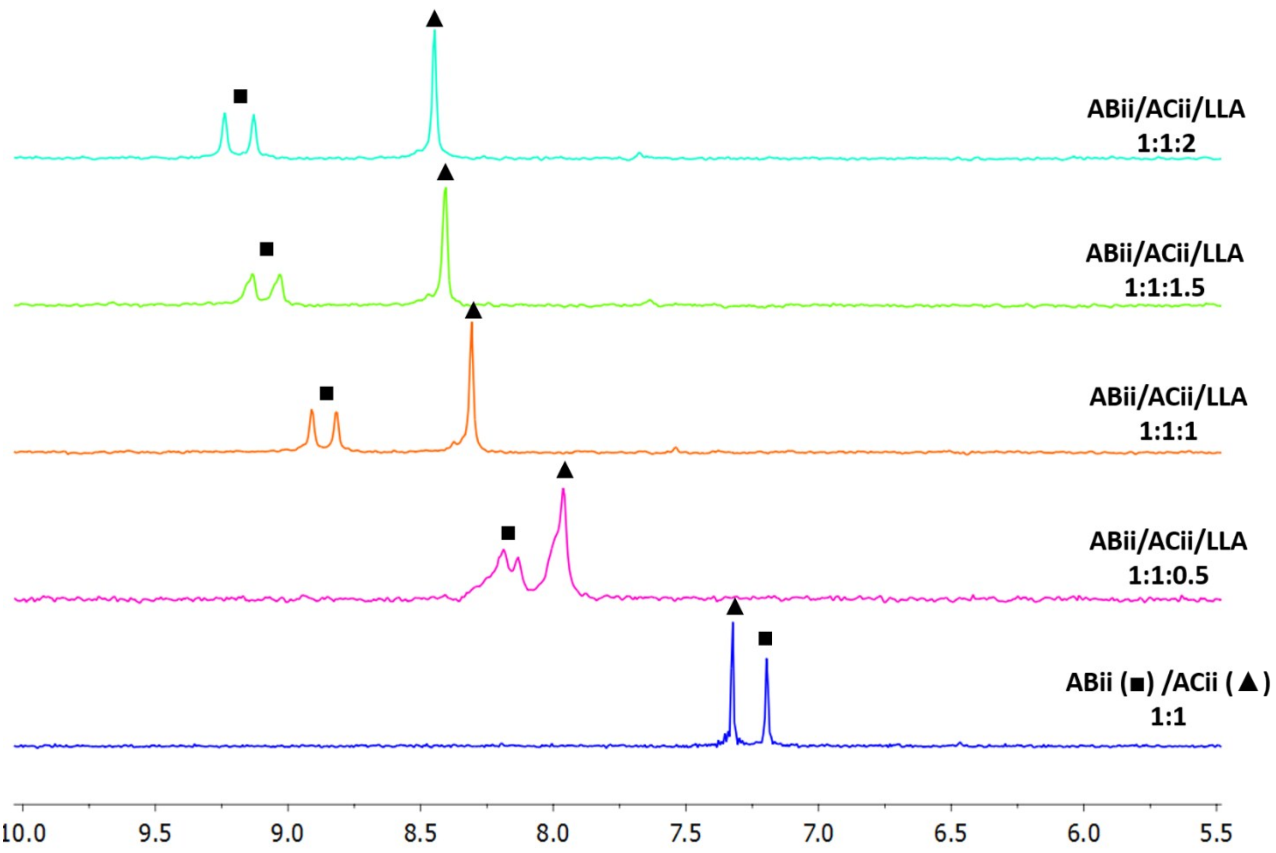


Figure S9. [31]P NMR competition titration (**ABii** vs **ACii** as hosts, LLA as guest).

