

Supporting Information

For

Structural dynamism of chiral sodium peraza- macrocycles complexes derived from cyclic peptoids

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List of abbreviations

DCM: dichloromethane

DIC: *N,N'*-diisopropylcarbodiimide

DIPEA: *N,N*-diisopropylethylamine

DMF: *N,N*-dimethylformamide

HFIP: 1,1,1,3,3,3-hexafluoro-2-propanol

HATU: *O*-(7-azabenzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate

RP-HPLC: reversed-phase high-performance liquid chromatography

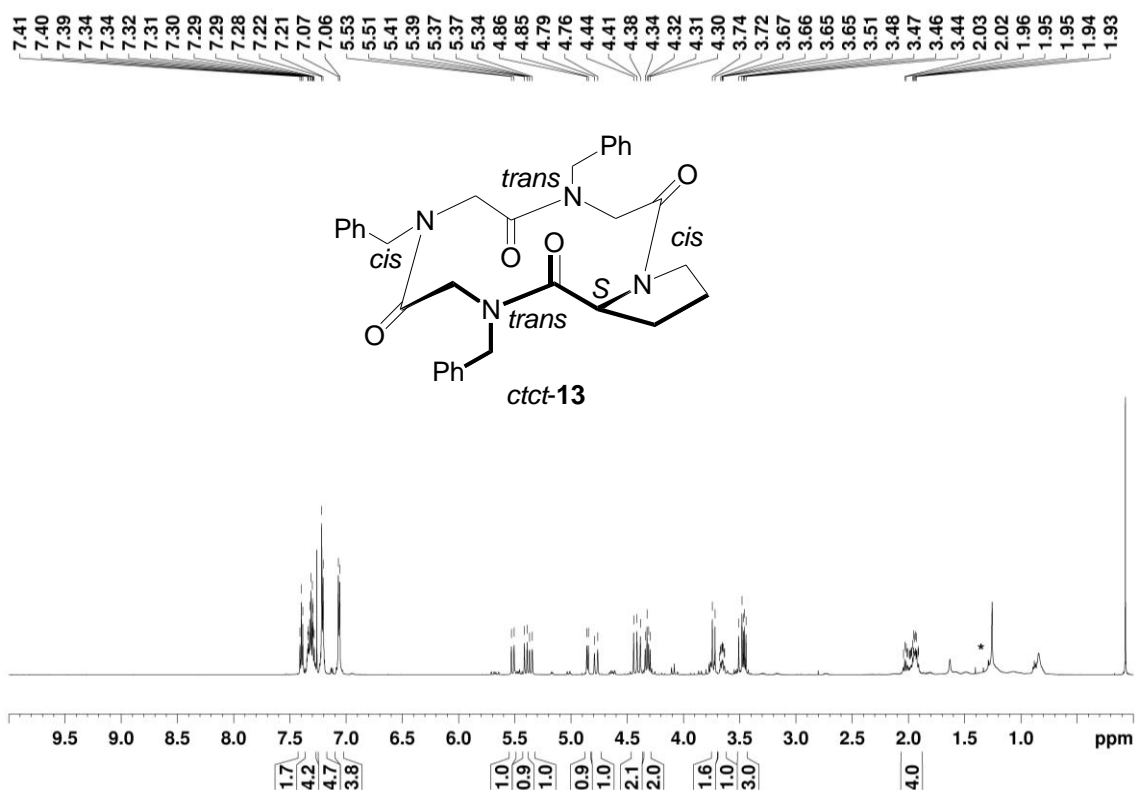
TFA: trifluoroacetic acid

TFE: 2,2,2-trifluoroethanol

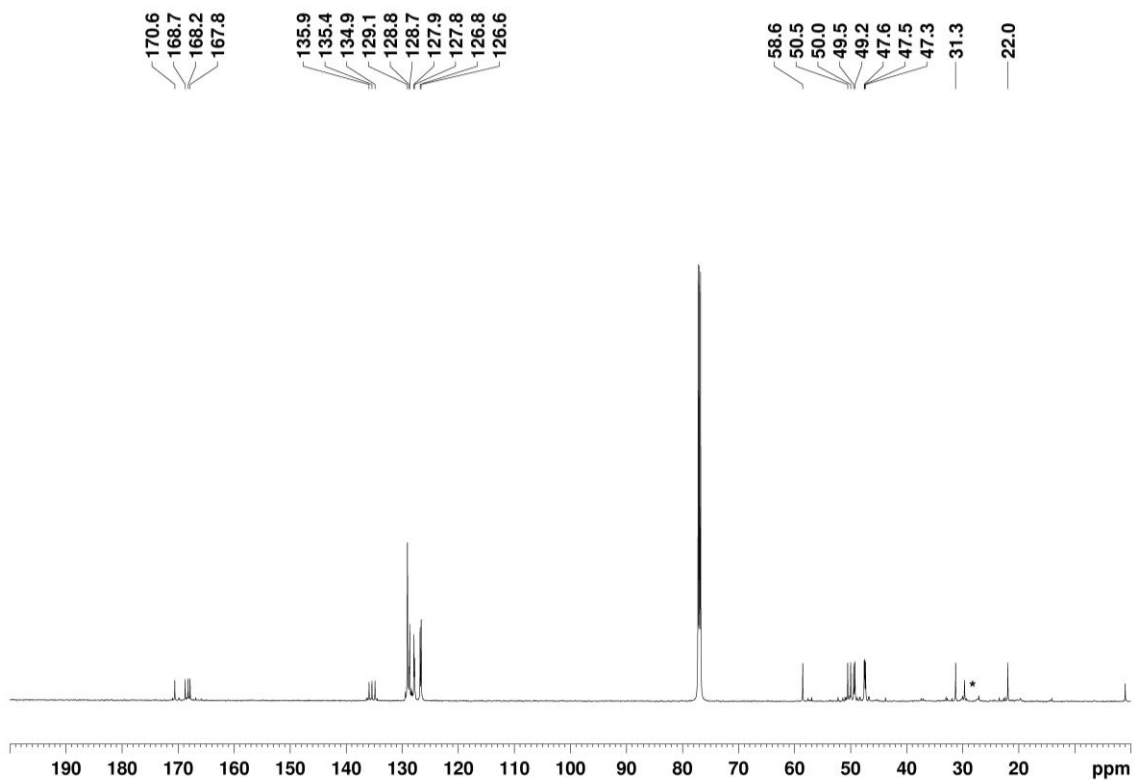
TFPB: tetrakis[3,5-bis(trifluoromethyl)phenyl]borate

1.0 ^1H -, ^{13}C NMR and two-dimensional spectra

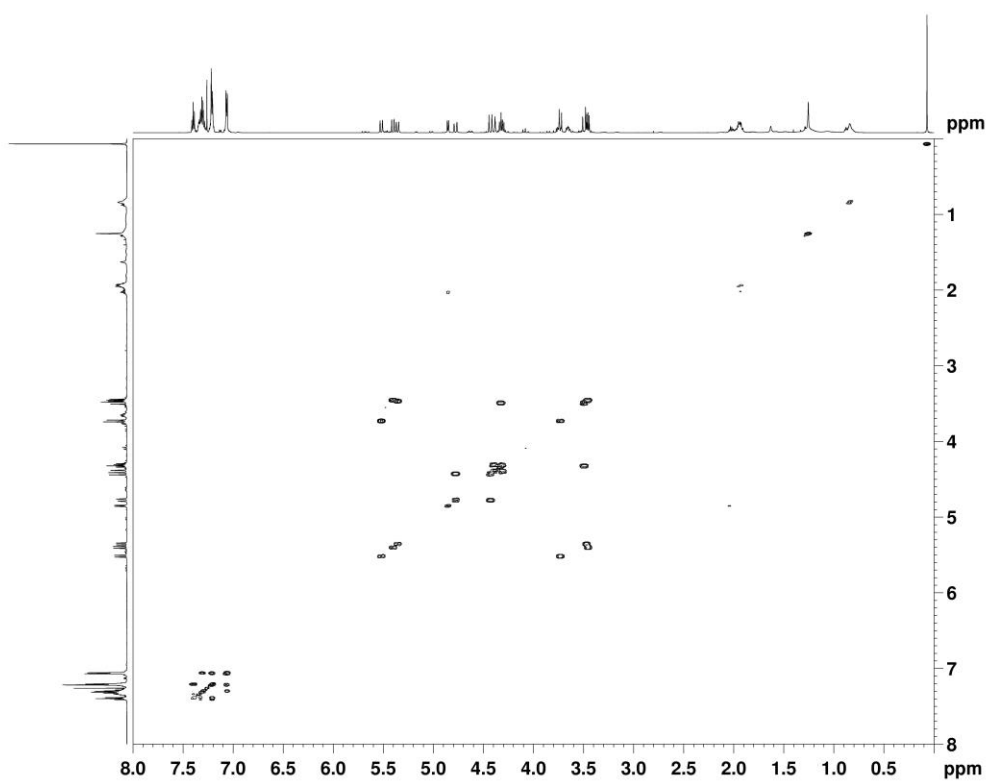
1.1 1D and 2D spectra of cyclic derivatives and their metal complexes



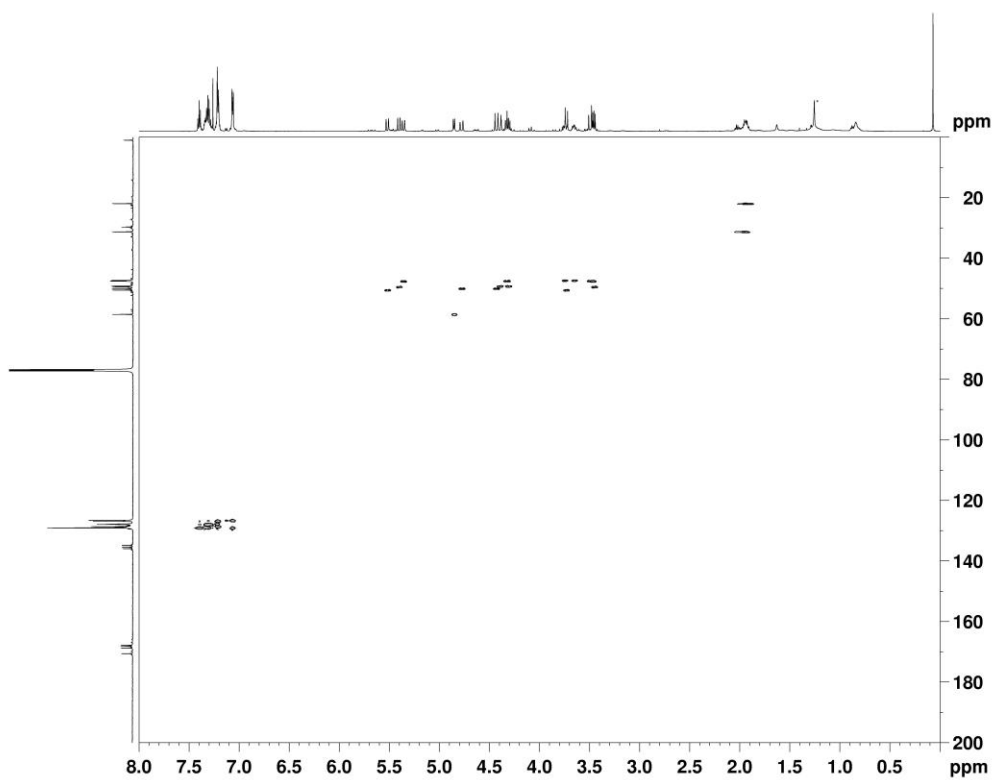
13: ^1H NMR (600 MHz, CDCl_3). Grease impurity labelled with an asterisk.



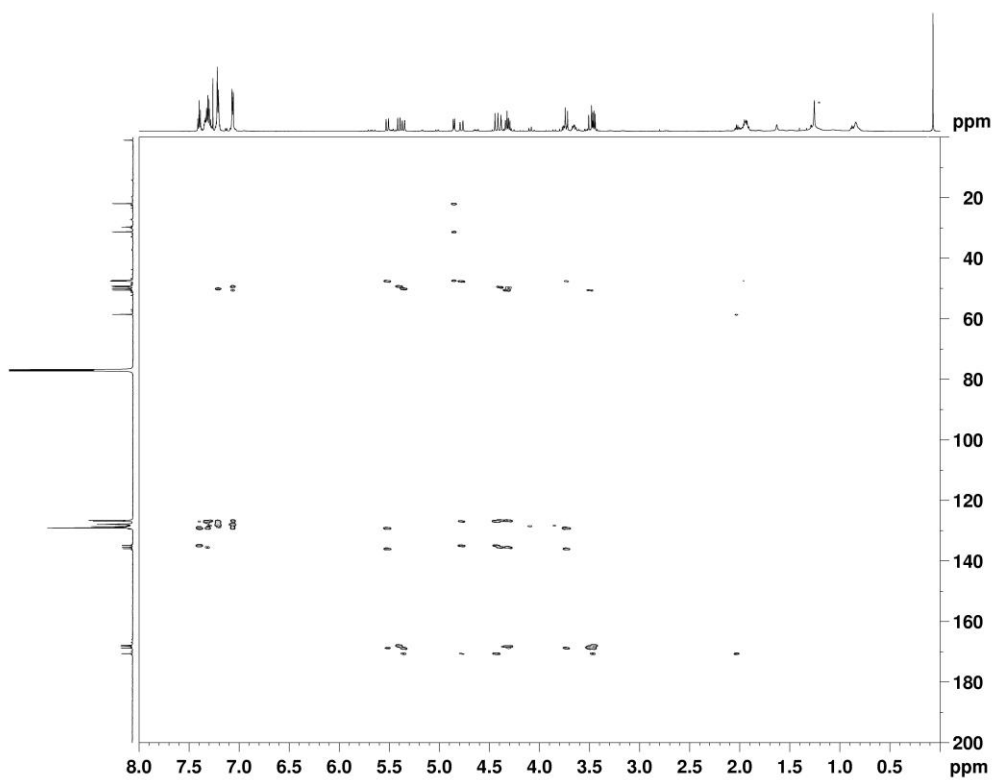
13: ^{13}C NMR (150 MHz, CDCl_3). Grease impurity labelled with an asterisk.



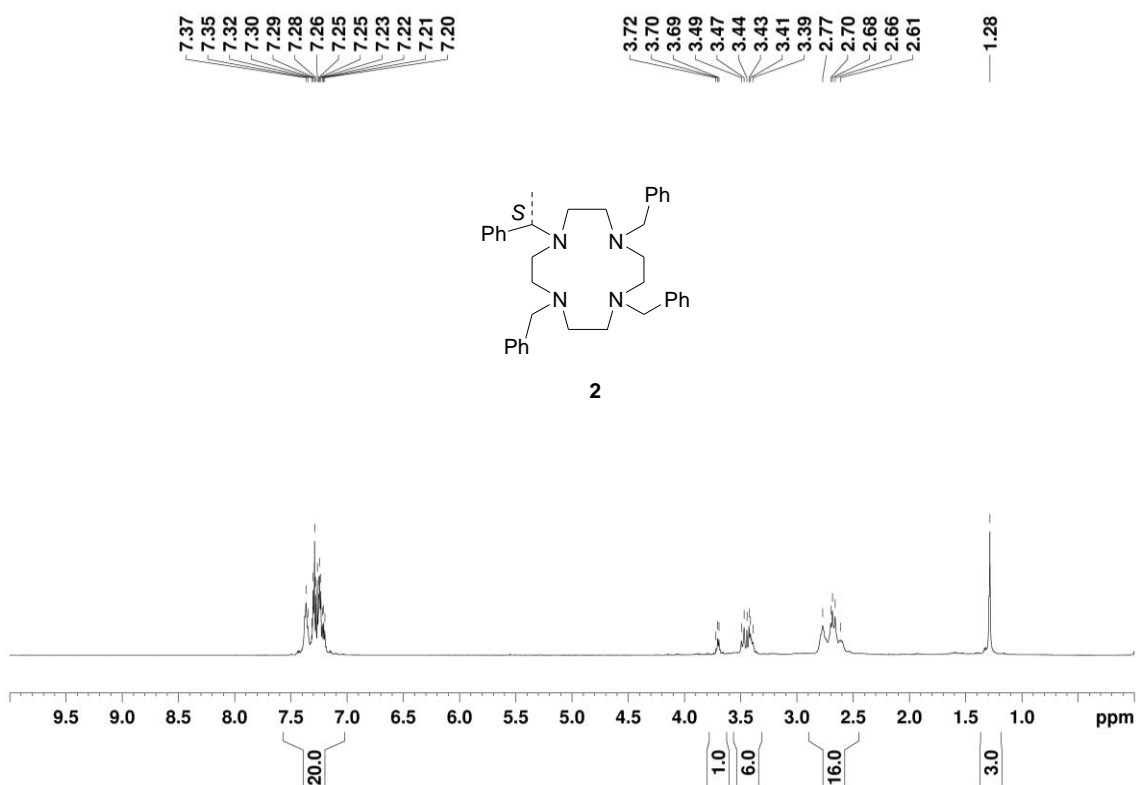
13: COSY NMR (600 MHz, CDCl₃)



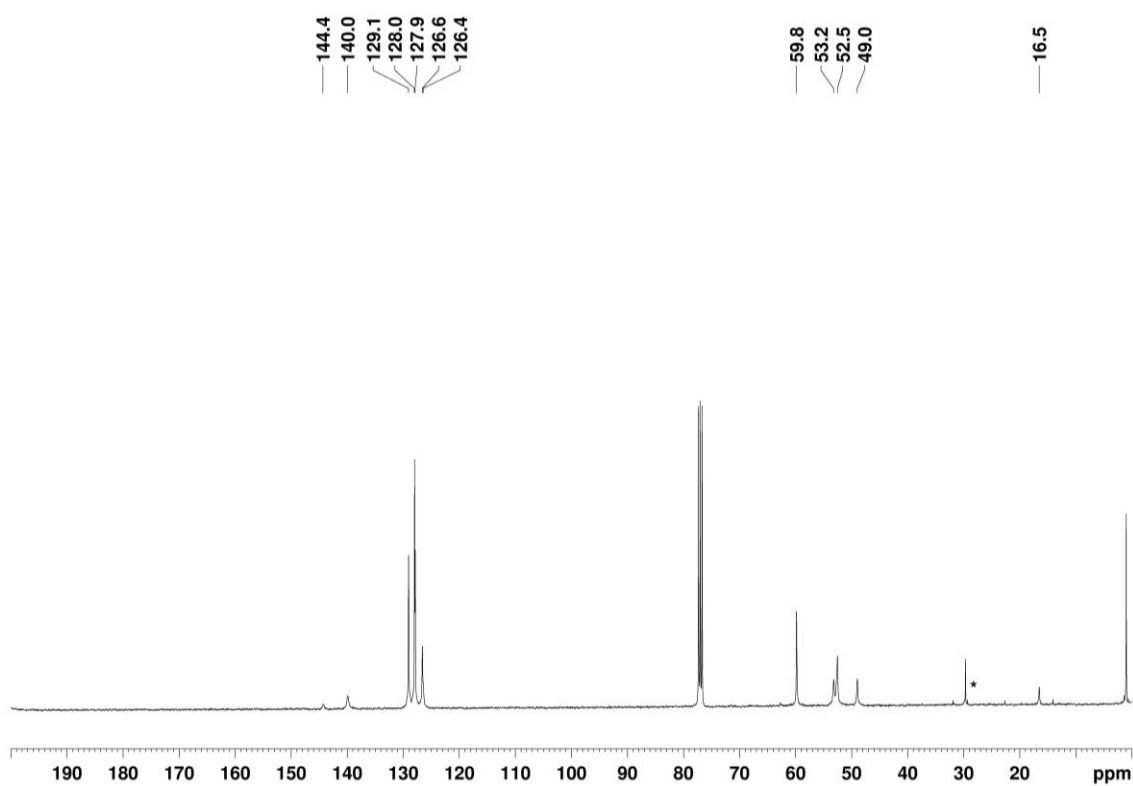
13: HSQC NMR (600 MHz, CDCl₃). Grease impurity labelled with an asterisk.



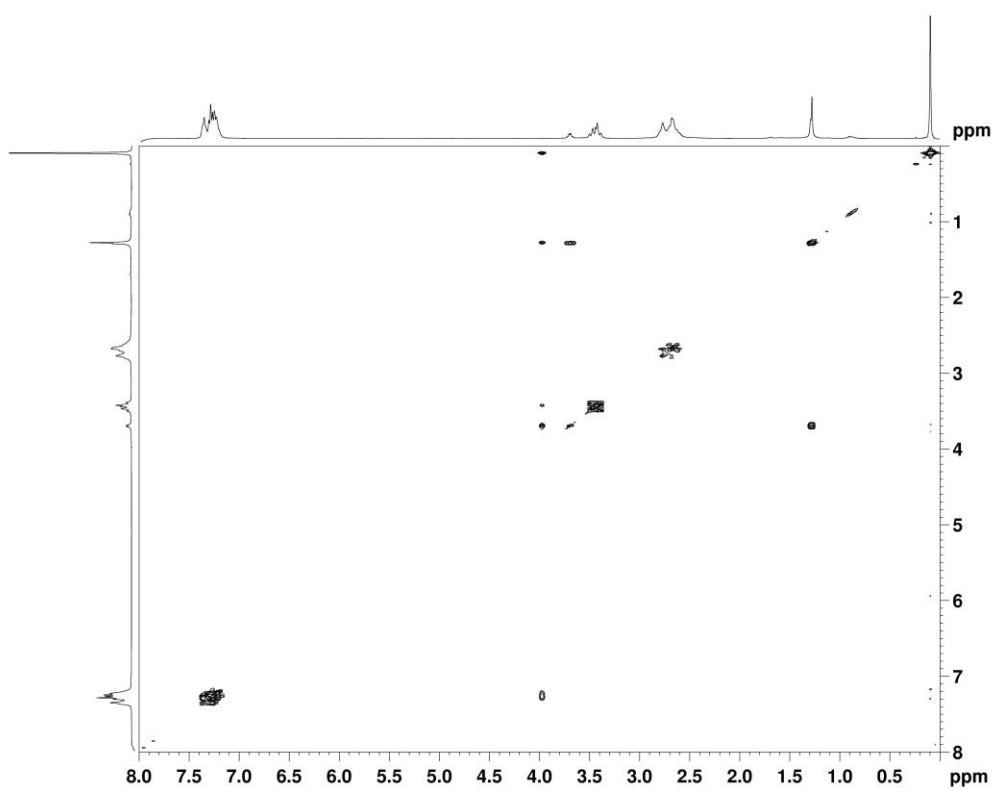
13: HMBC NMR (600 MHz, CDCl_3). Grease impurity labelled with an asterisk.