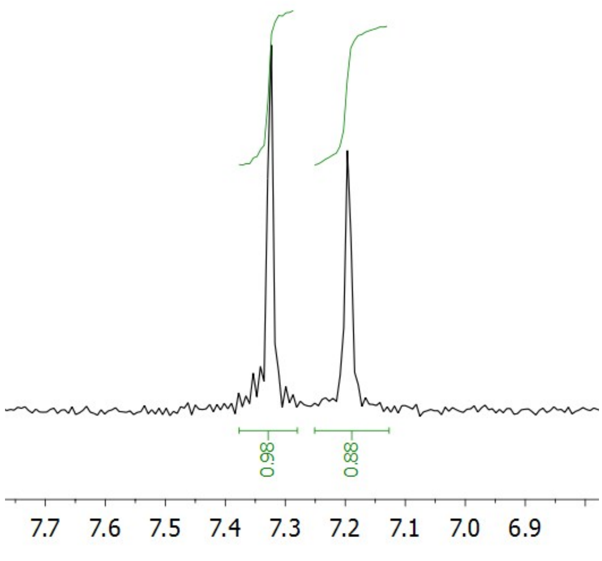


Figure S10. [31]P NMR spectrum of the **ABii/ACii** mixture at 1:1 ratio. (162 MHz, $CDCl_3$).

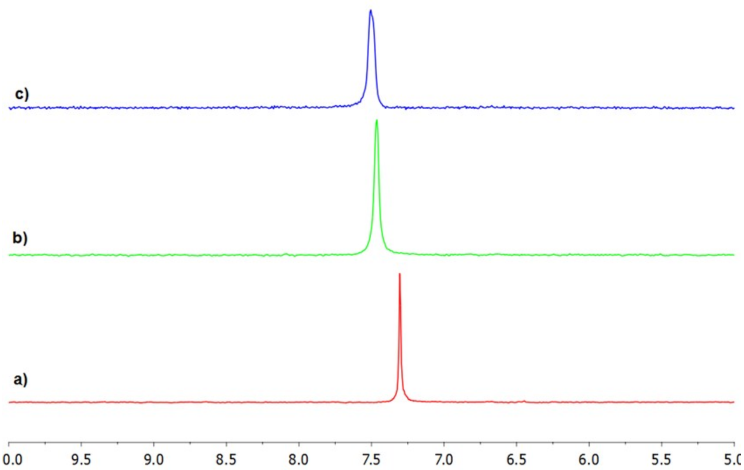


Figure S11. ^{31}P NMR competition experiment with LLA and Ethanol as competitive guest, and **ACii** as host. (162 MHz, $CDCl_3$). a) **ACii**; b) **ACii**/LLA 1:0.4. c) **ACii**/LLA/Ethanol 1:0.4:0.4.

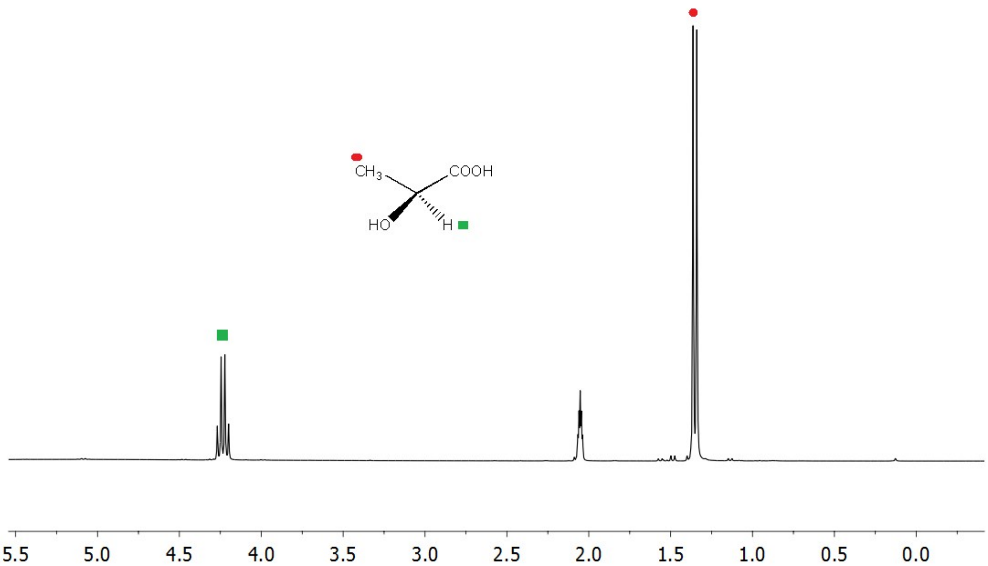


Figure S12. ^{1}H NMR spectrum of commercial L-lactic acid (300 MHz, d_6-acetone, 298K)