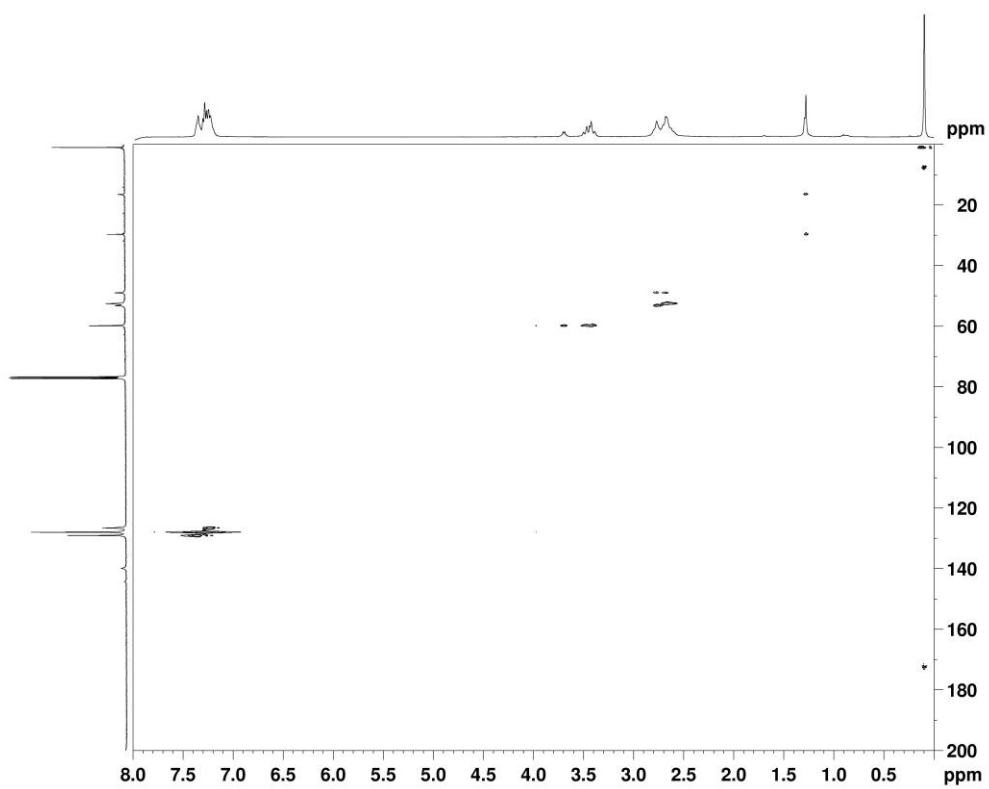
2: ^1H NMR (600 MHz, CDCl_3). Grease at 1.29 overlap with the doublet at 1.28 ppm.



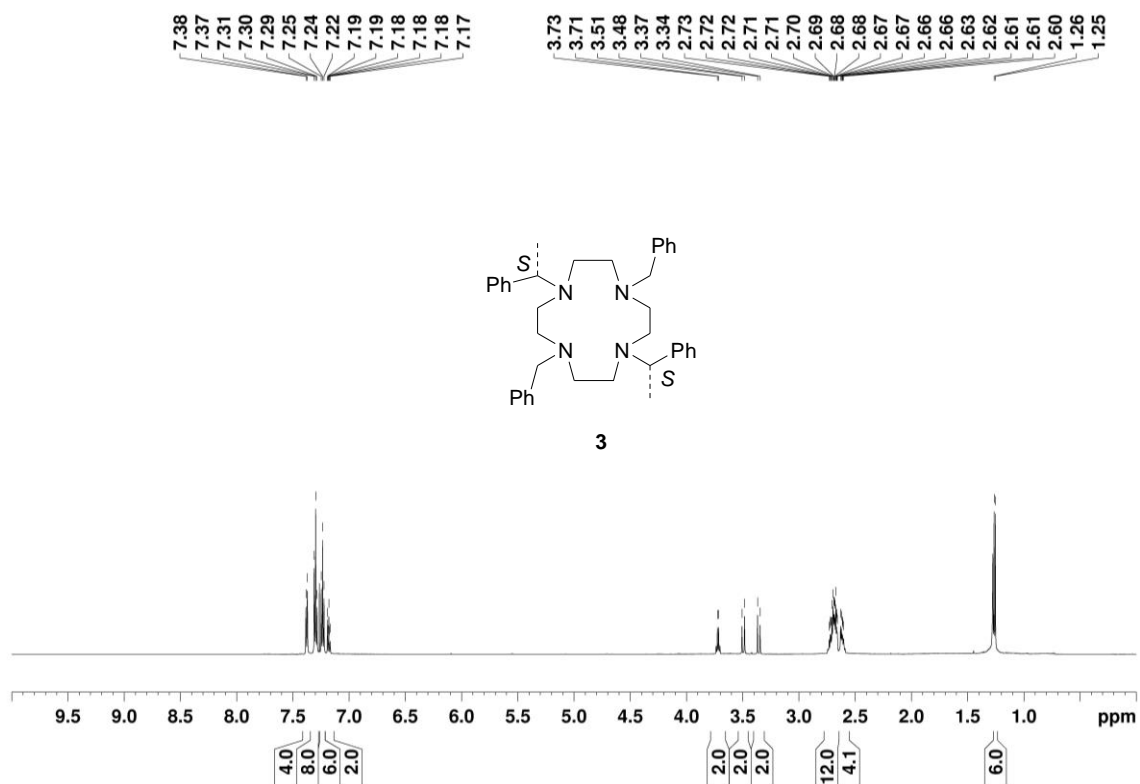
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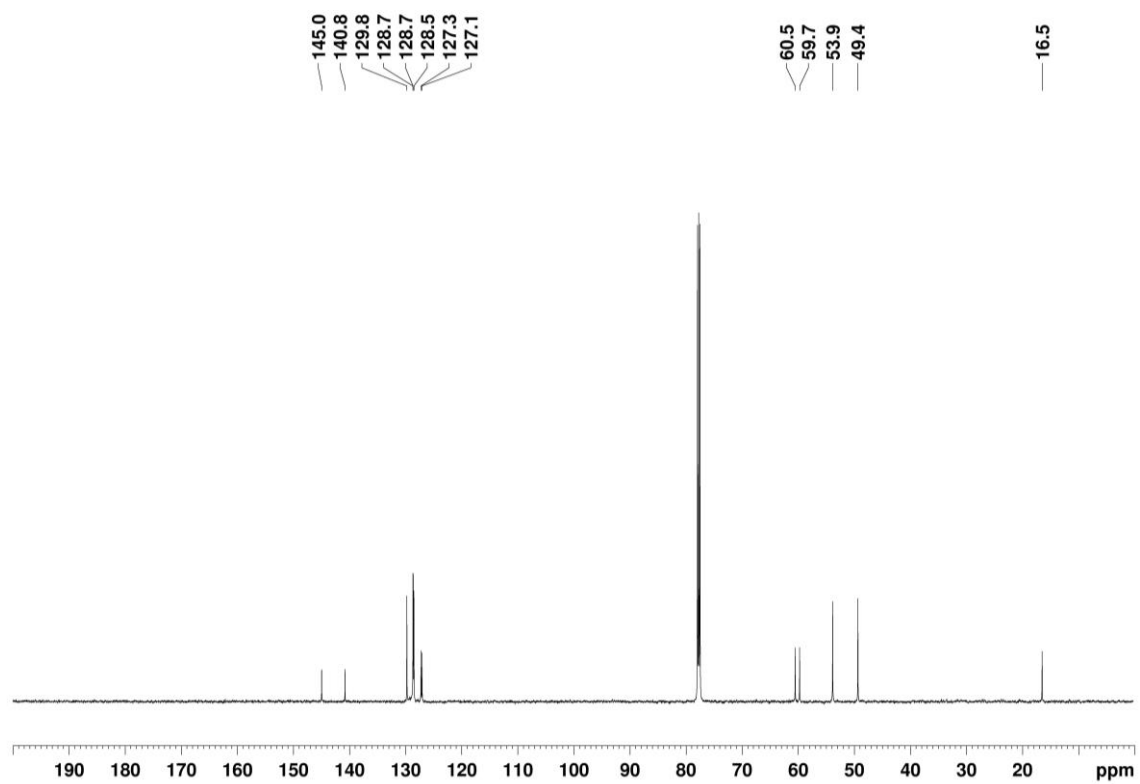
2: COSY NMR (400 MHz, CDCl₃)



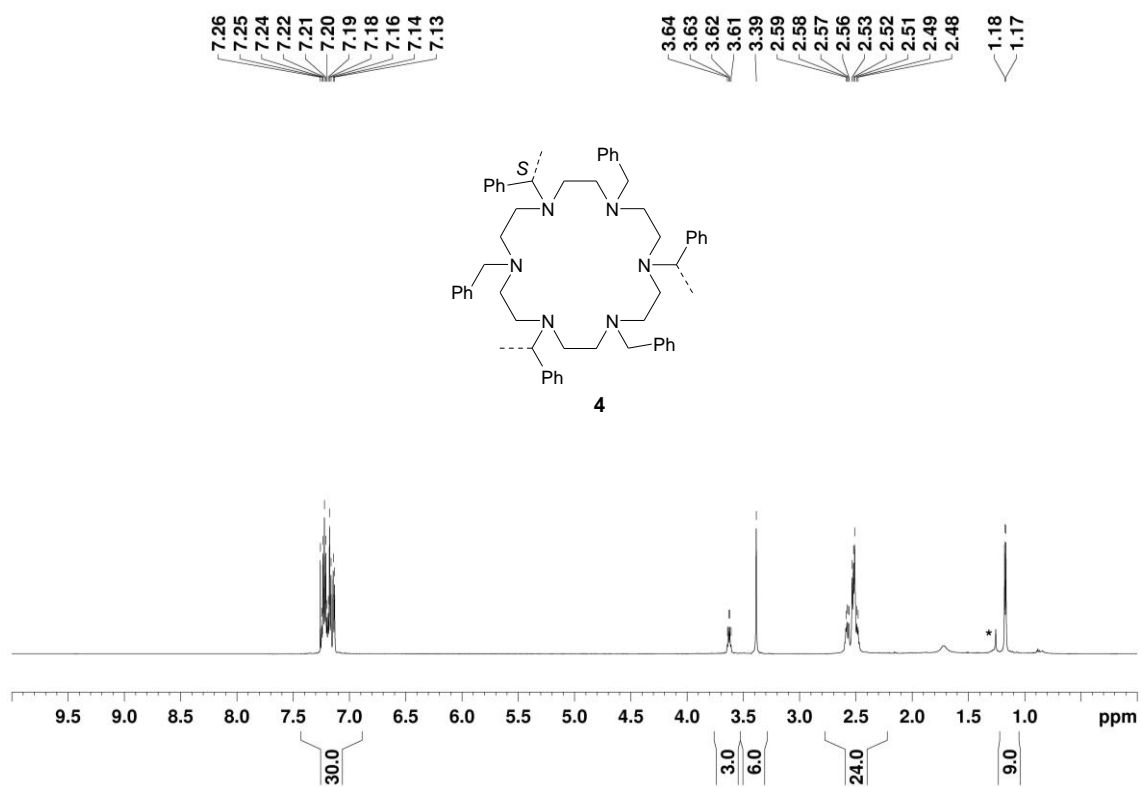
2: HSQC NMR (400 MHz, CDCl_3)



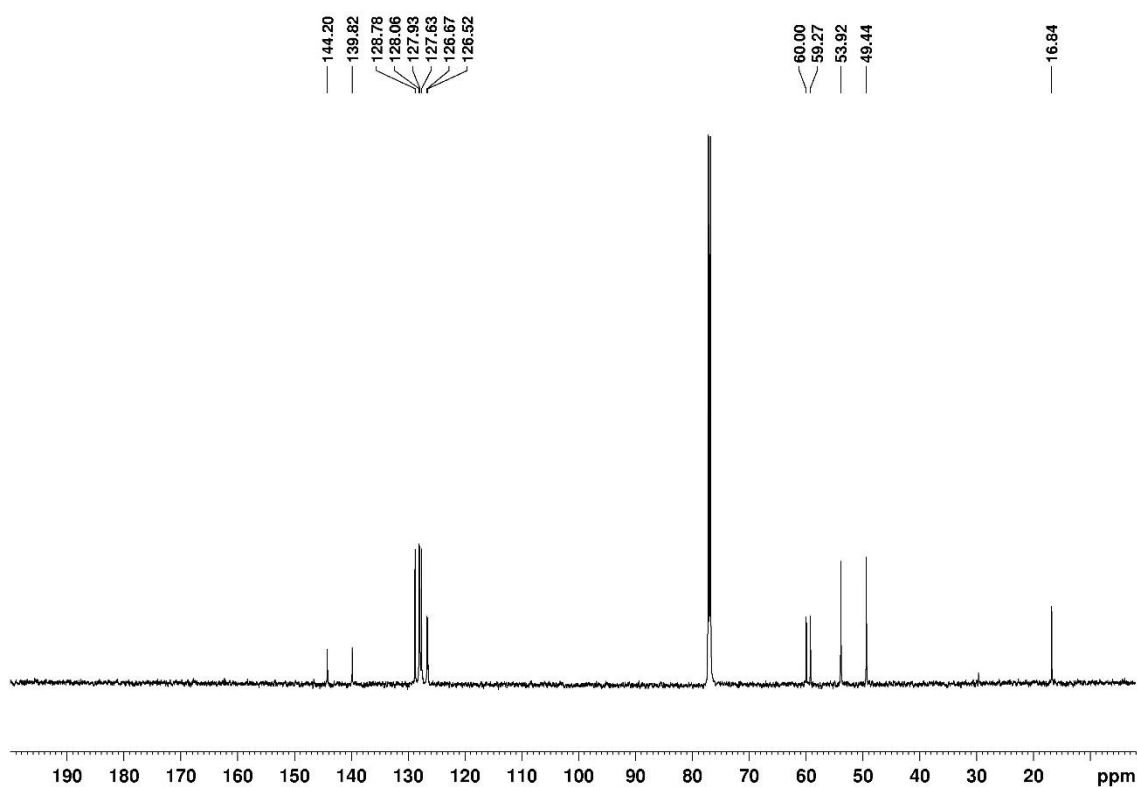
3: ^1H NMR (600 MHz, CDCl_3)



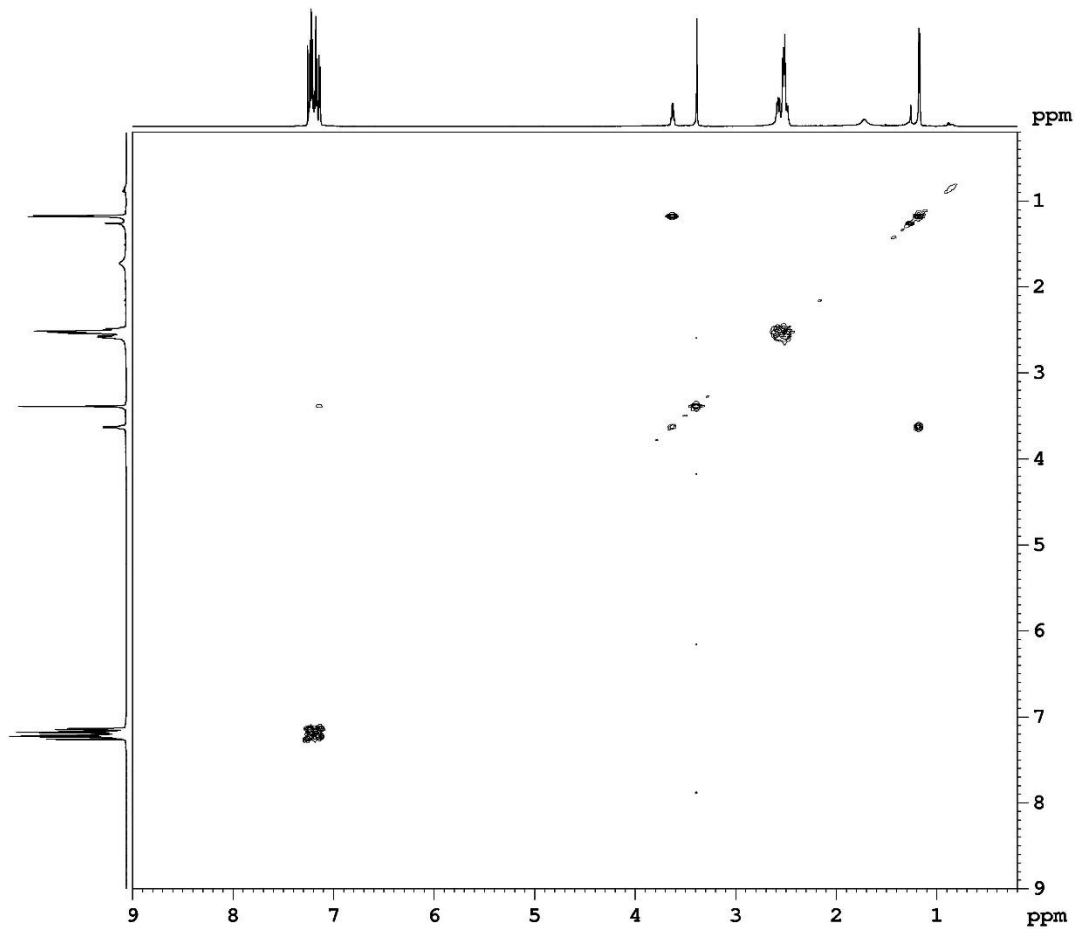
3: ^{13}C NMR (150 MHz, CDCl_3). Grease impurity labelled with an asterisk.



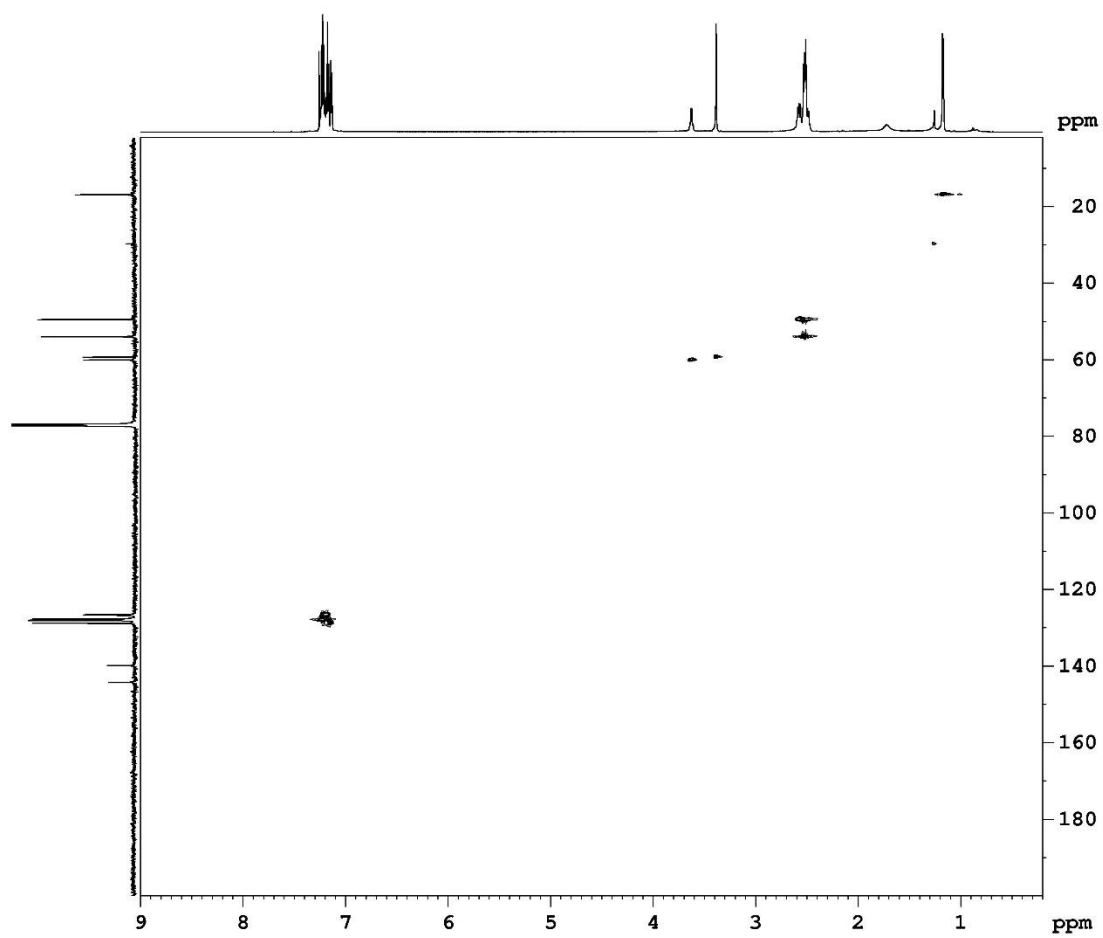
4: ¹H NMR (600 MHz, CDCl₃). Grease impurity labelled with an asterisk.



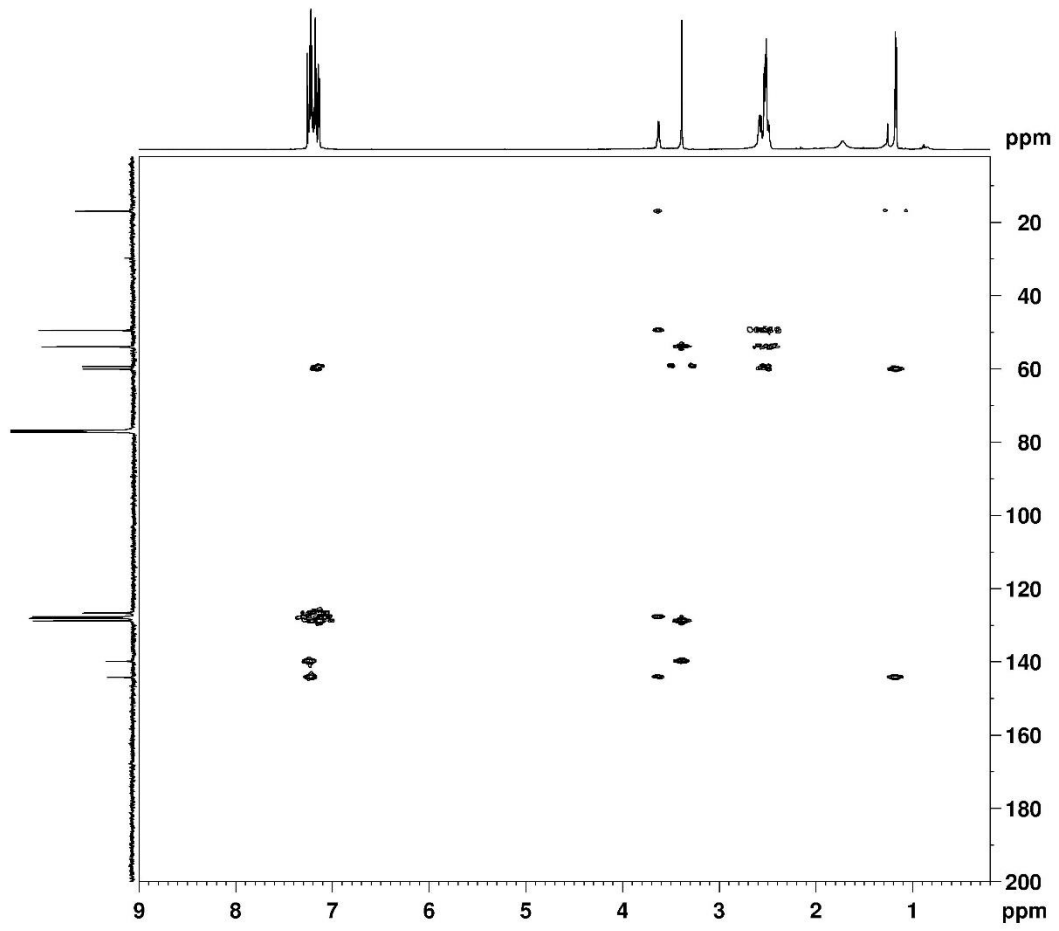
4: ¹³C NMR (150 MHz, CDCl₃)