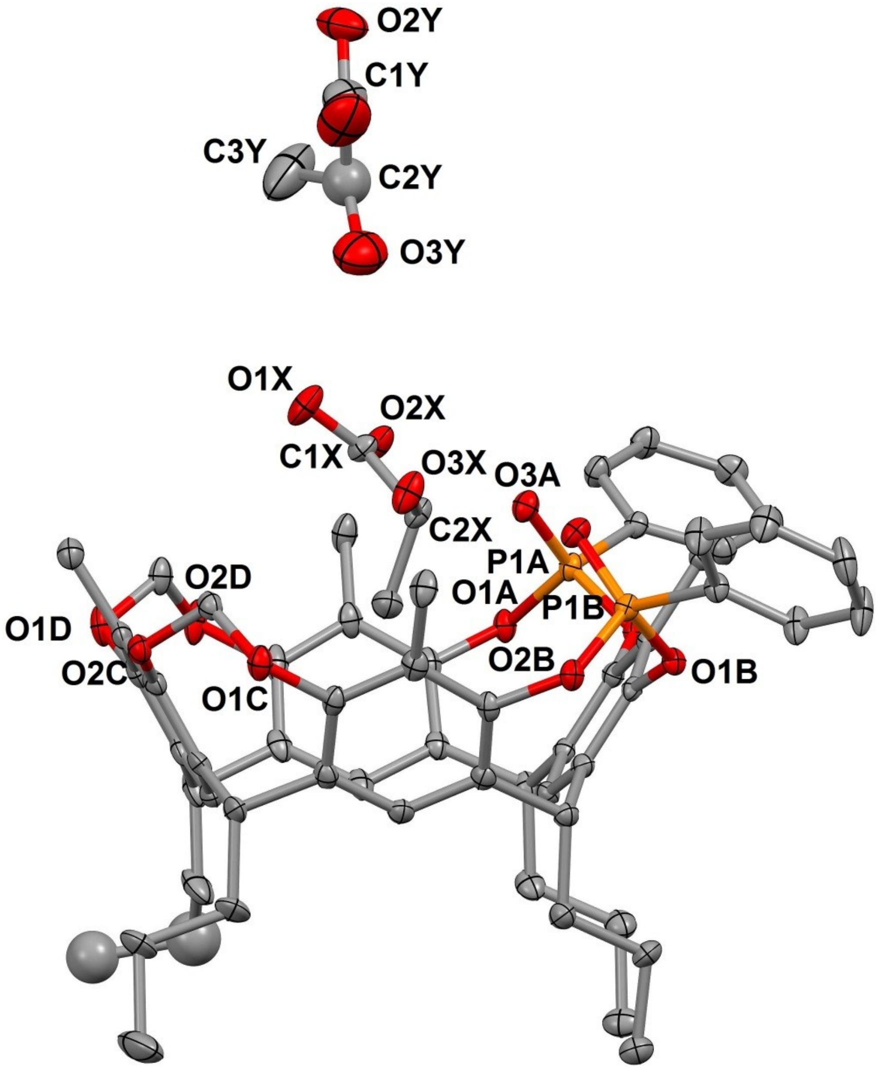


Figure S13. Ortep view (20% probability level) with partial labeling scheme of **ABii[C_3H_7, CH_3, Ph]•$C_3H_6O_6$•$C_3H_6O_6$•C_6H_{14}**. Hydrogen atoms have been omitted for clarity.