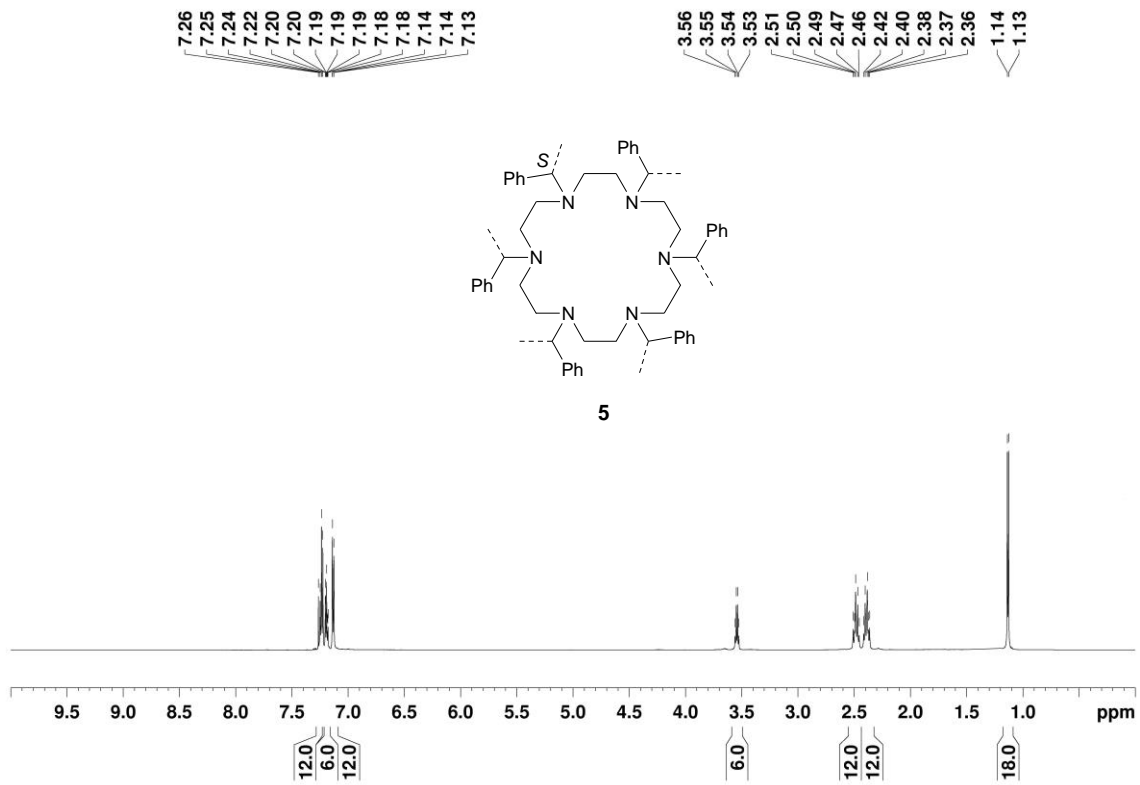
4: COSY NMR (600 MHz, CDCl₃)



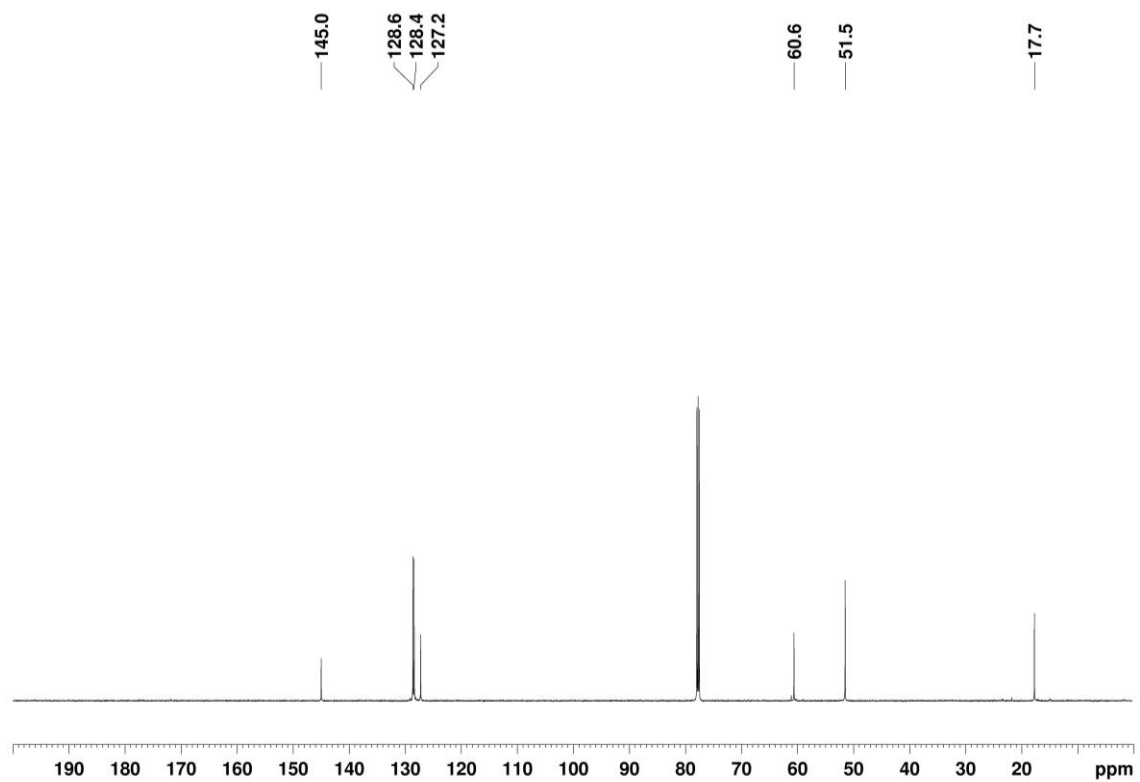
4: HSQC NMR (600 MHz, CDCl_3)



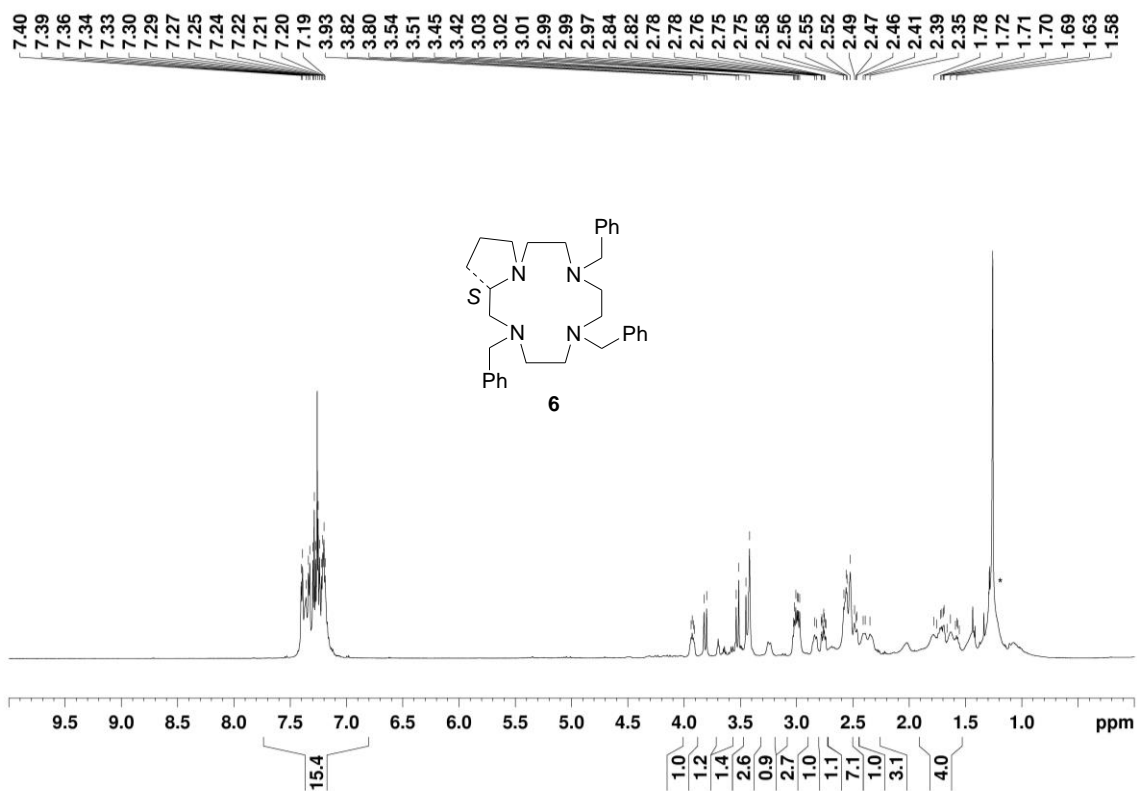
4: HMBC NMR (600 MHz, CDCl₃)



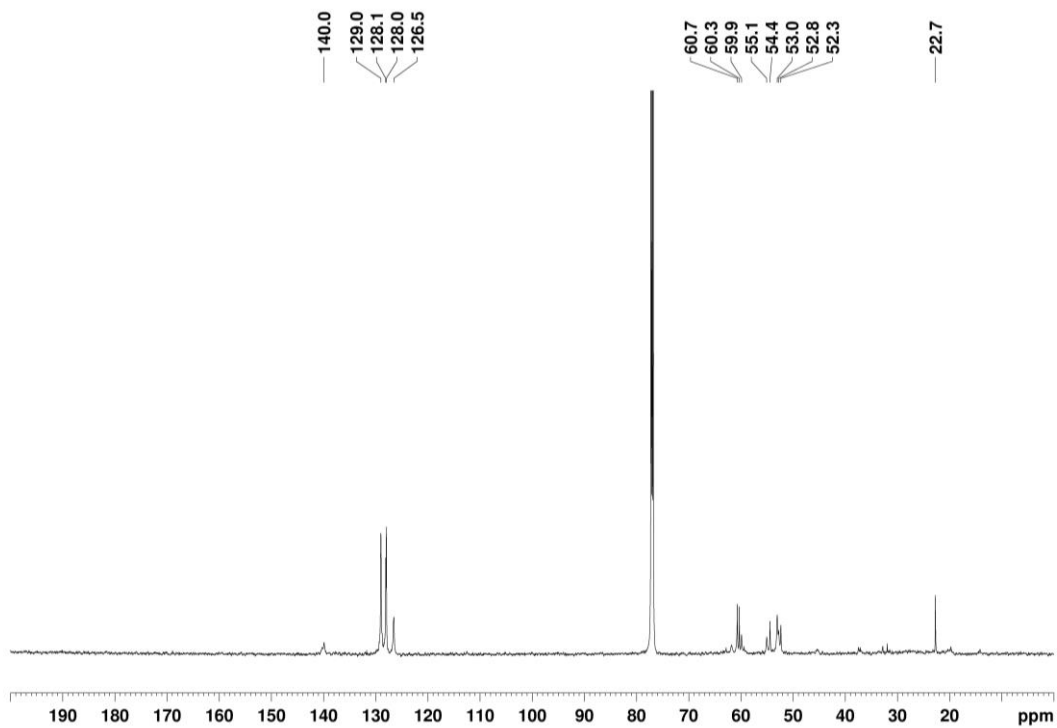
5: ^1H NMR (600 MHz, CDCl_3)



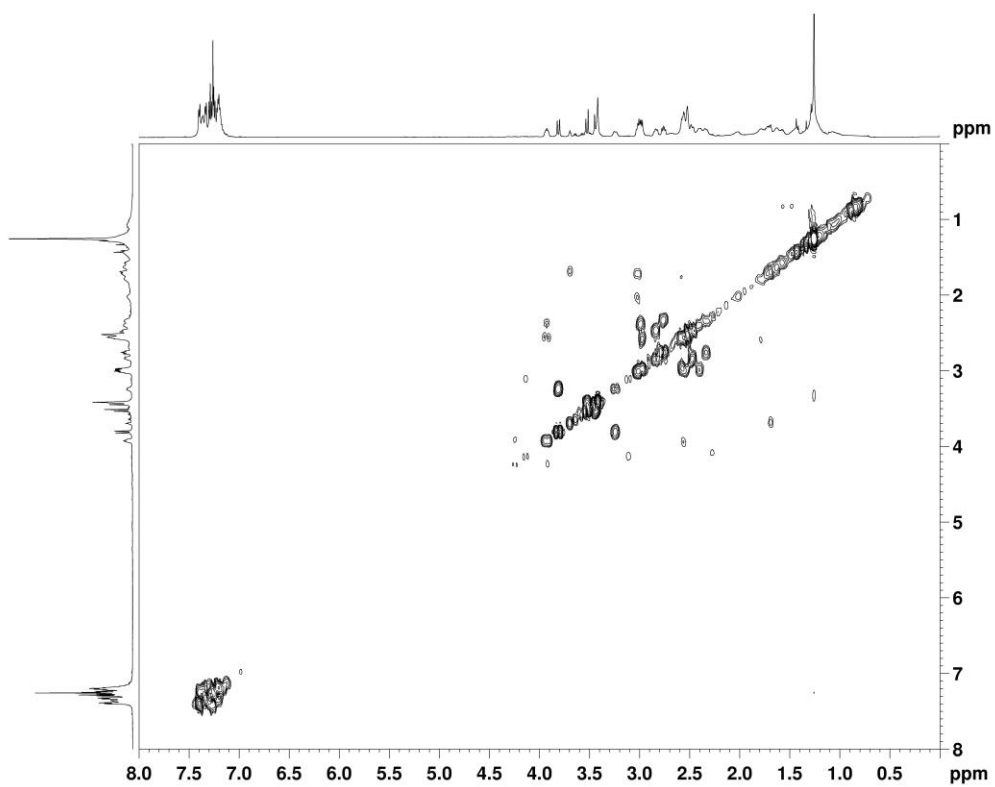
5: ^{13}C NMR (150 MHz, CDCl_3)



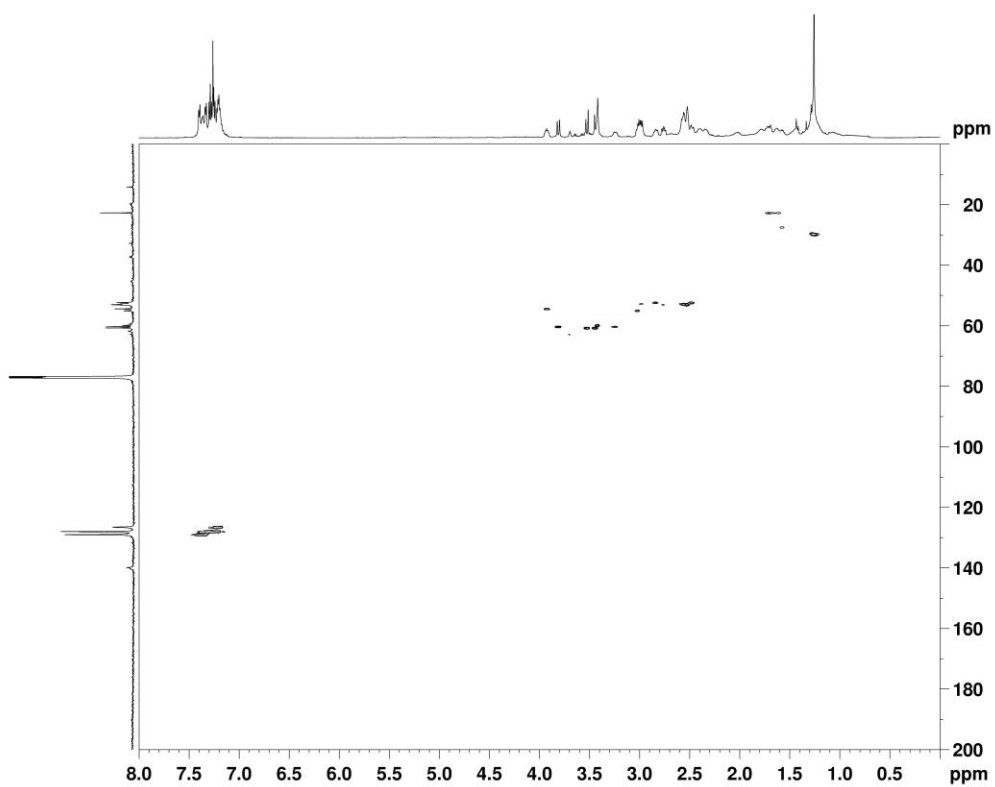
6: ^1H NMR (600 MHz, CDCl_3). Grease impurity labelled with an asterisk.



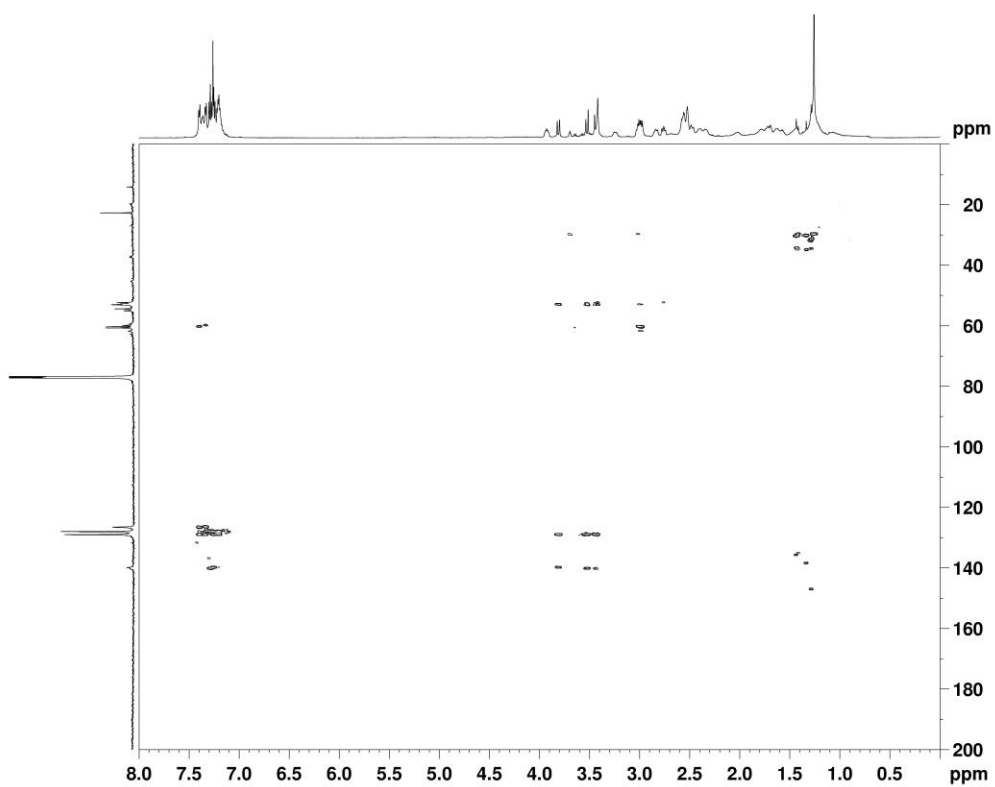
6: ^{13}C NMR (150 MHz, CDCl_3)



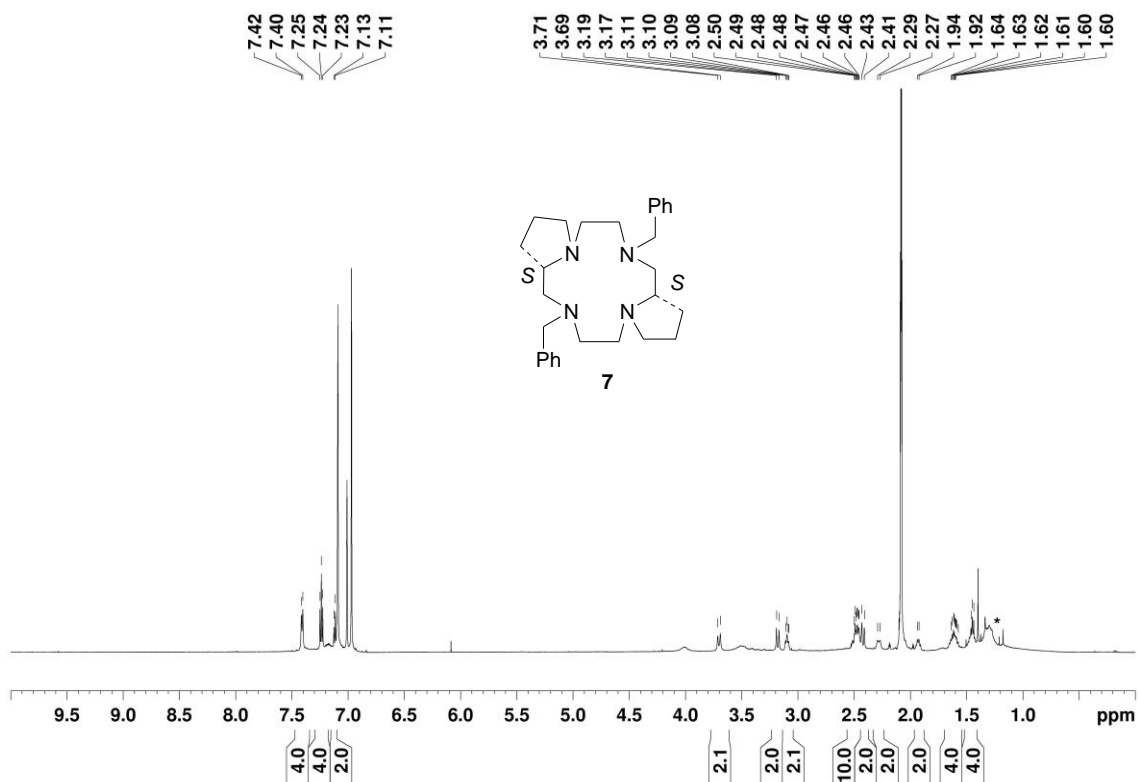
6: COSY NMR (600 MHz, CDCl₃)



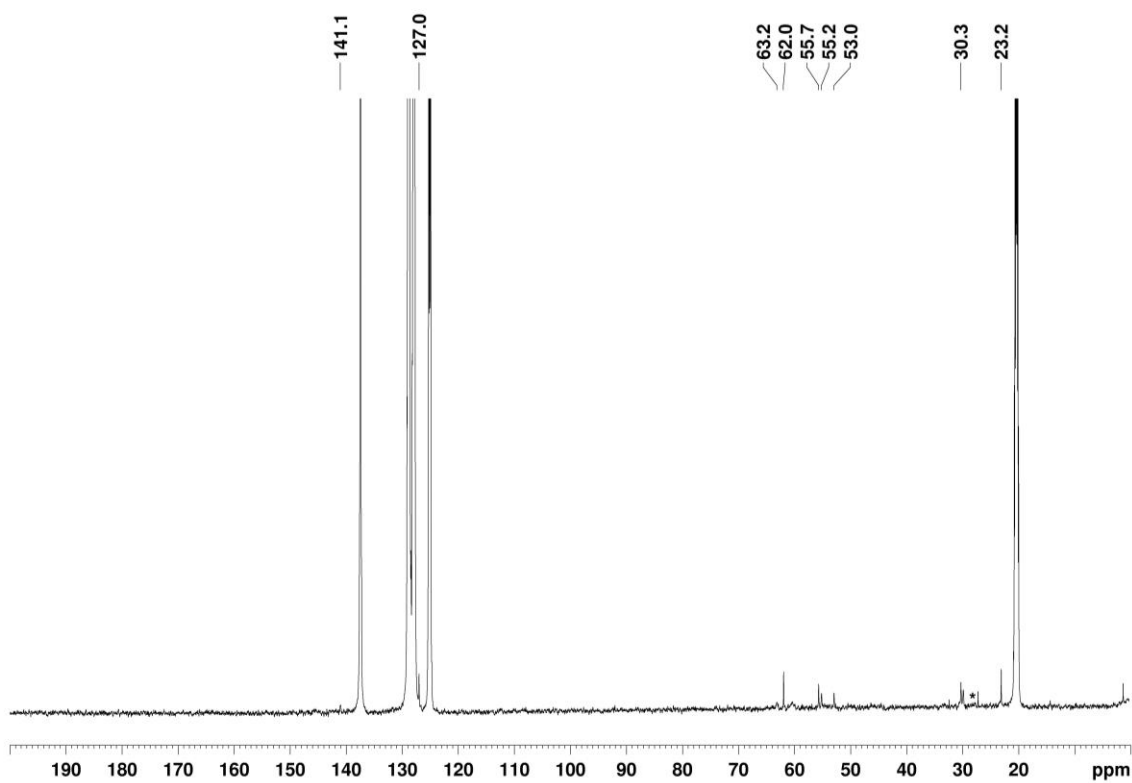
6: HSQC NMR (600 MHz, CDCl₃)