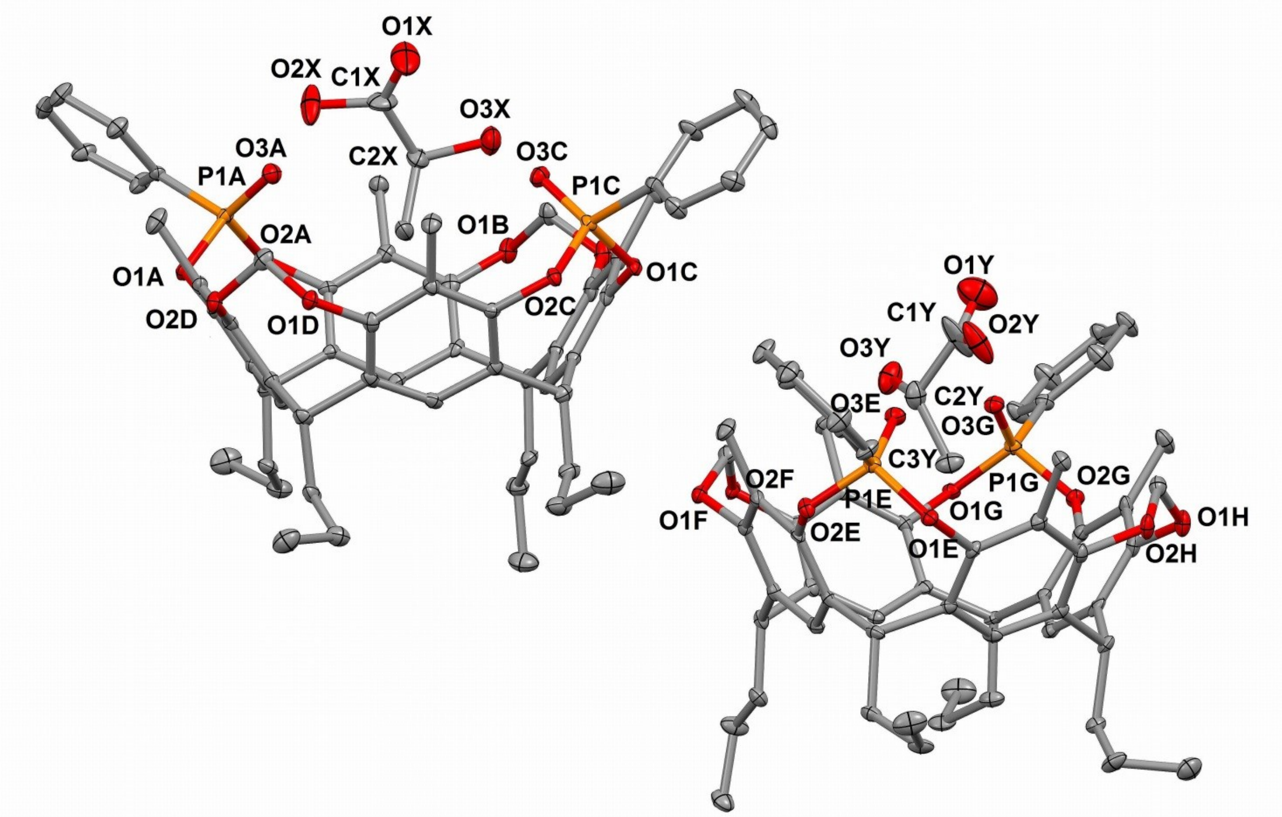


Figure S14. Ortep view (20% probability level) with partial labeling scheme of the two indipendent complexes **ACii[C_3H_7, CH_3, Ph]•$C_3H_6O_6$**. Hydrogen atoms have been omitted for clarity.