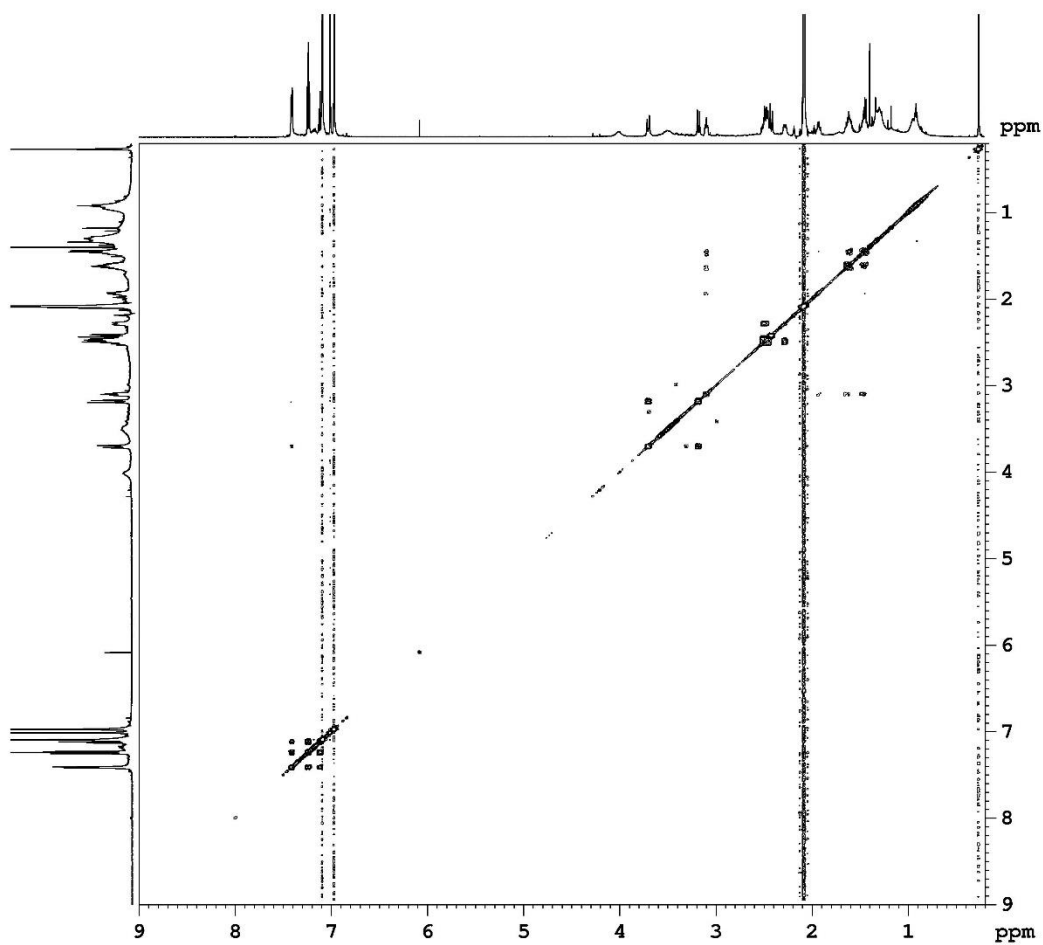
6: HMBC NMR (600 MHz, CDCl₃)



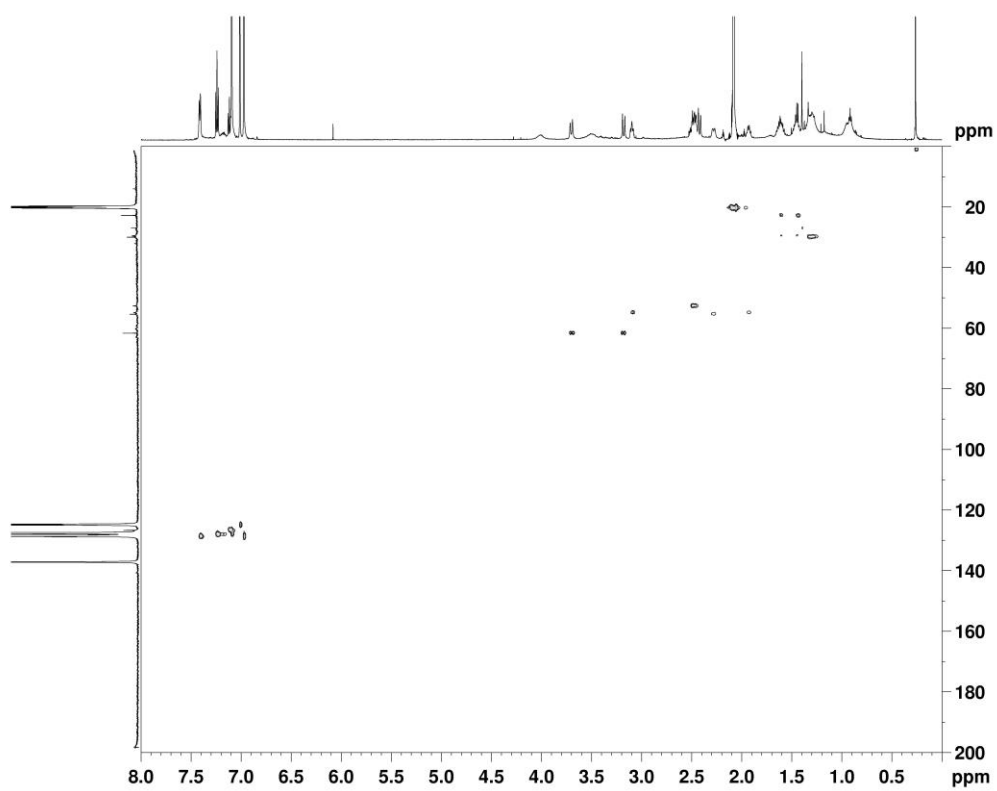
7: ¹H NMR (600 MHz, C₆D₅CD₃)



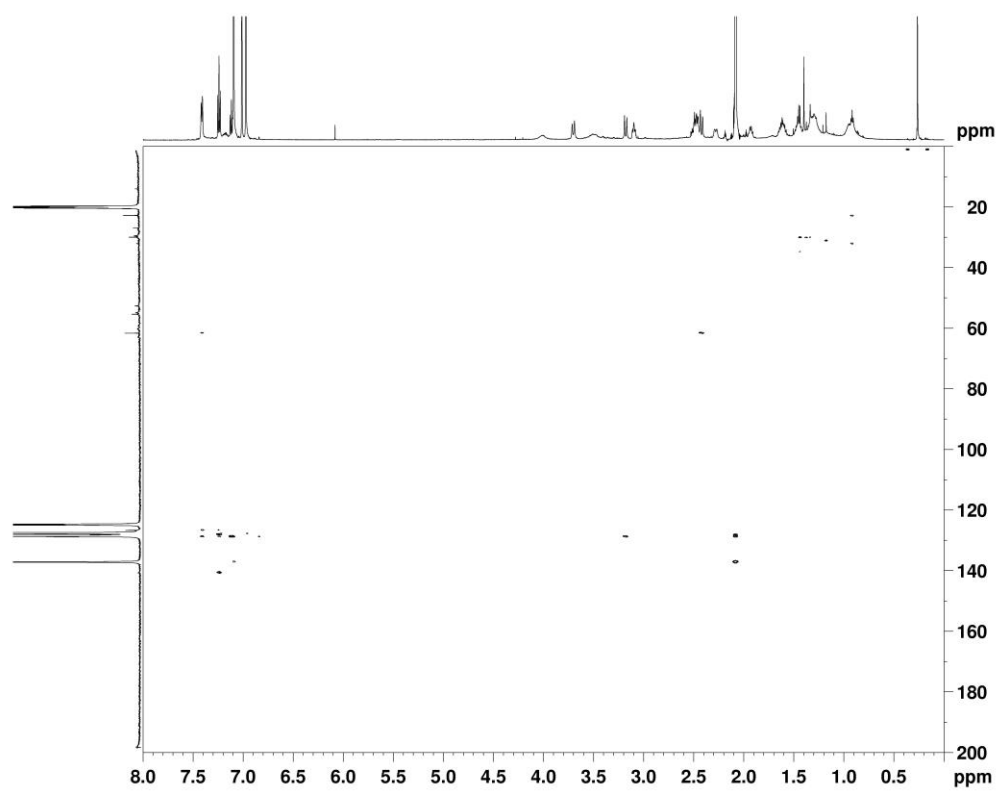
7: ¹³C NMR (150 MHz, C₆D₅CD₃). Impurities labelled with an asterisk.



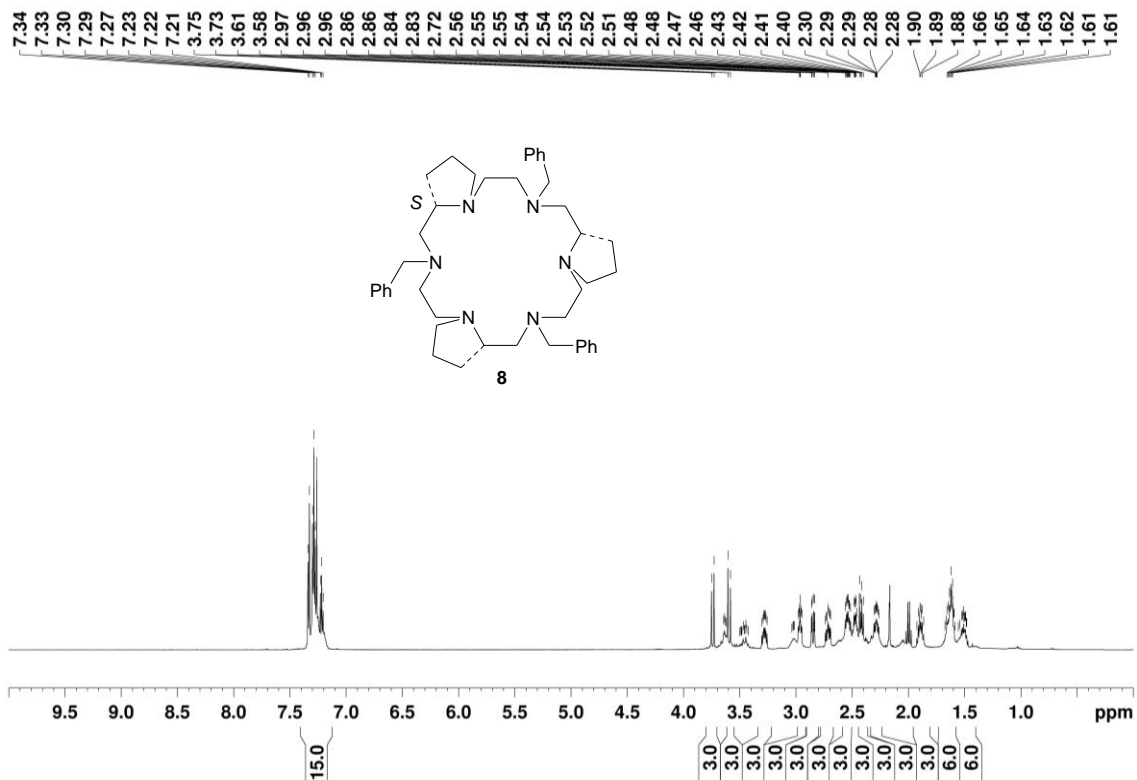
7: COSY NMR (600 MHz, C₆D₅CD₃)



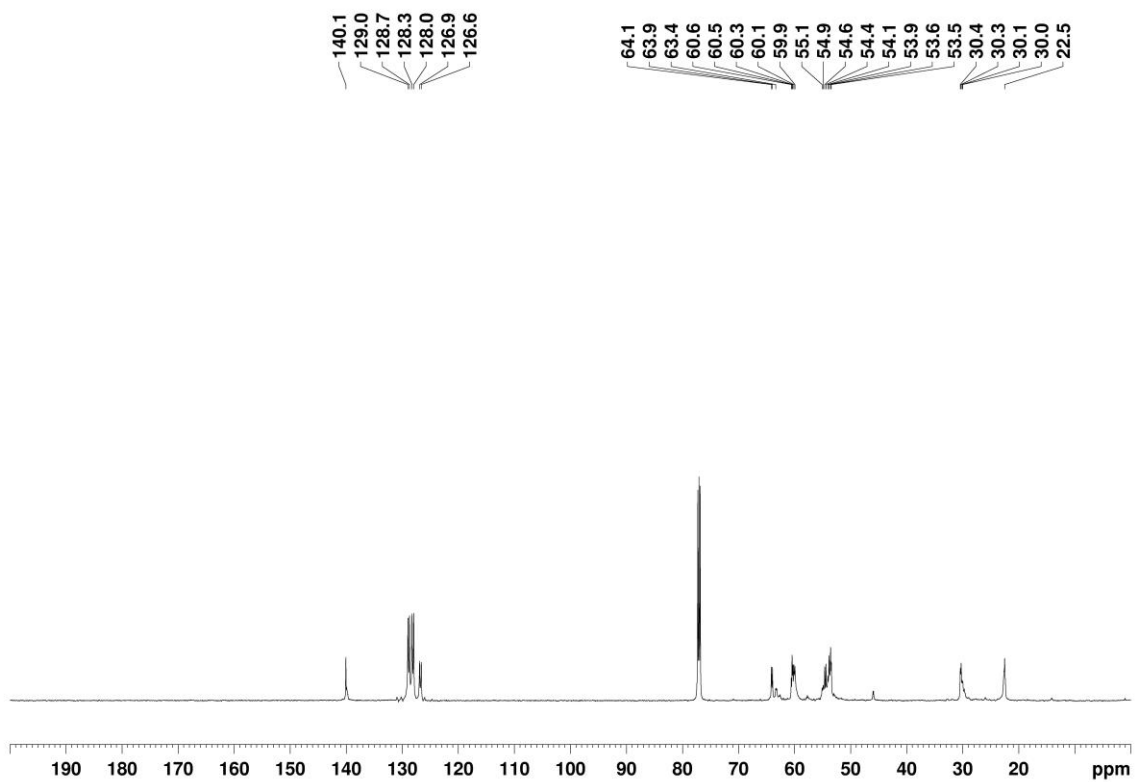
7: HSQC NMR (600 MHz, $\text{C}_6\text{D}_5\text{CD}_3$)



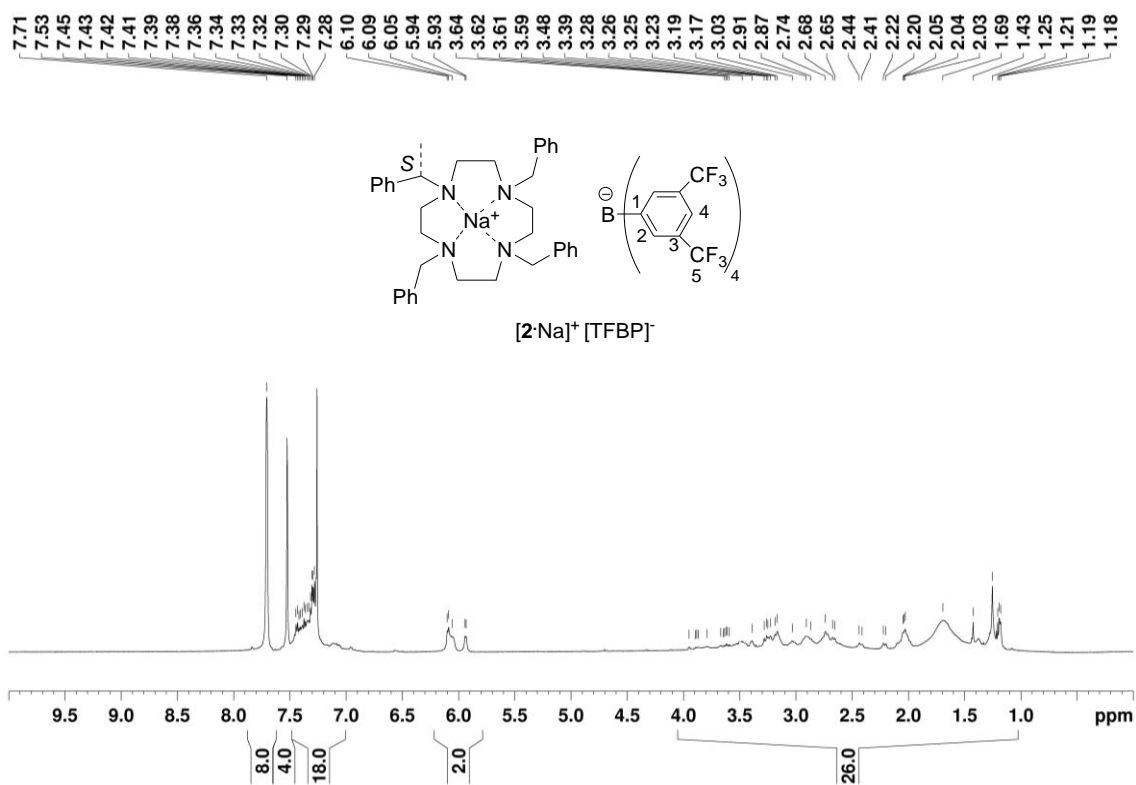
7: HMBC NMR (600 MHz, C₆D₅CD₃)



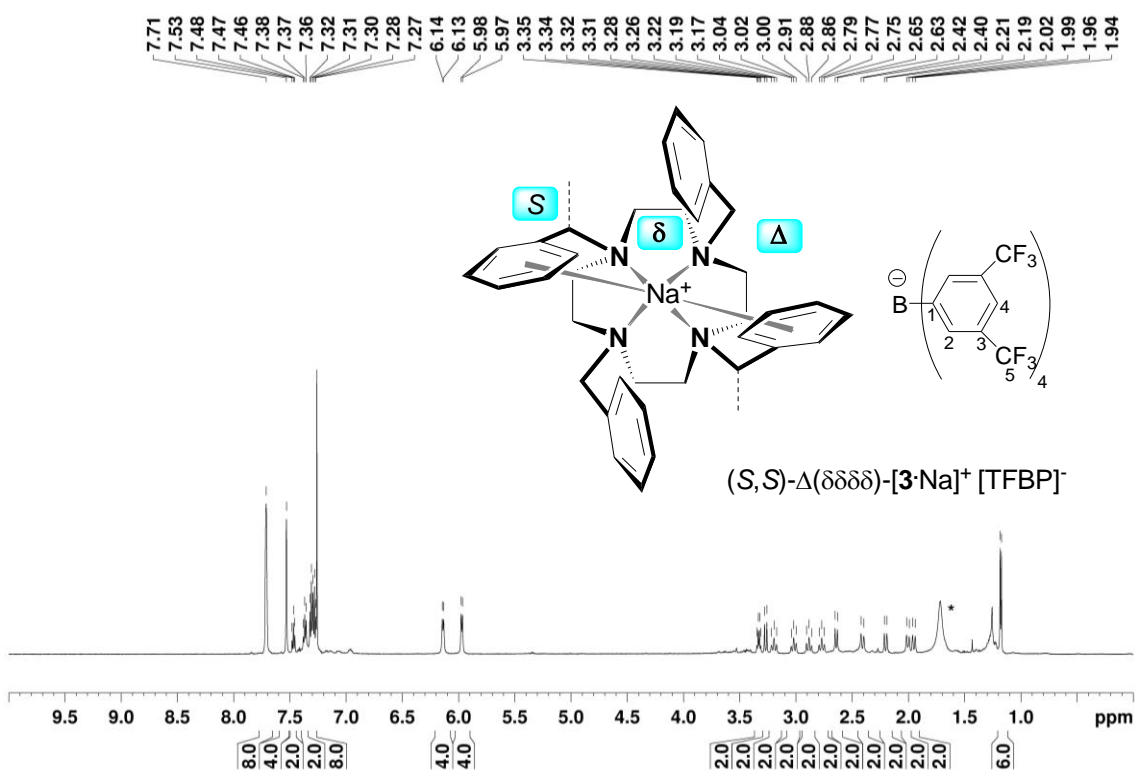
8: ¹H NMR (600 MHz, CDCl₃)



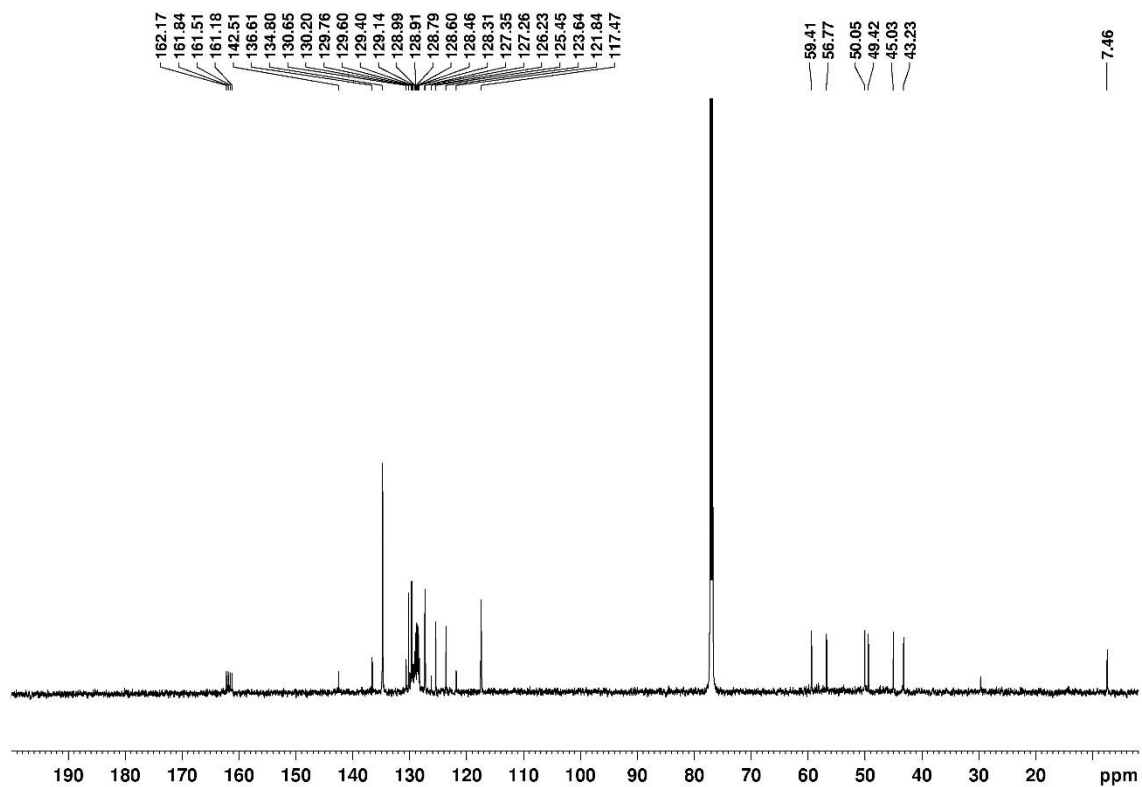
8: ¹³C NMR (150 MHz, CDCl₃)



[2·Na]⁺TFPB⁻: ¹H NMR (600 MHz, CDCl₃).



[3·Na]⁺TFPB⁻: ¹H NMR (600 MHz, CDCl₃). Water impurity labelled with an asterisk.



$[3\cdot\text{Na}]^+\text{TFPB}^-$: ^{13}C NMR (150 MHz, CDCl_3).

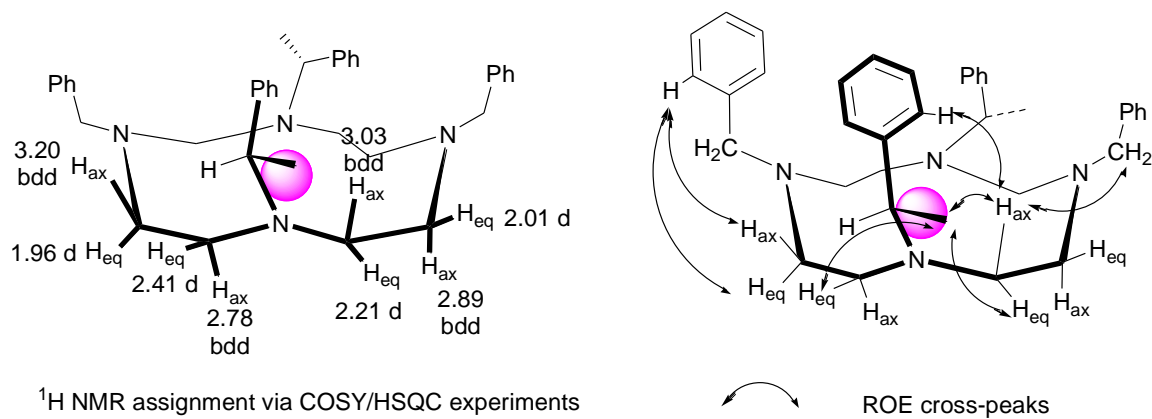
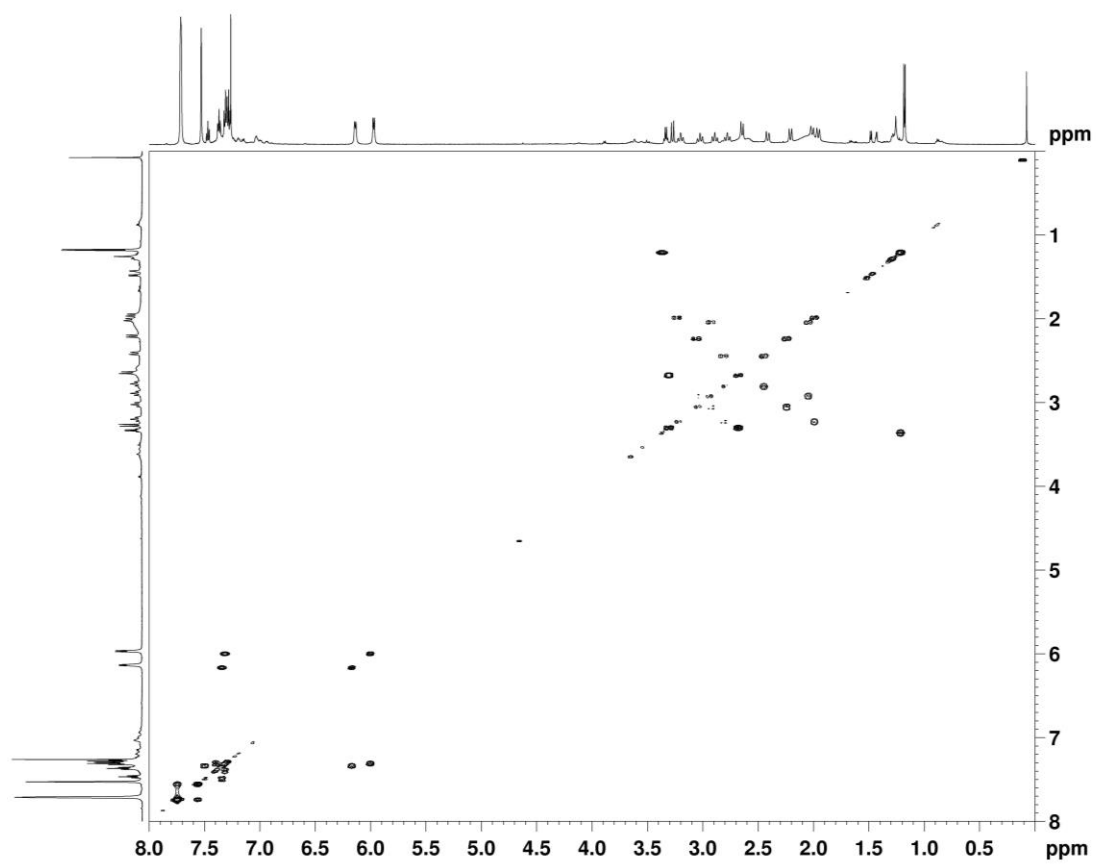
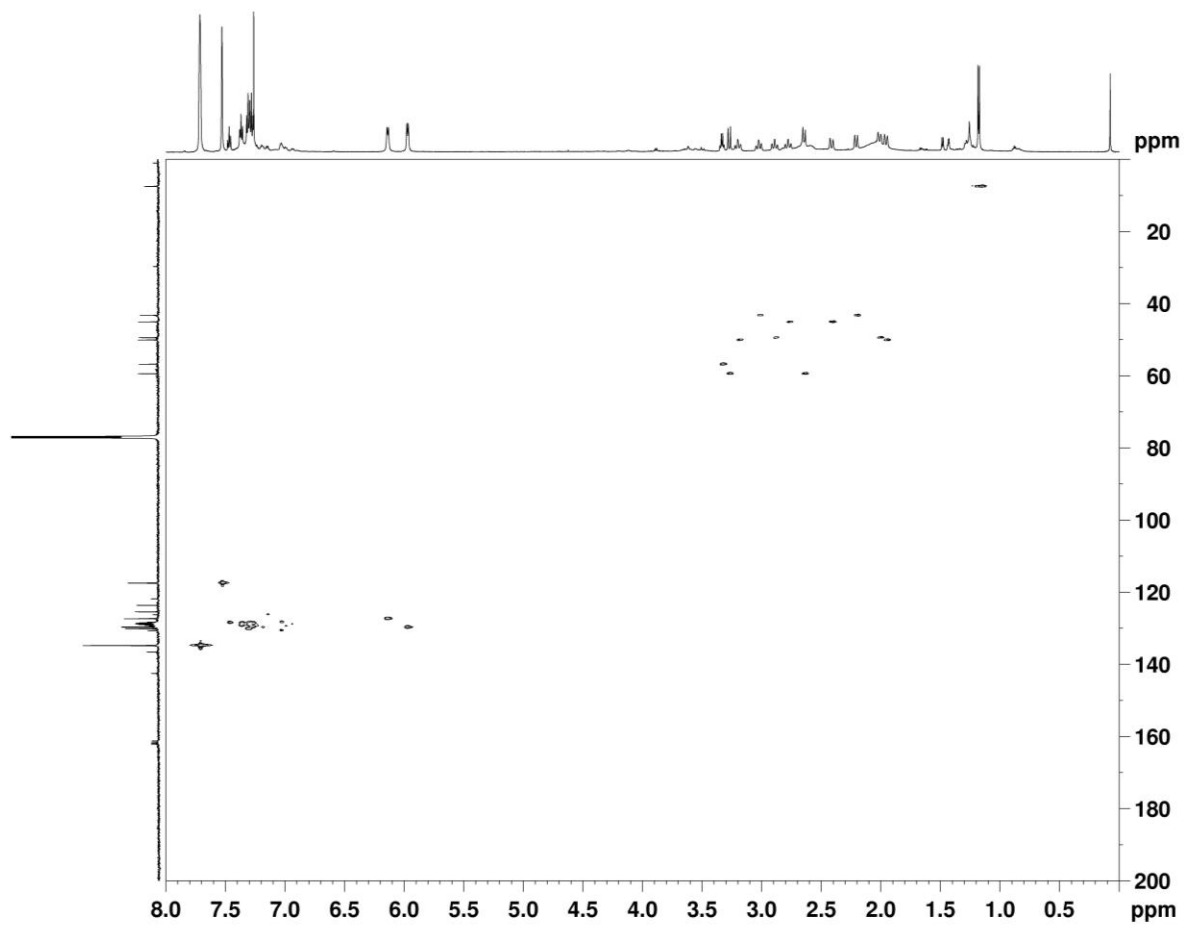


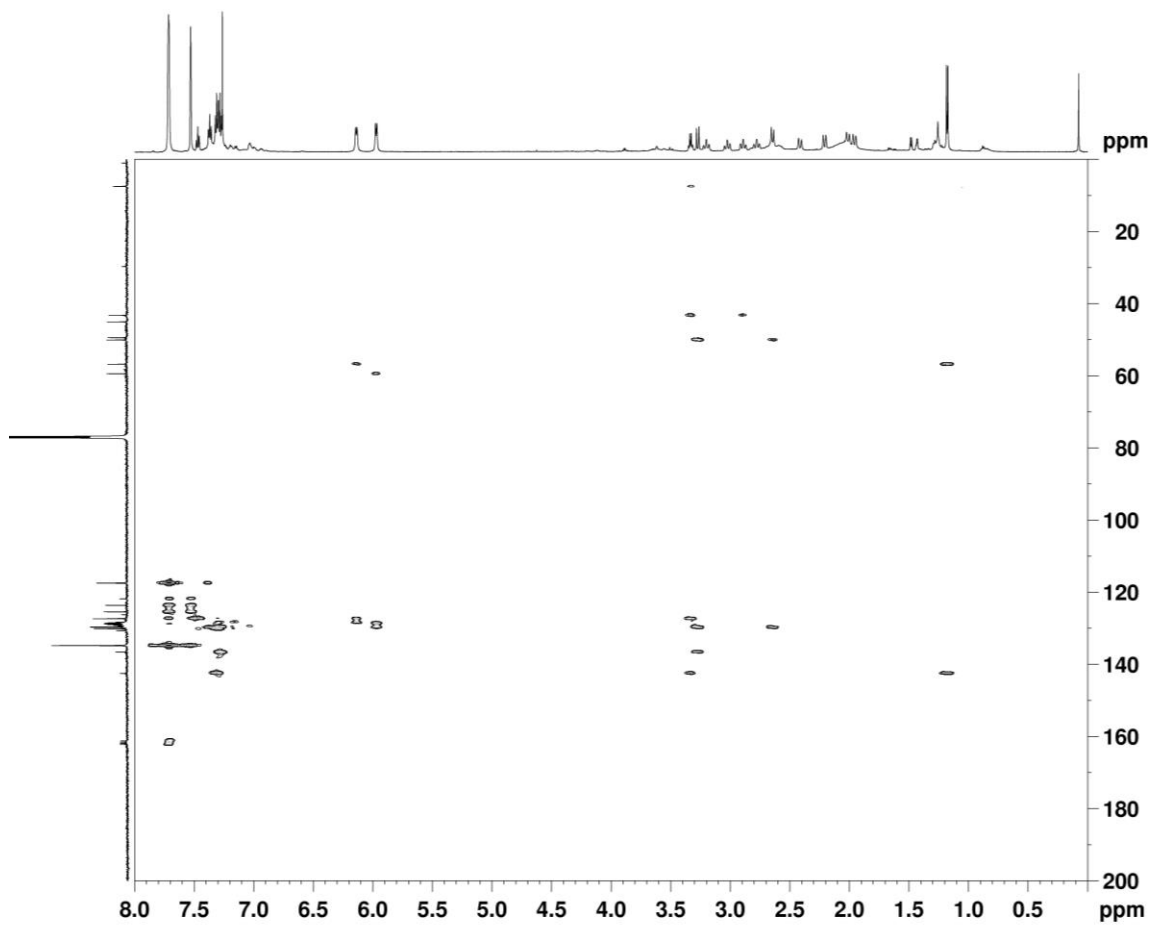
Figure S1. ^1H NMR assignment for complex $[3\cdot\text{Na}]^+\text{TFPB}^-$.



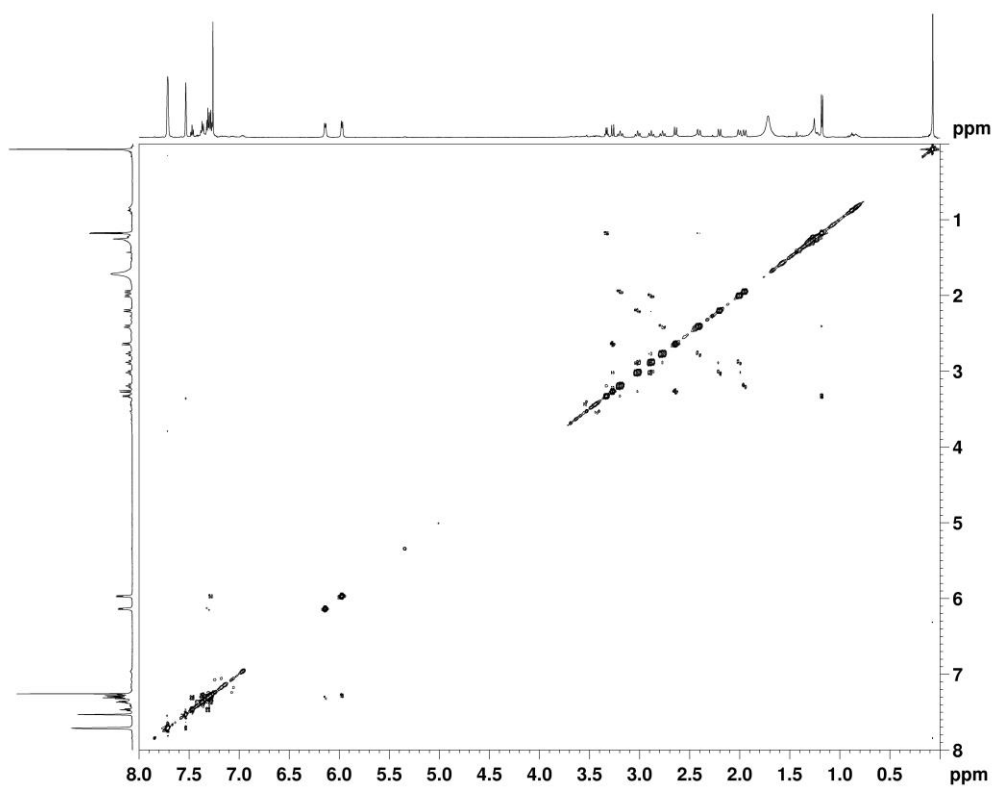
[3·Na]⁺TFPB⁻: COSY NMR (600 MHz, CDCl₃)



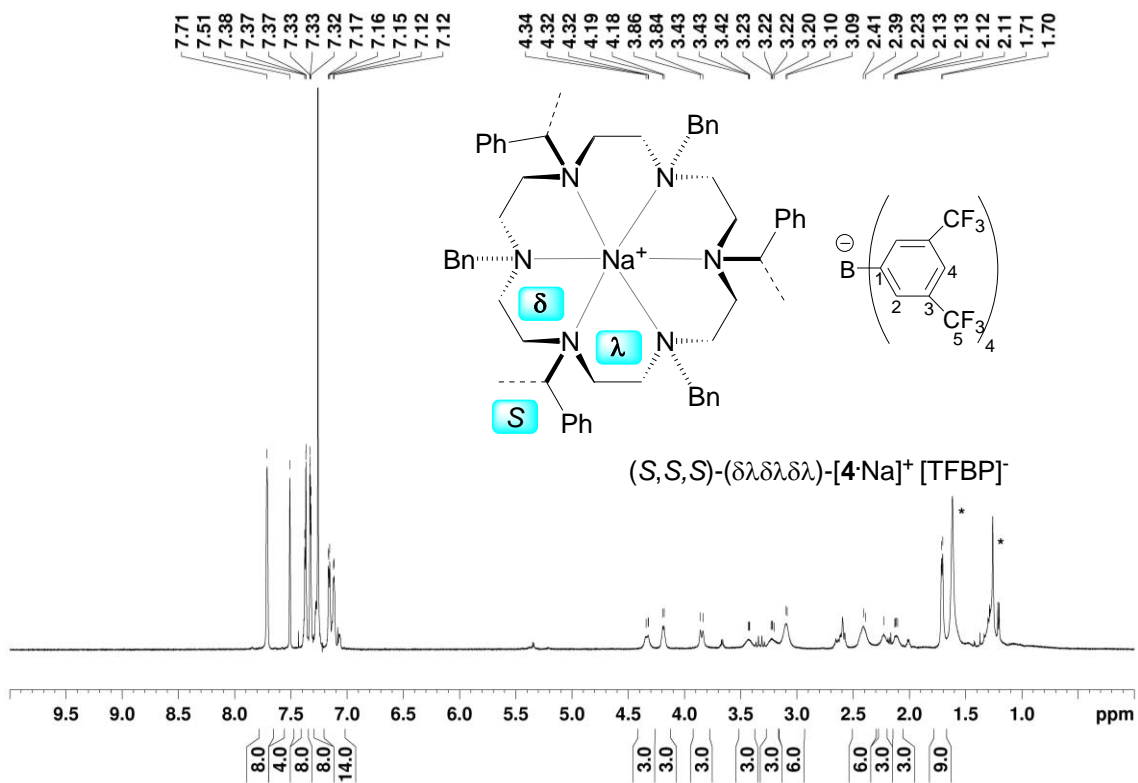
[3·Na]⁺TFPB⁻: HSQC NMR (600 MHz, CDCl₃)



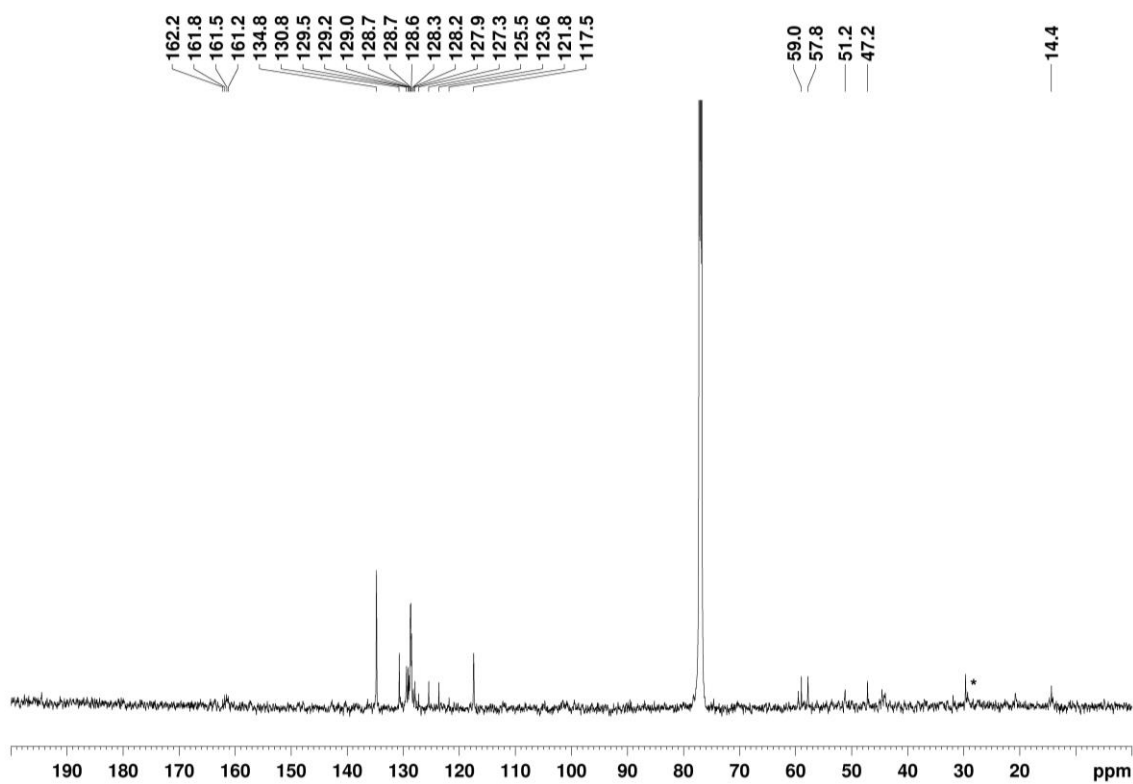
$[3 \cdot Na]^+ TFPB^-$: HMBC NMR (600 MHz, $CDCl_3$)



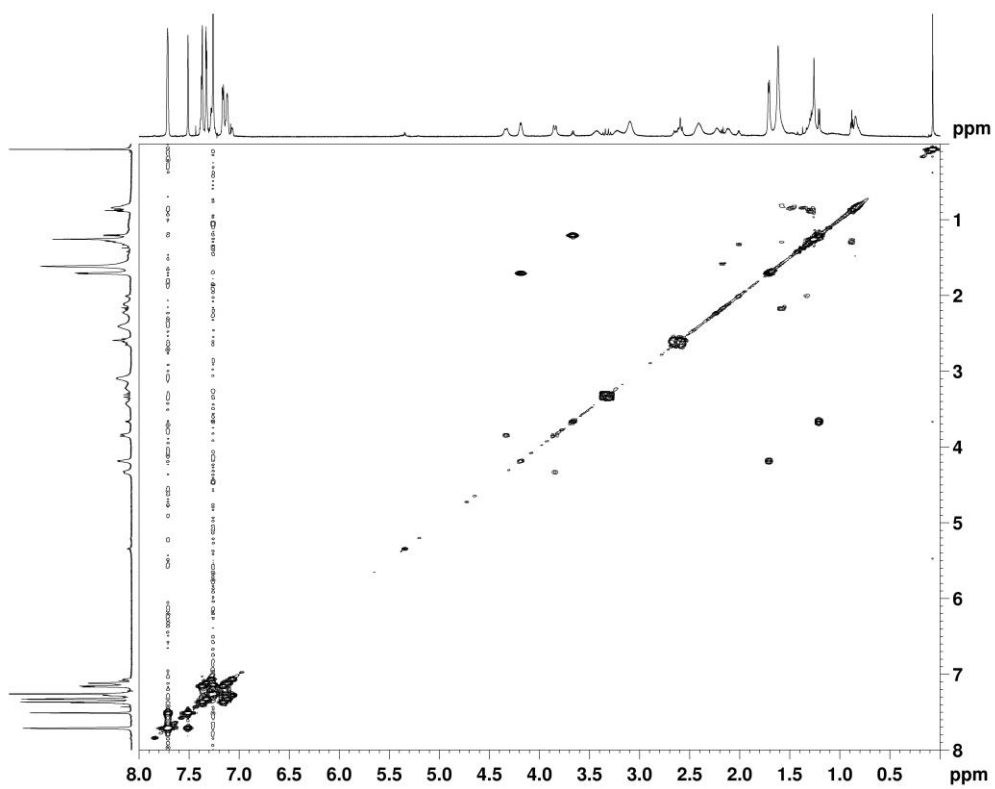
[3·Na]⁺TFPB⁻: ROESY NMR (600 MHz, CDCl₃)



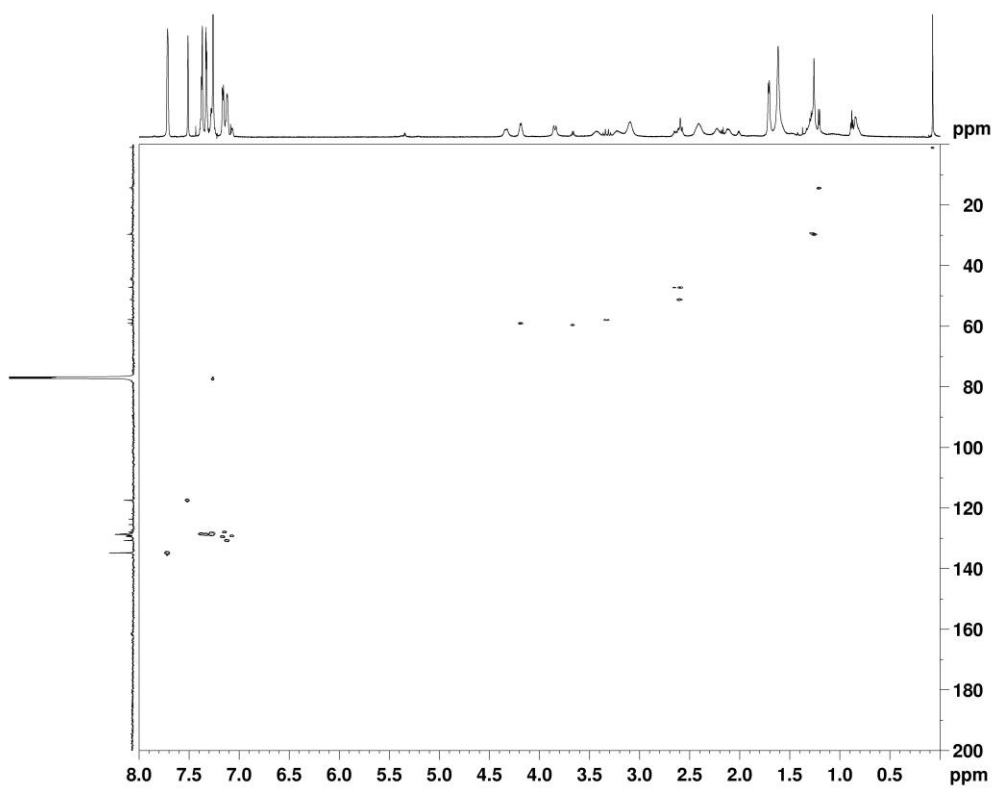
$[4\cdot Na]^+ [TFBP]^-$: 1H NMR (600 MHz, $CDCl_3$) Water and grease impurities are labelled with asterisks.