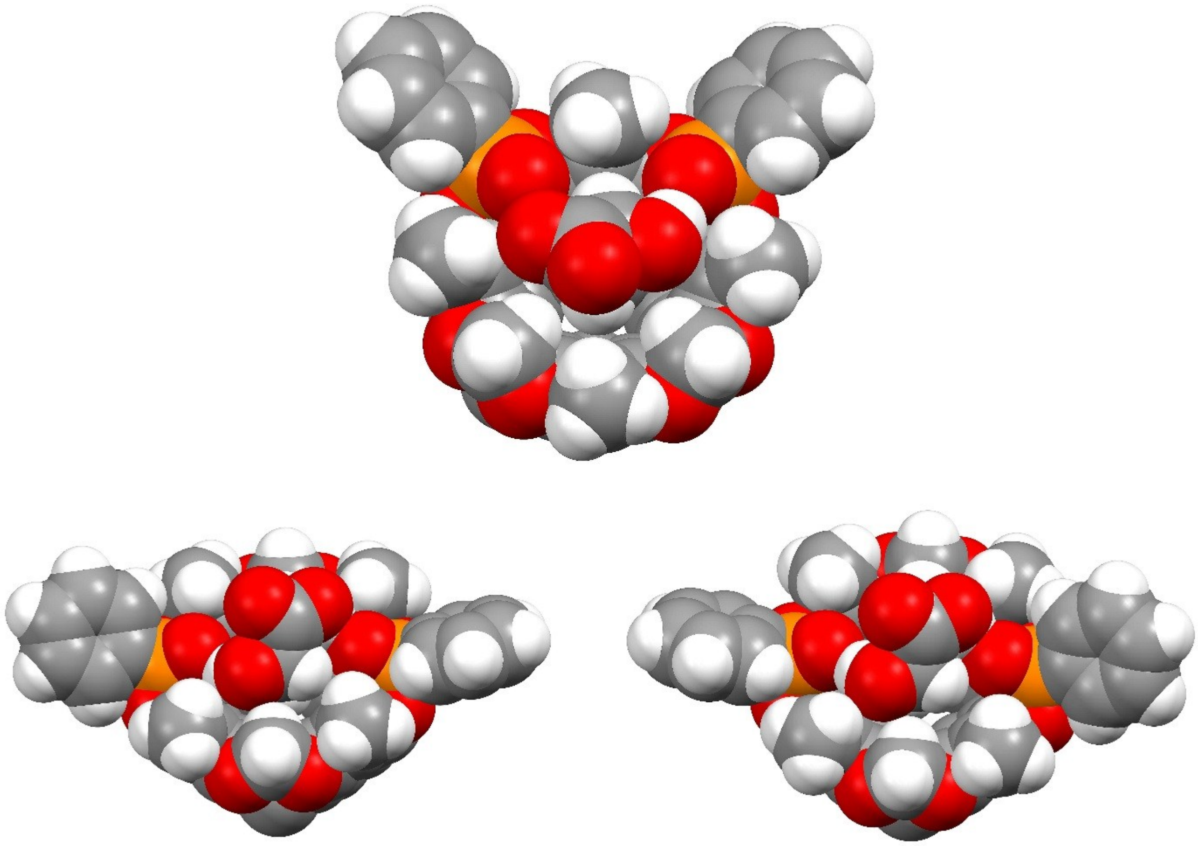
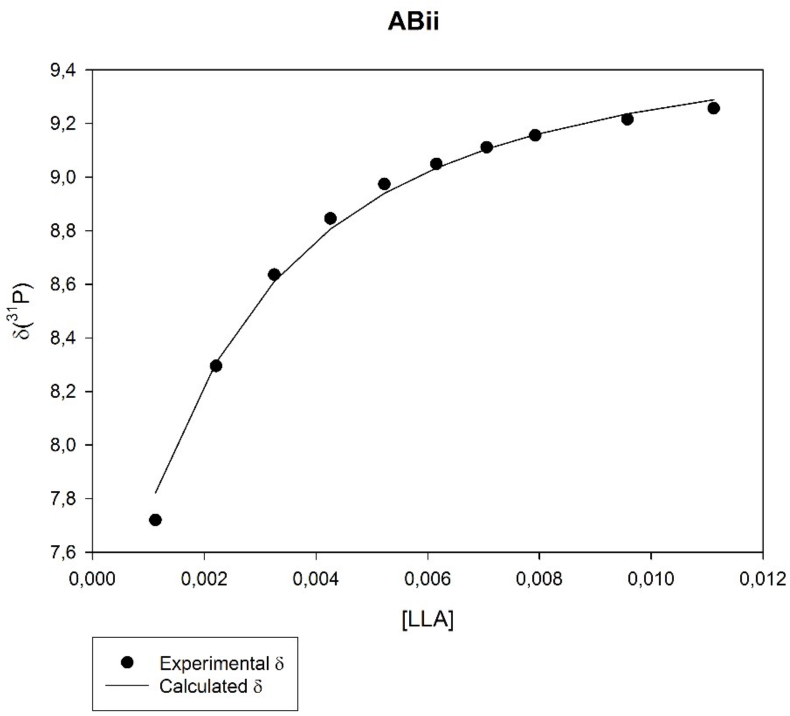


Figure S15. Space and filling view of the two complexes **LLA@ABii** (above) and **LLA@ACii** (below, both independent complexes are shown). The alkylic chains at the lower rim have been omitted for clarity. The steric hindrance provided by the frontal methylene bridges is evident for the **ACii** isomer, but it is not present for the **ABii** one.