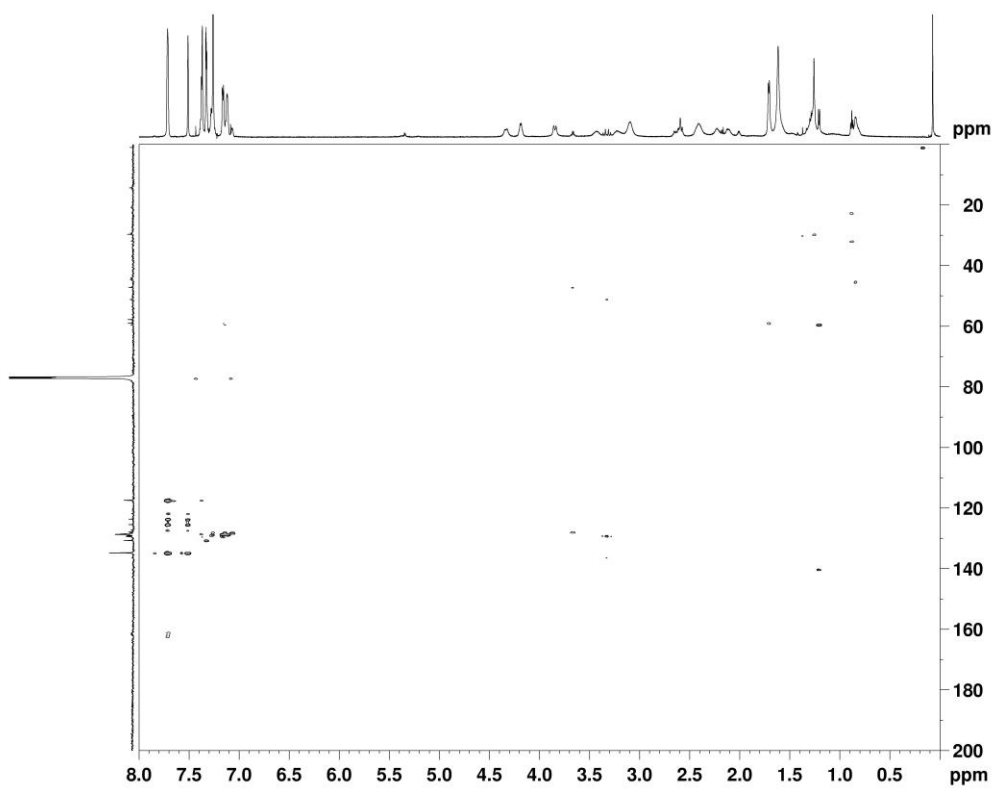
$[4\cdot Na]^+ [TFBP]^-$: ^{13}C NMR (600 MHz, $CDCl_3$). Grease impurity labelled with an asterisk.



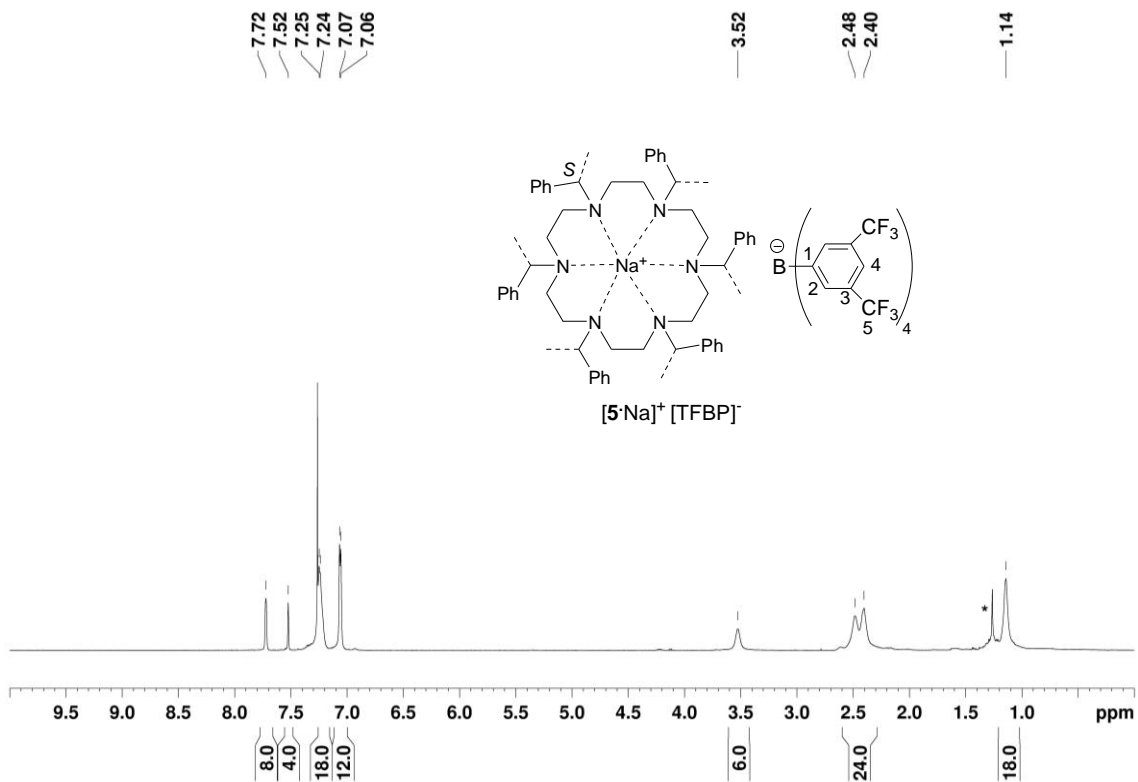
[4-Na]⁺TFPB⁻: COSY NMR (600 MHz, CDCl₃)



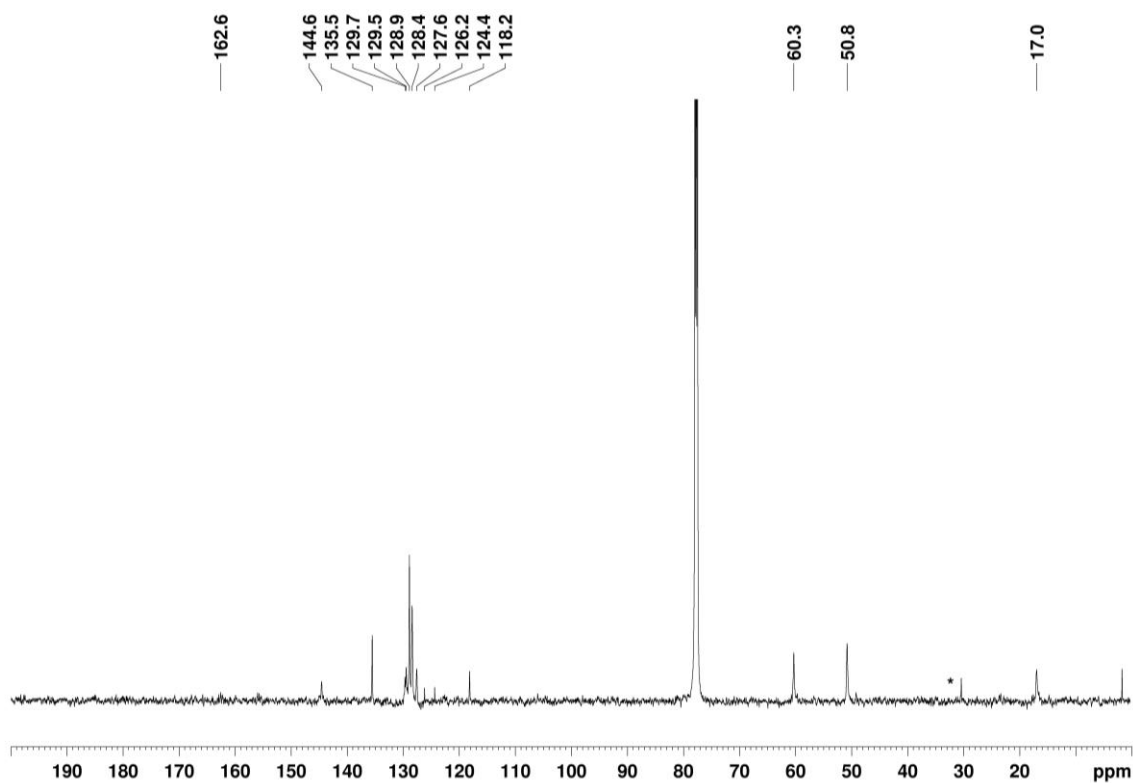
[4·Na]⁺TFPB⁻: HSQC NMR (600 MHz, CDCl₃)



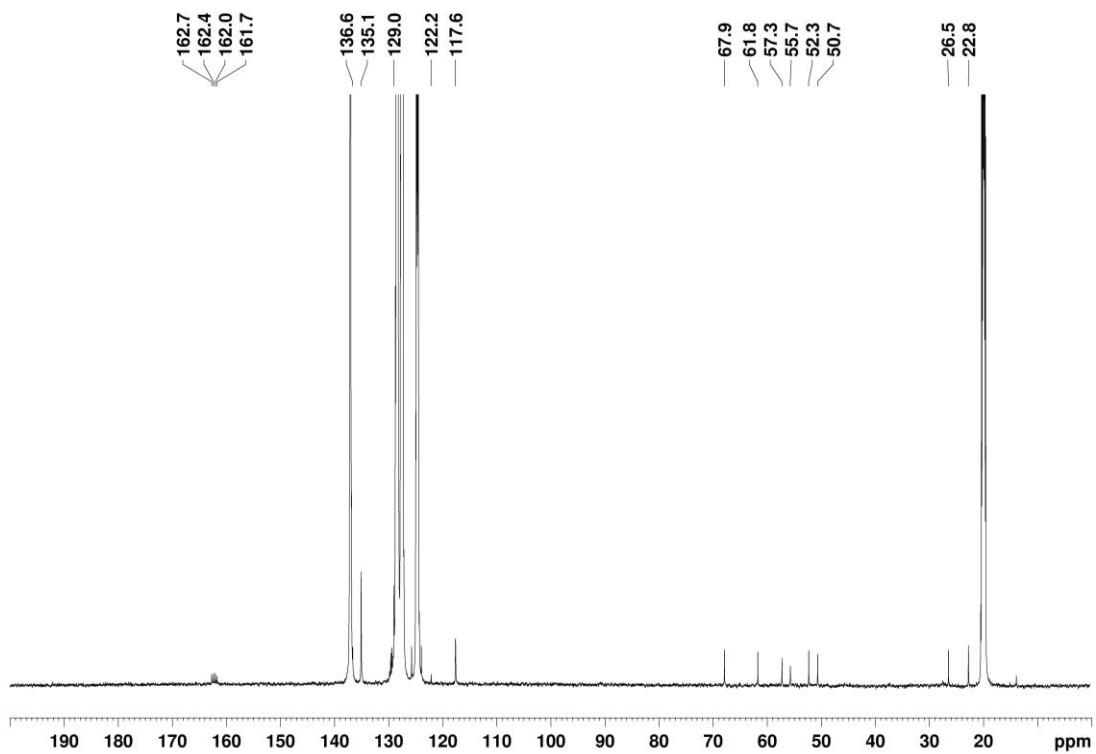
[4·Na]⁺TFPB: HMBC NMR (600 MHz, CDCl₃)



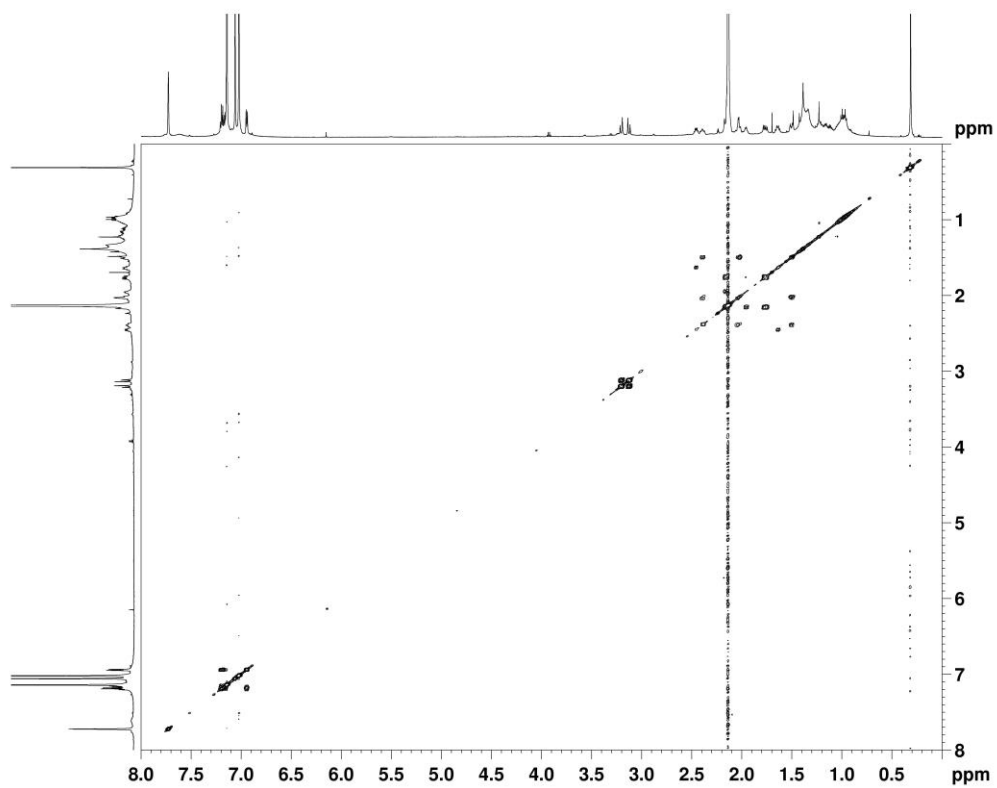
$[5\cdot\text{Na}]^+\text{TFPB}$: $^1\text{H NMR}$ (600 MHz, CDCl_3). Grease impurity labelled with an asterisk.



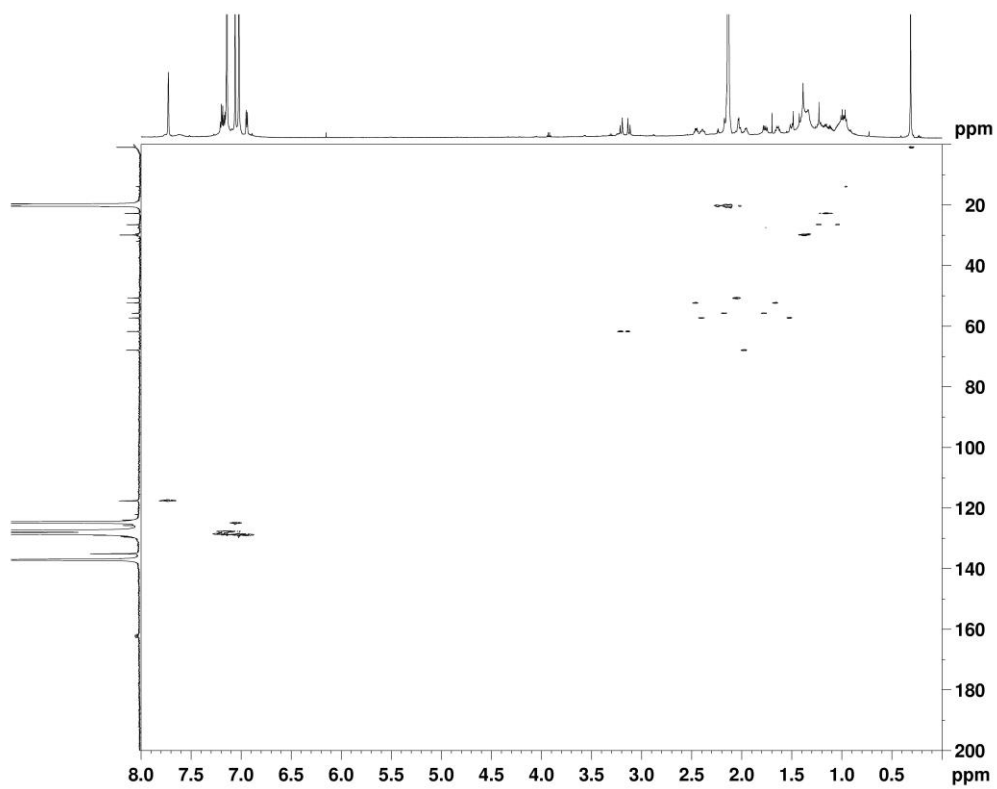
$[5\cdot\text{Na}]^+\text{TFPB}$: $^{13}\text{C NMR}$ (150 MHz, CDCl_3). Grease impurity labelled with an asterisk.



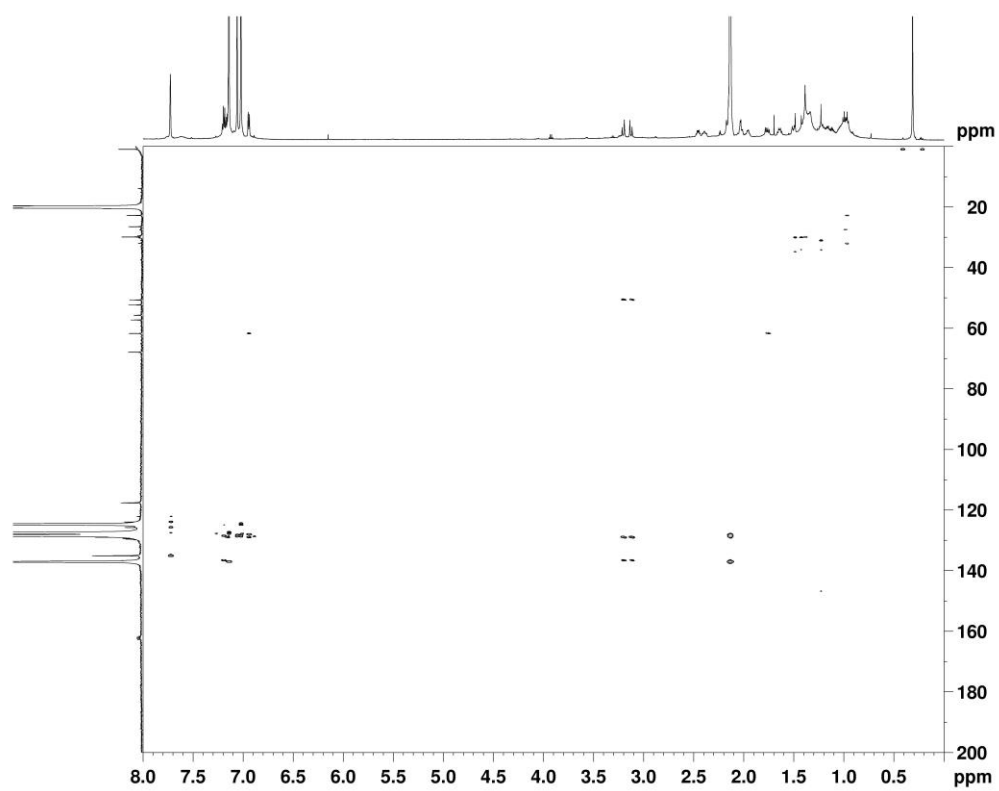
[7-Na]⁺TFPB⁻: ¹³C NMR (150 MHz, C₆D₅CD₃)



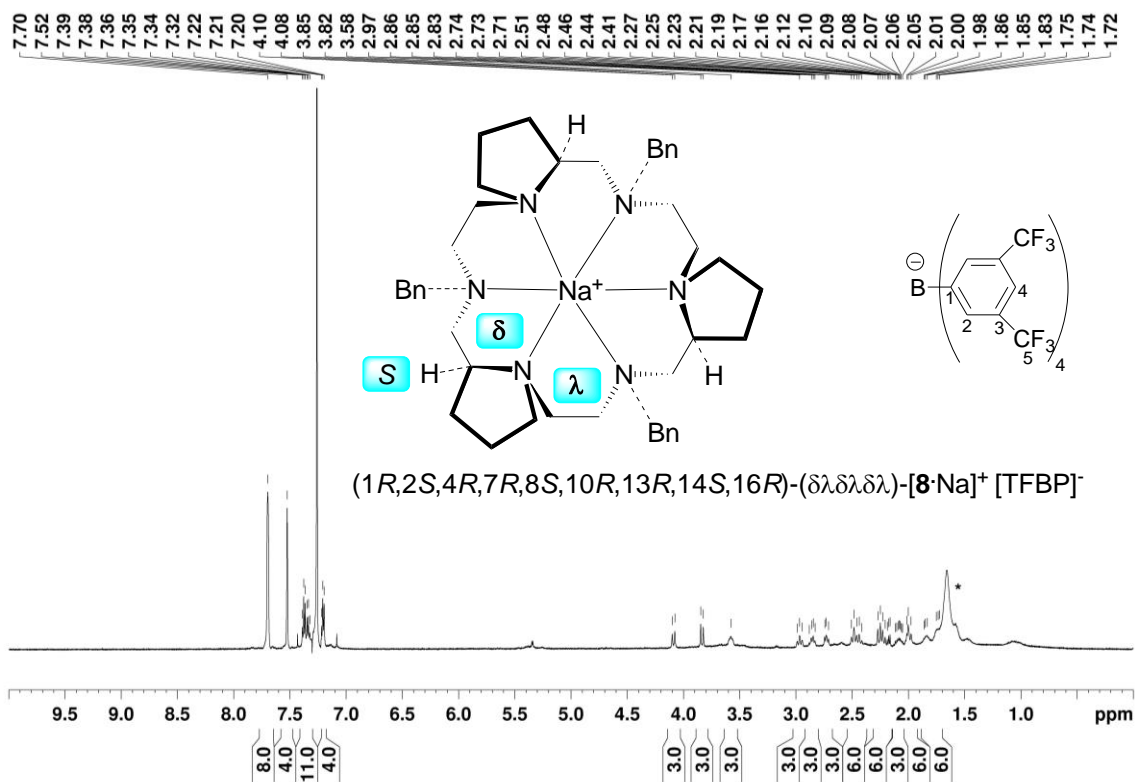
[7-Na]⁺TFPB⁻: COSY NMR (600 MHz, C₆D₅CD₃)



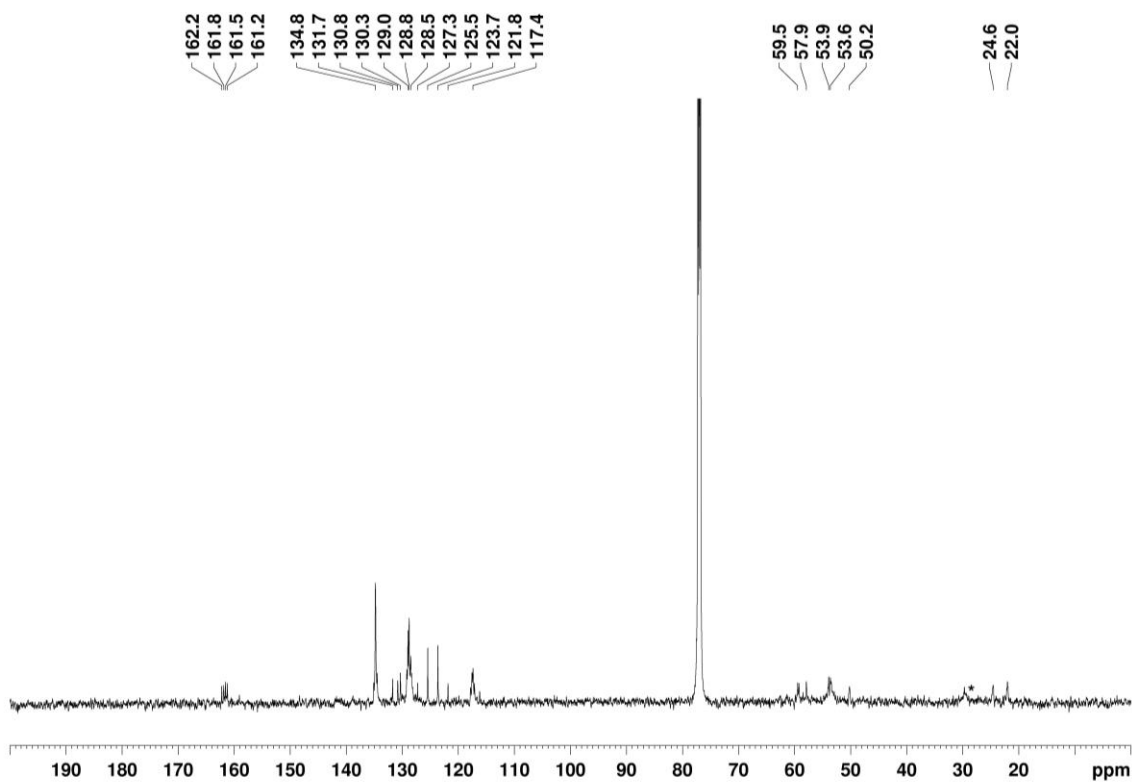
[7·Na]⁺TFPB: HSQC NMR (600 MHz, C₆D₅CD₃)



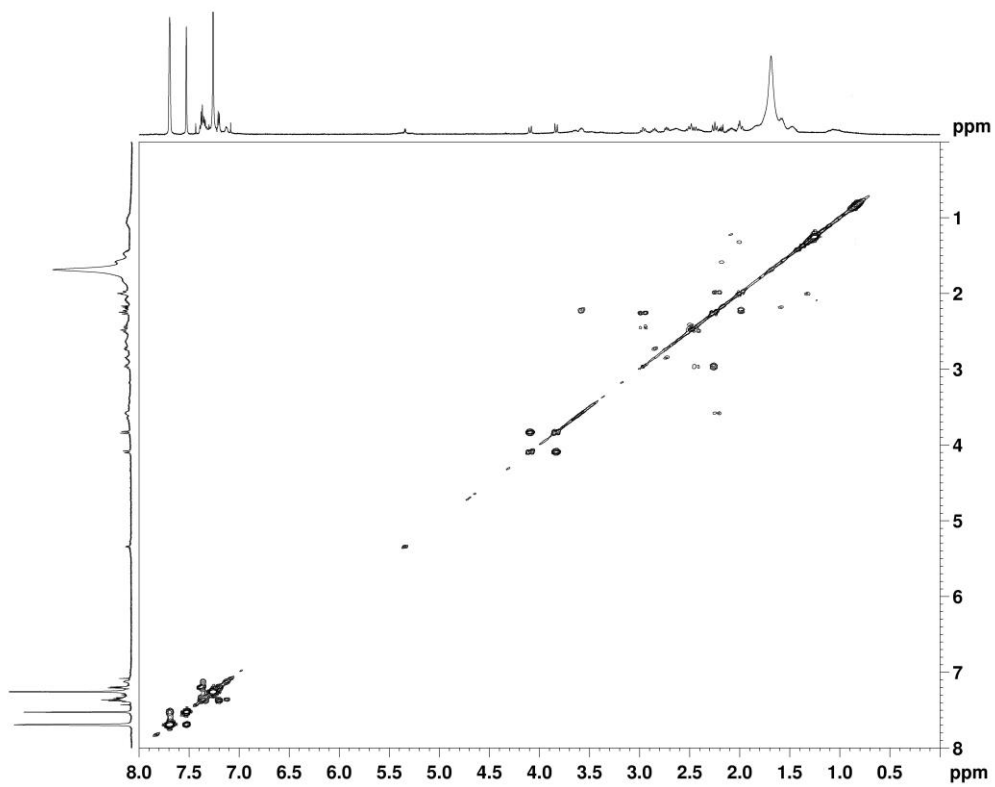
[7·Na]⁺TFPB: HMBC NMR (600 MHz, C₆D₅CD₃)



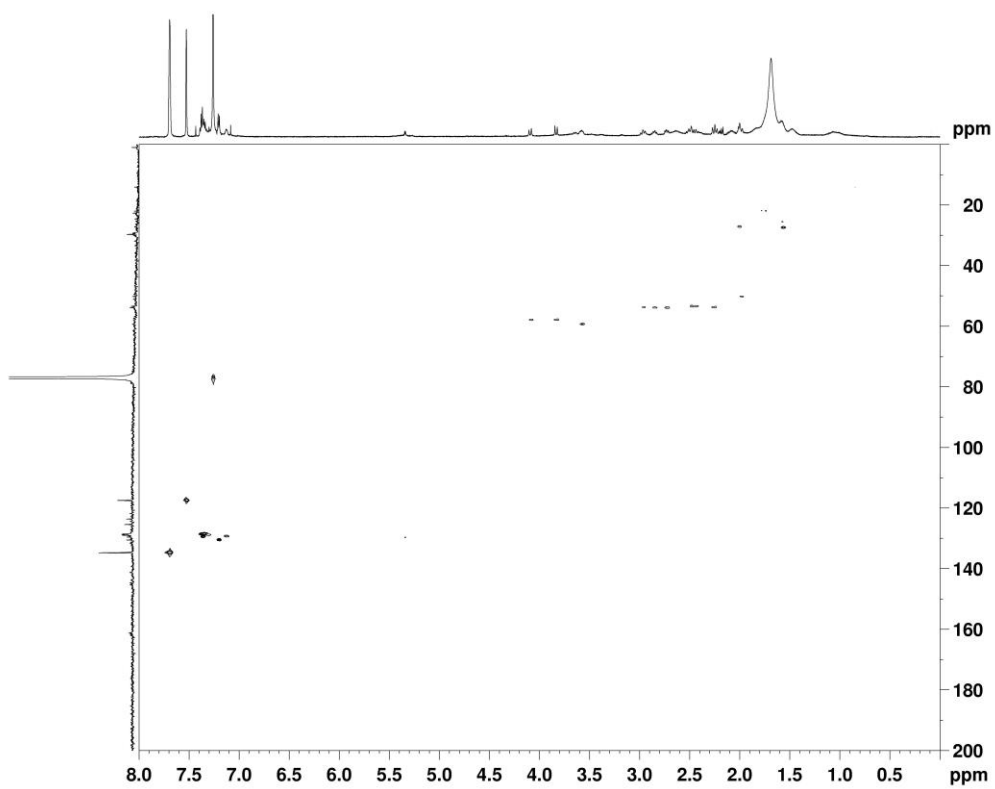
[8·Na]⁺TFPB: ¹H NMR (600 MHz, CDCl₃). Water impurity labelled with an asterisk.



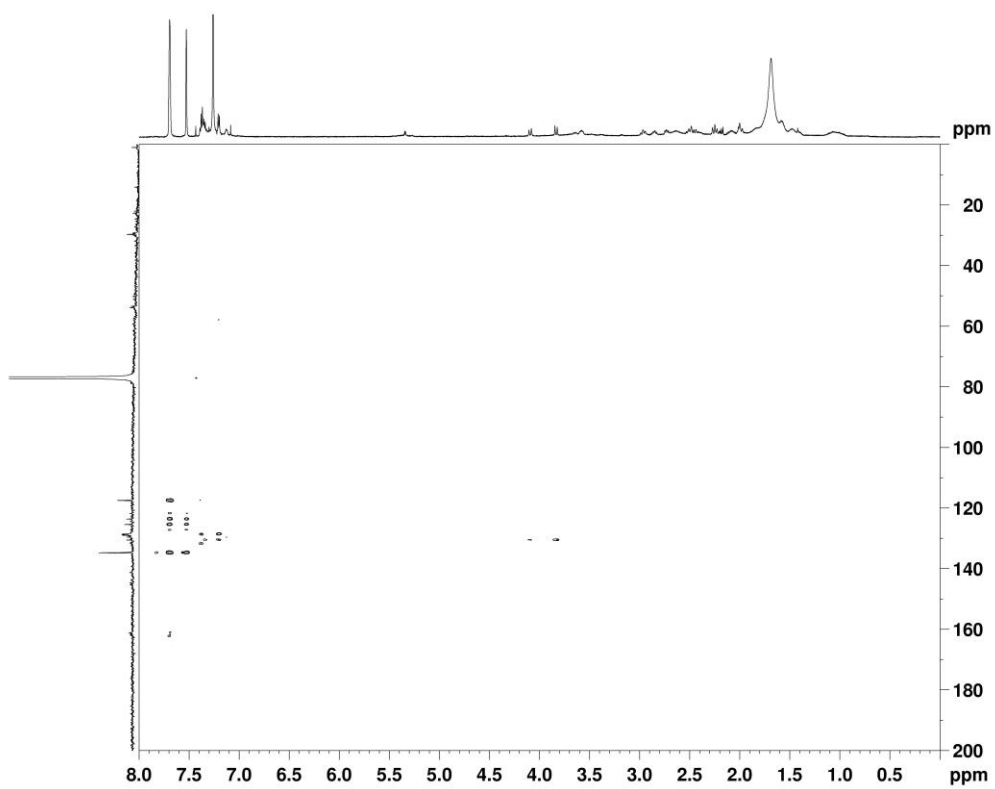
[8·Na]⁺TFPB: ¹³C NMR (150 MHz, CDCl₃). Grease impurity labelled with an asterisk.



[8·Na]⁺TFPB⁻: COSY NMR (600 MHz, CDCl₃)



[8·Na]⁺TFPB⁻: HSQC NMR (600 MHz, CDCl₃)



[8·Na]⁺TFPB⁻: HMBC NMR (600 MHz, CDCl₃)

2.2 ^1H NMR titrations with NaTFPB (Figures S2-S9)

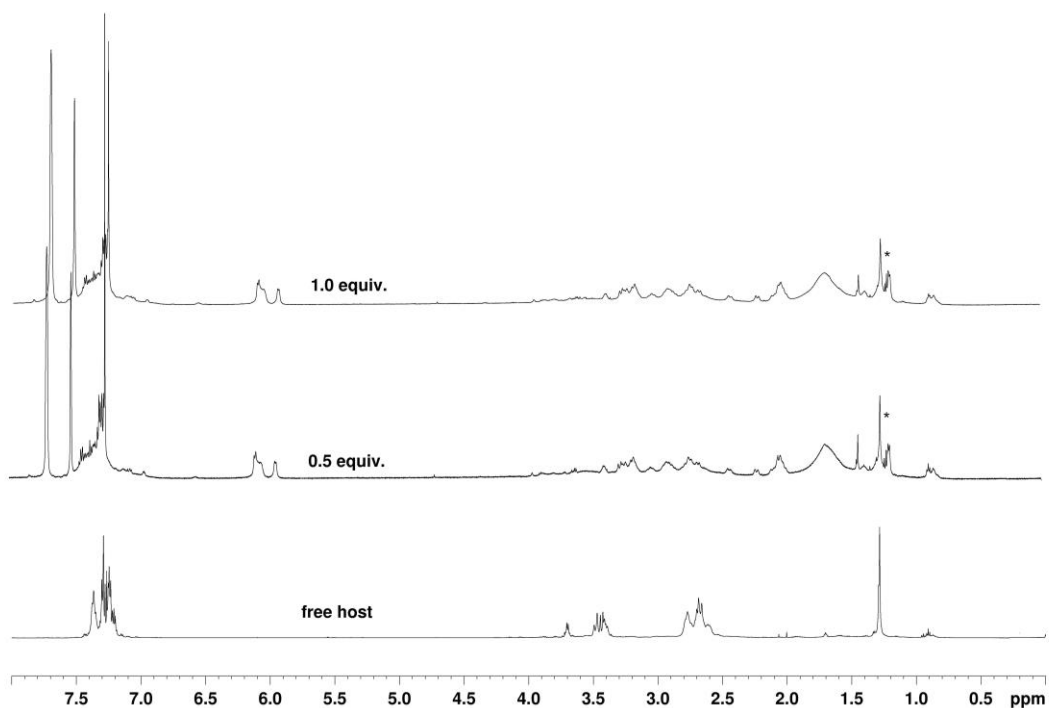


Figure S2. Quantitative step-wise addition of NaTFPB to **2**. ^1H NMR (600 MHz, CDCl_3 , 298 K, 5.0 mM solution). Grease impurity labelled with an asterisk.

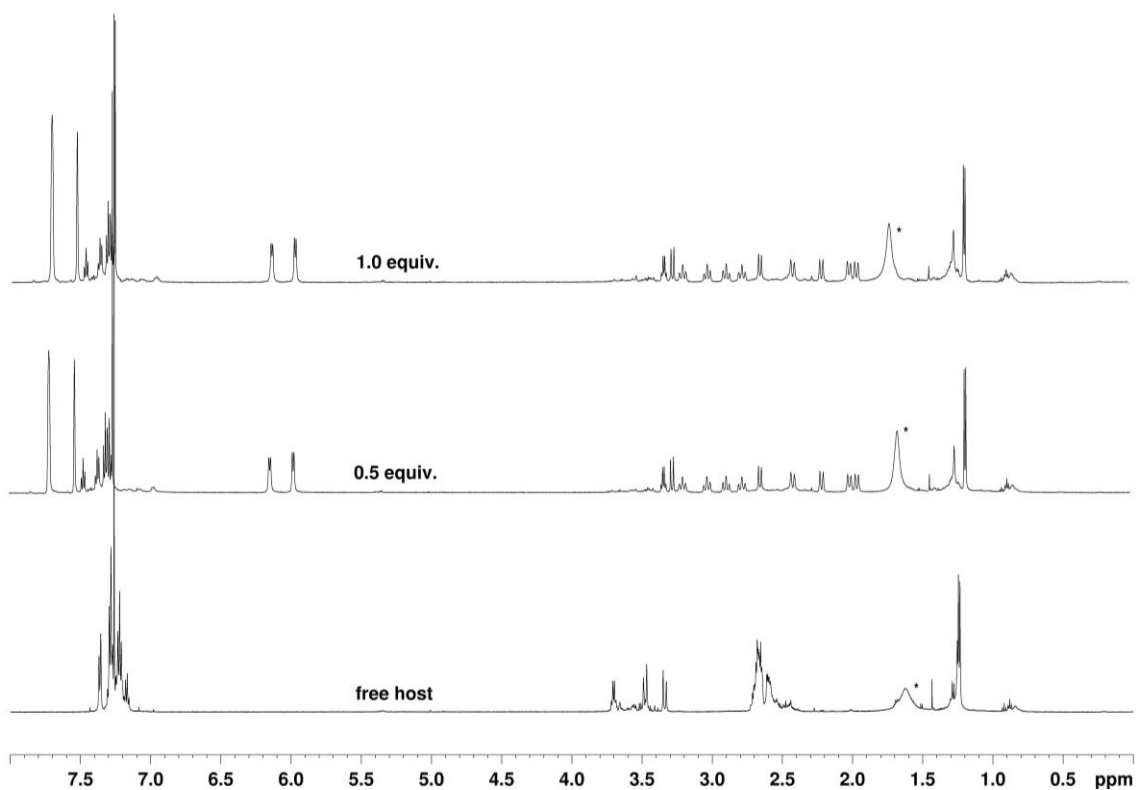


Figure S3. Quantitative step-wise addition of NaTFPB to **3**. ^1H NMR (600 MHz, CDCl_3 , 298 K, 5.0 mM solution). Water impurity labelled with an asterisk.

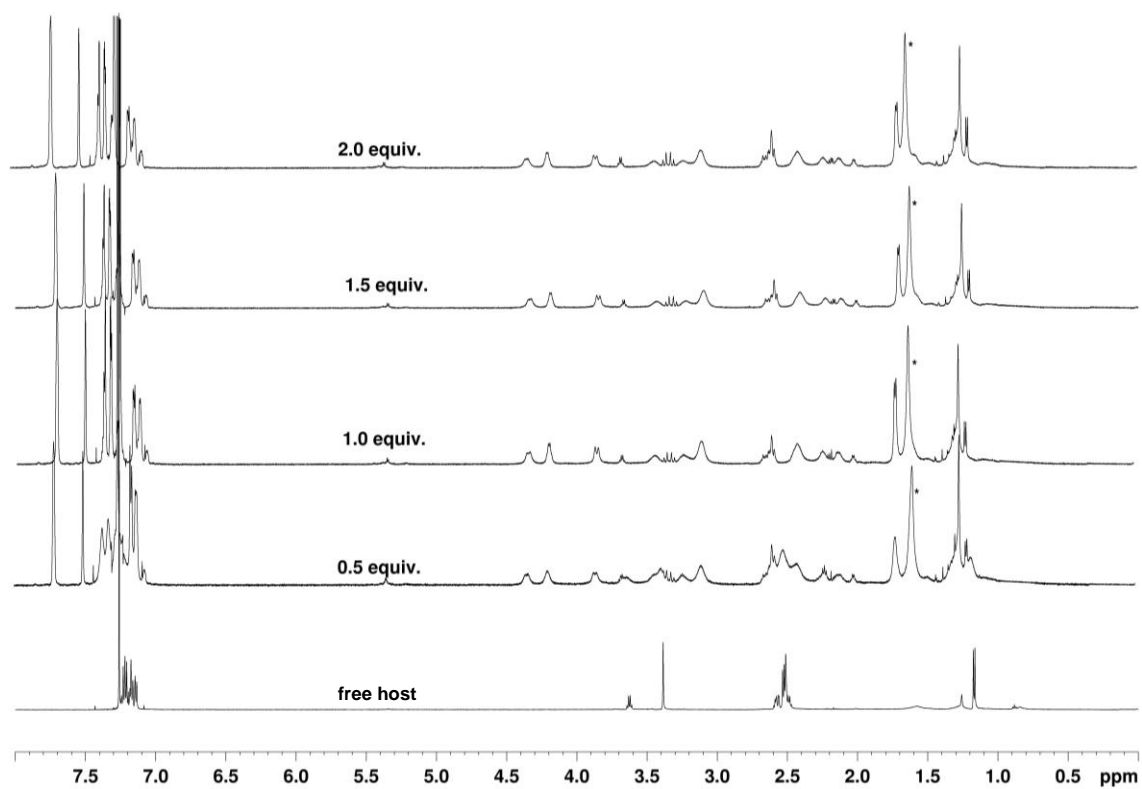


Figure S4. Quantitative step-wise addition of NaTFPB to **4**. ^1H NMR (600 MHz, CDCl_3 , 298 K, 5.0 mM solution). Water impurities are labelled with an asterisk.

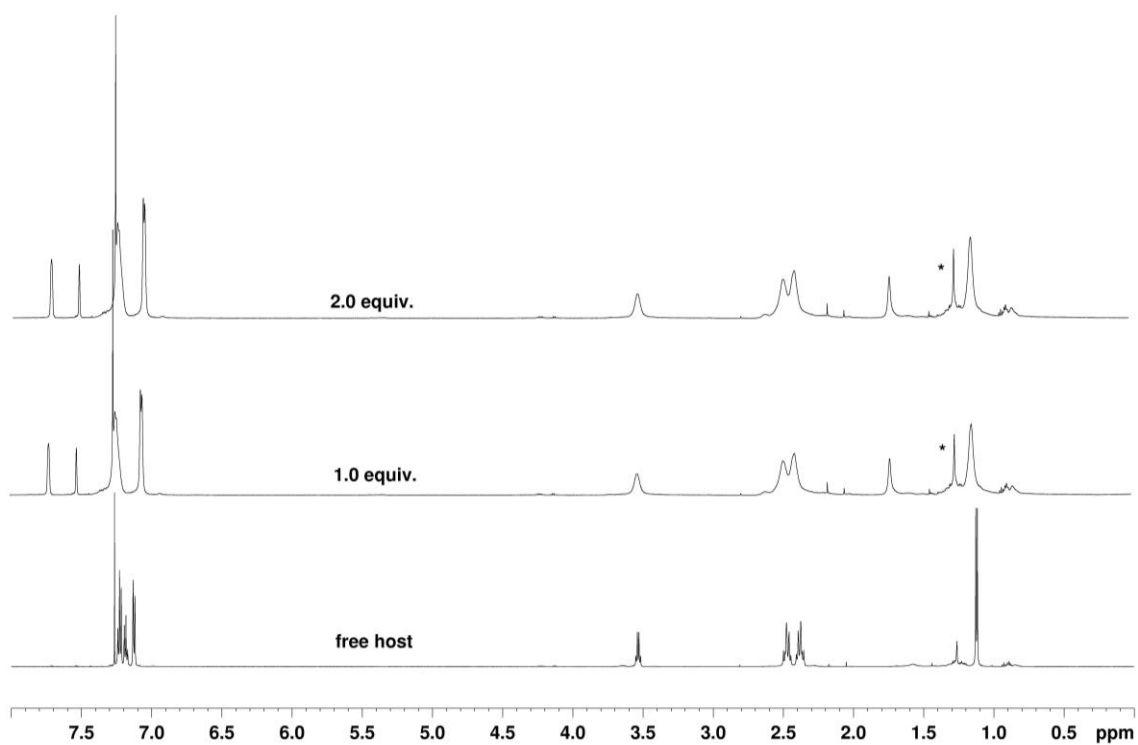


Figure S5. Quantitative step-wise addition of NaTFPB to **5**. ^1H NMR (600 MHz, CDCl_3 , 298 K, 5.0 mM solution). Water impurities are labelled with an asterisk.