ABii				ACii			
Preparation of the samples							
[ABii]$_0$ = 1.71 mM (0.84 mg in 500 μL of $CDCl_3$) **[LLA]$_0$ =** 57.4 mM (20.7 mg in 4.0 mL of $CDCl_3$)				**[ACii]$_0$ =** 1.51 mM (0.74 mg in 500 μL of $CDCl_3$) **[LLA]$_0$ =** 57.4 mM (20.7 mg in 4.0 mL of $CDCl_3$)			
NMR measurements							
#	**[ABii]**	**[LLA]**	**δ(^{31}P)**	**#**	**[ACii]**	**[LLA]**	**δ(^{31}P)**
0	1,71E-03	0,00E+00	7,060	0	1,51E-03	0,00E+00	7,295
1	1,68E-03	1,13E-03	7,720	1	1,48E-03	1,13E-03	7,614
2	1,65E-03	2,21E-03	8,295	2	1,45E-03	2,21E-03	7,958
3	1,62E-03	3,25E-03	8,636	3	1,42E-03	3,25E-03	8,141
4	1,59E-03	4,26E-03	8,846	4	1,40E-03	4,26E-03	8,256
5	1,56E-03	5,22E-03	8,974	5	1,37E-03	5,22E-03	8,329
6	1,53E-03	6,16E-03	9,049	6	1,35E-03	6,16E-03	8,370
7	1,50E-03	7,06E-03	9,111	7	1,32E-03	7,06E-03	8,407
8	1,48E-03	7,92E-03	9,156	8	1,30E-03	7,92E-03	8,436
9	1,43E-03	9,57E-03	9,215	9	1,28E-03	8,76E-03	8,459
10	1,38E-03	1,11E-02	9,257	10	1,26E-03	9,57E-03	8,472
				11	1,24E-03	1,04E-02	8,491
Association constant determination							
K_a = 6.74·10^2 ± 0.065 M^{-1} R^2 = 0.993				**K_a = 5.37·10^2 ± 0.065 M^{-1}** R^2 = 0.987			

Table S1. ^{31}P NMR titrations data for the determination of association constants.



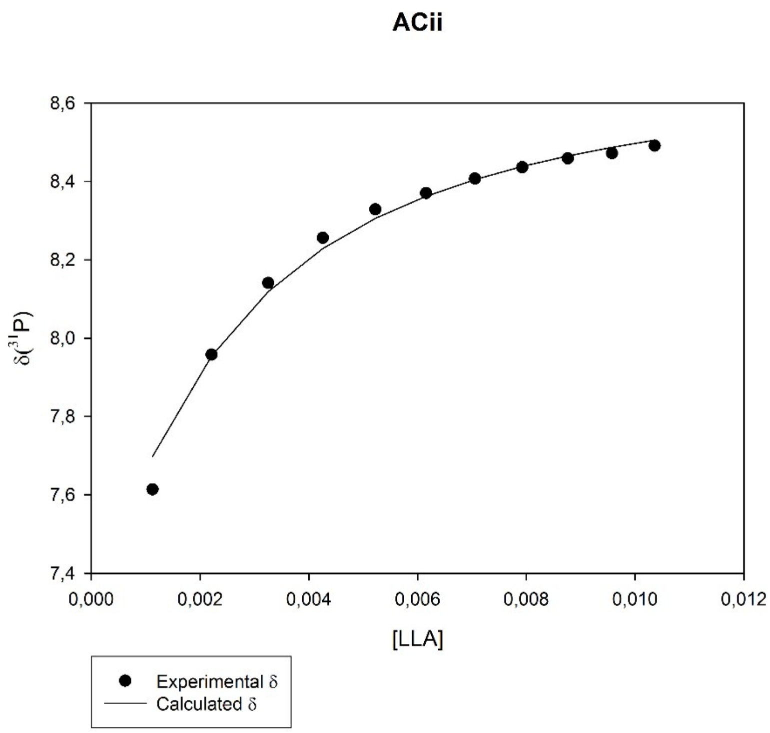


Figure S16. Fitting curves of ^{31}P NMR titrations for **ABii** (top) and **ACii** (bottom).