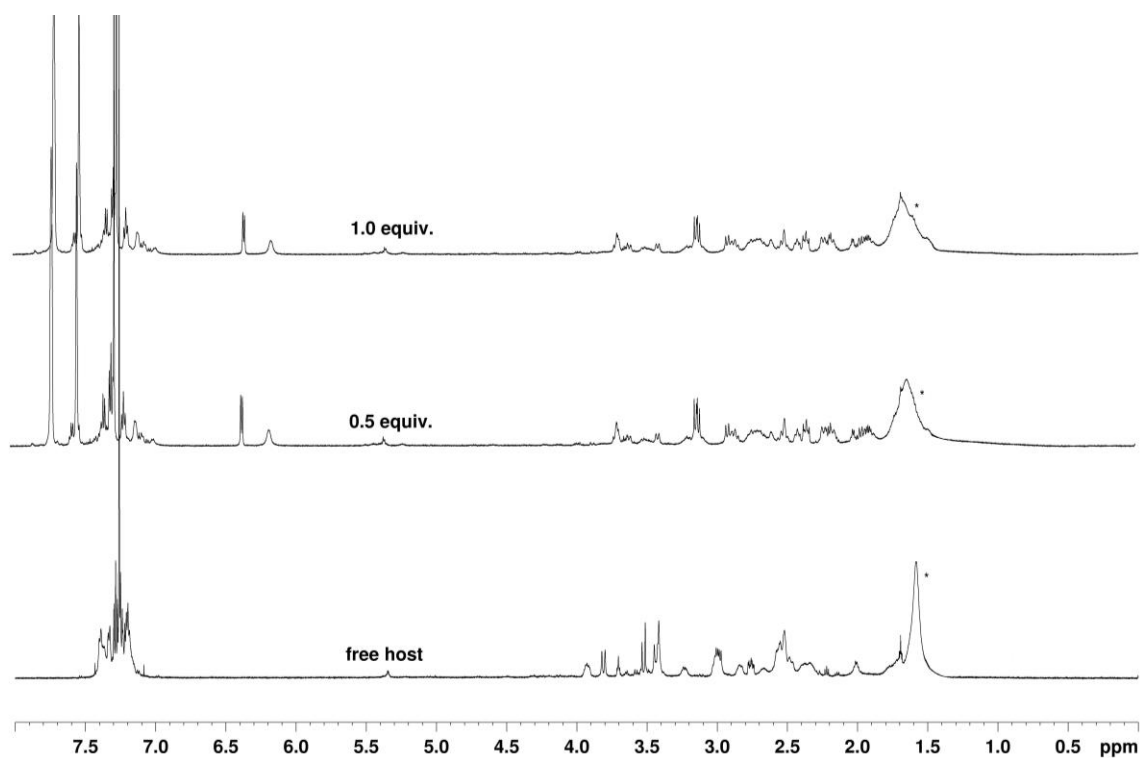


Figure S6. Quantitative step-wise addition of NaTFPB to **6**. ^1H NMR (600 MHz, CDCl_3 , 298 K, 5.0 mM solution). Water impurities are labelled with an asterisk.

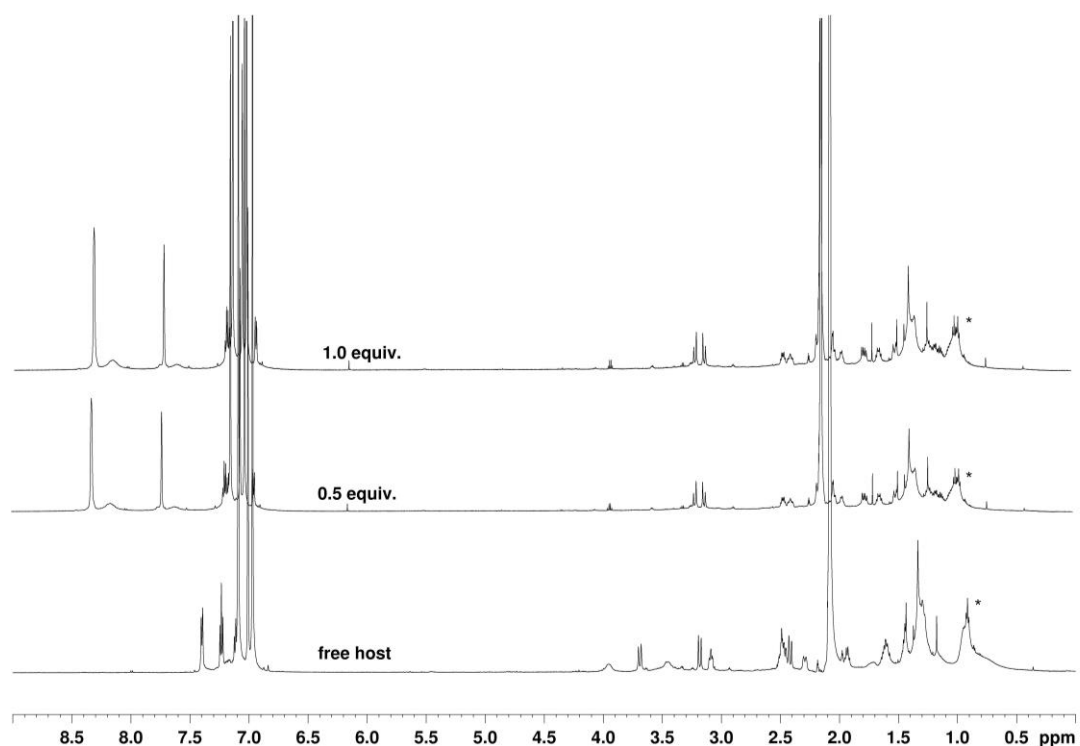


Figure S7. Quantitative step-wise addition of NaTFPB to **7**. ^1H NMR (600 MHz, $\text{C}_6\text{D}_5\text{CD}_3$, 298 K, 5.0 mM solution). Grease impurity labelled with an asterisk.

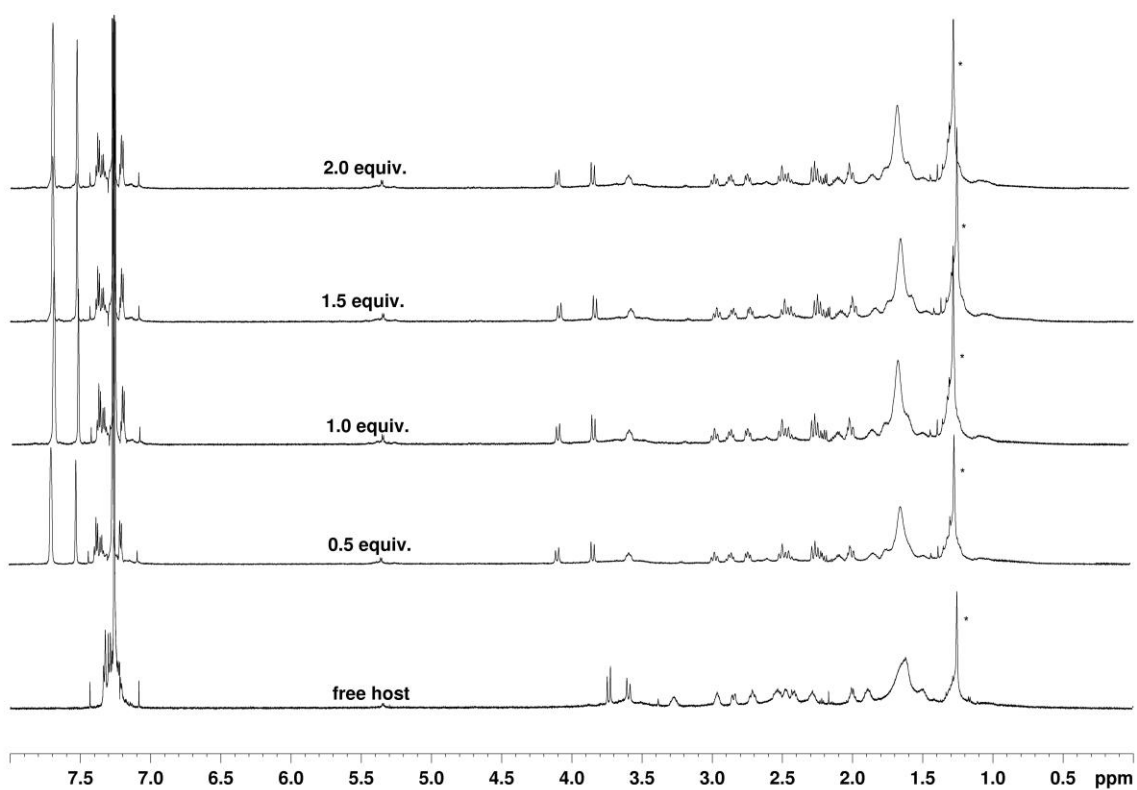


Figure S8. Quantitative step-wise addition of NaTFPB to **8**. ^1H NMR (600 MHz, CDCl_3 , 298 K, 5.0 mM solution). Grease impurities are labelled with an asterisk.

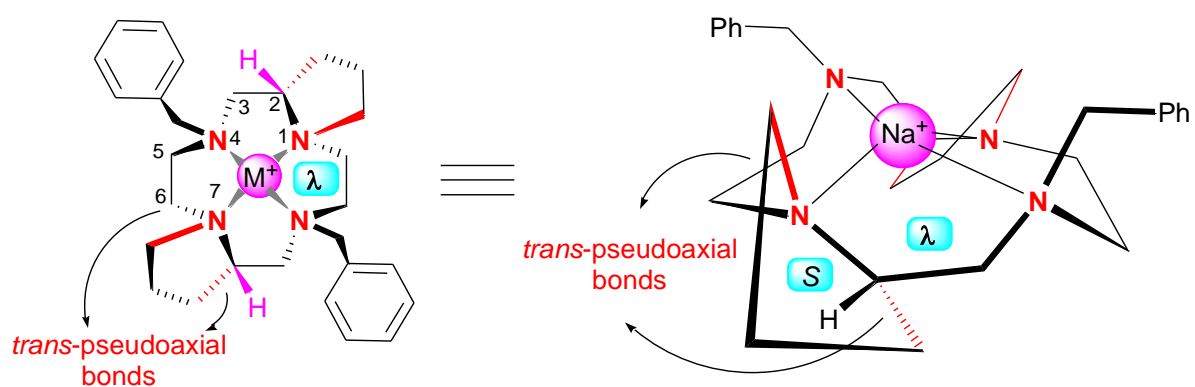


Figure S9. Schematic structures of geometrically implausible (1*S*,2*S*,4*R*,7*S*,8*S*,10*R*)-(λλλλ)-[**7**-Na]⁺ model (top and side view).

2.0 HPLC Chromatograms

Conditions: 5 → 100% A in 30 min (A, 0.1% TFA in acetonitrile, B, 0.1% TFA in water);
flow: 1 mL min⁻¹, 220 nm.

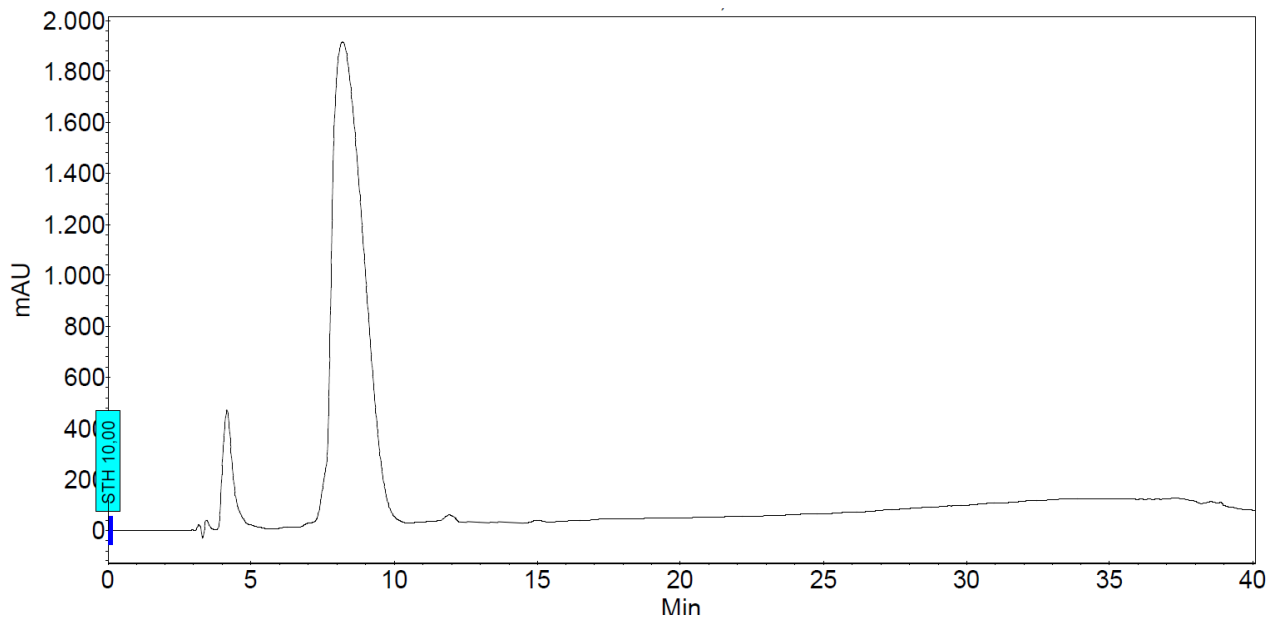


Figure S10. HPLC analysis of **16**

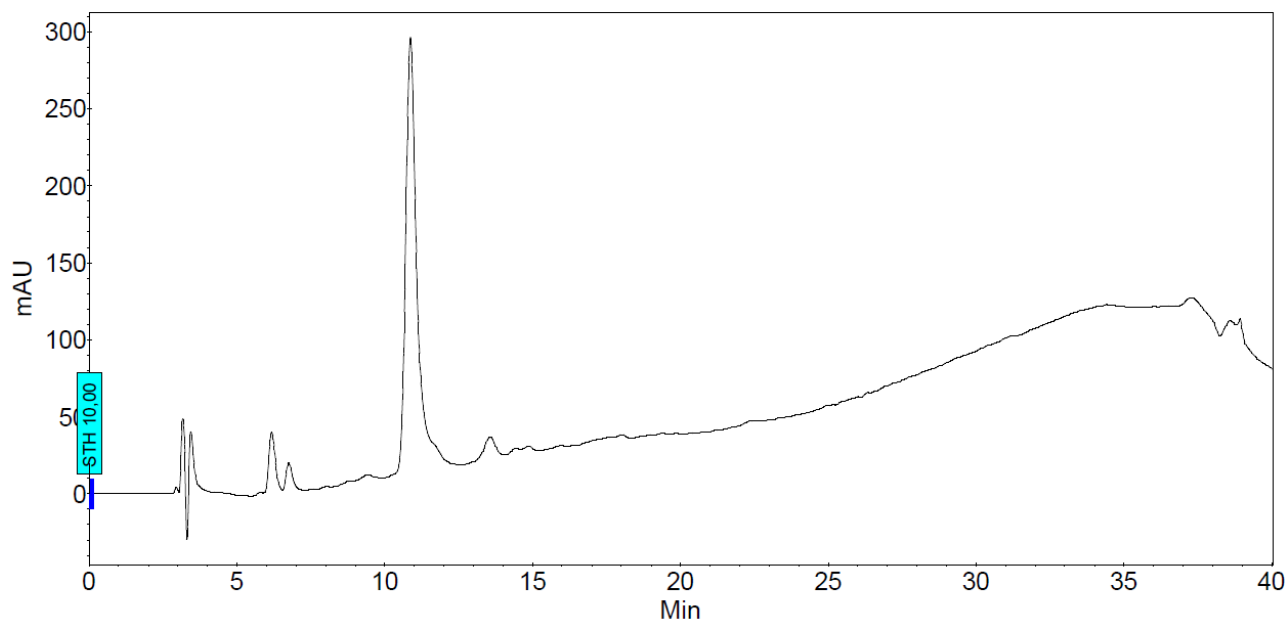


Figure S11. HPLC analysis of **13**

3.0 UV-Vis Spectra (Figures S12-S18)

All UV-Vis spectra were acquired in acetonitrile, $C = 0.003 \text{ mg mL}^{-1}$

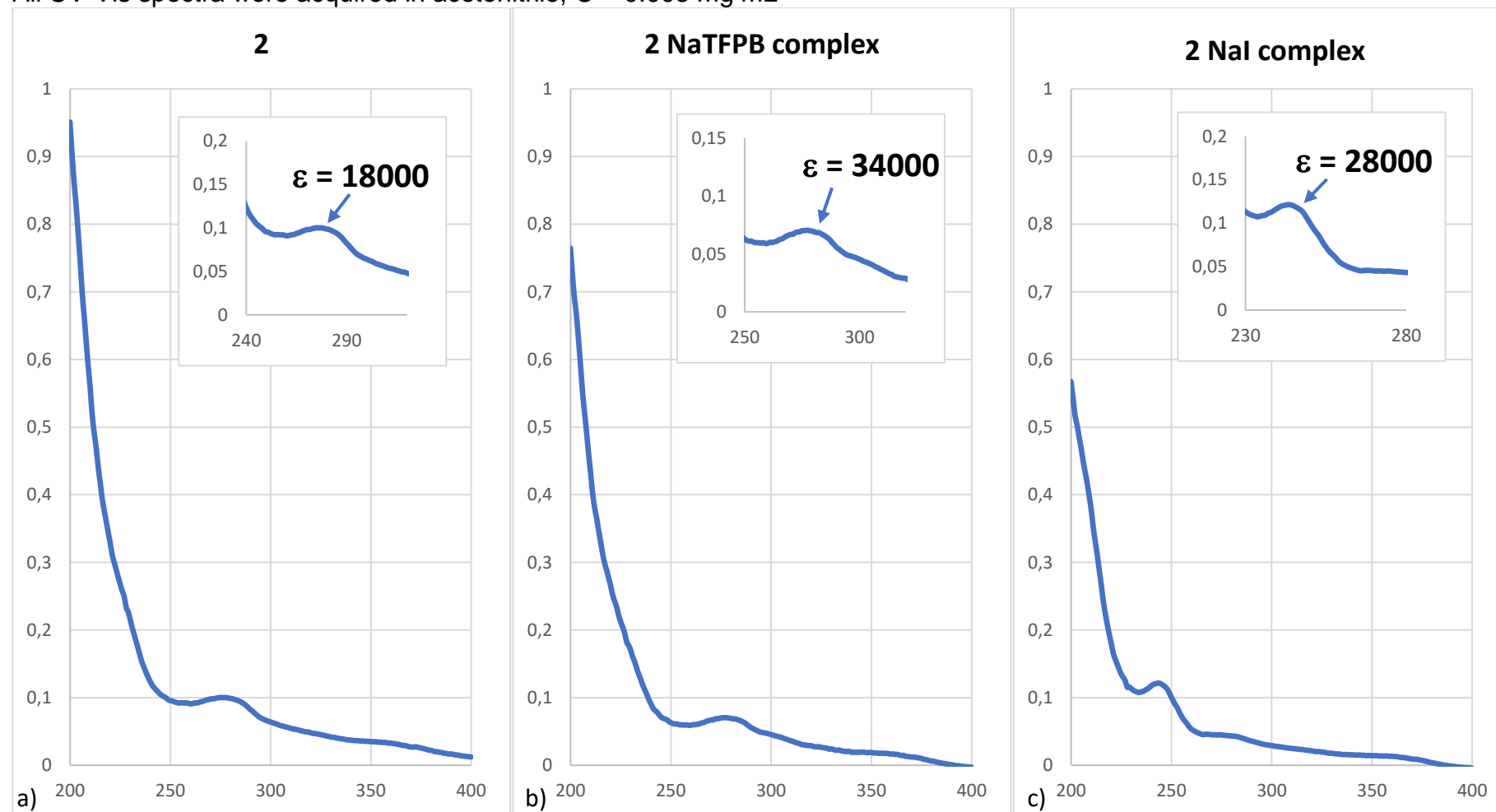


Figure S12. UV-Vis spectra of a) **2** (λ_{max} 275 nm, $\pi \rightarrow \pi^*$); b) **2** as NaTFPB complex (λ_{max} 277 nm, $\pi \rightarrow \pi^*$); c) **2** as NaI complex (λ_{max} 244 nm, $\pi \rightarrow \pi^*$).

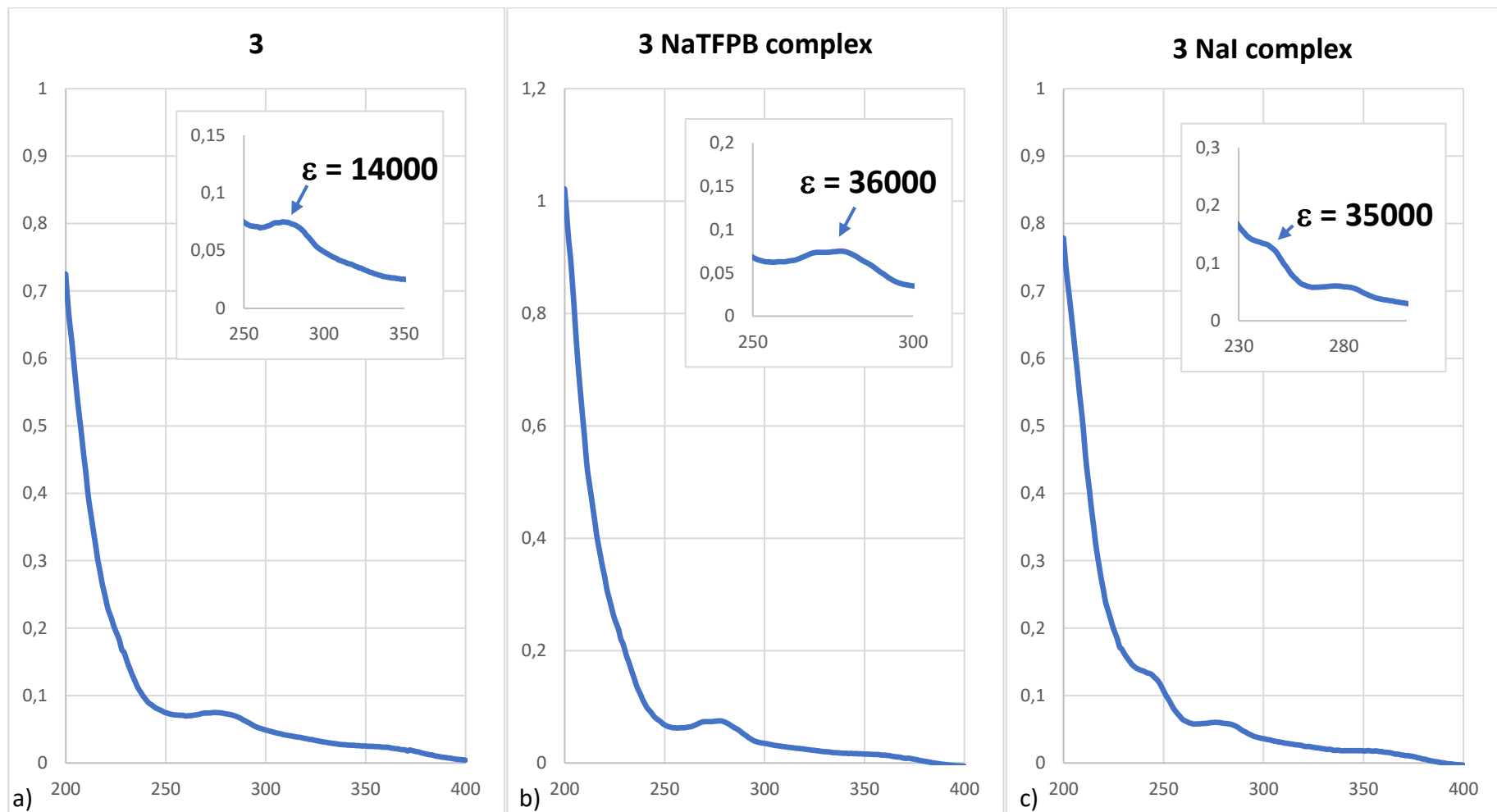


Figure S13. UV-Vis spectra of a) **3** (λ_{max} 274 nm, $\pi \rightarrow \pi^*$); b) **3** as NaTFPB complex (λ_{max} 277 nm, $\pi \rightarrow \pi^*$); c) **3** as NaI complex (λ_{max} 234 nm, $\pi \rightarrow \pi^*$).

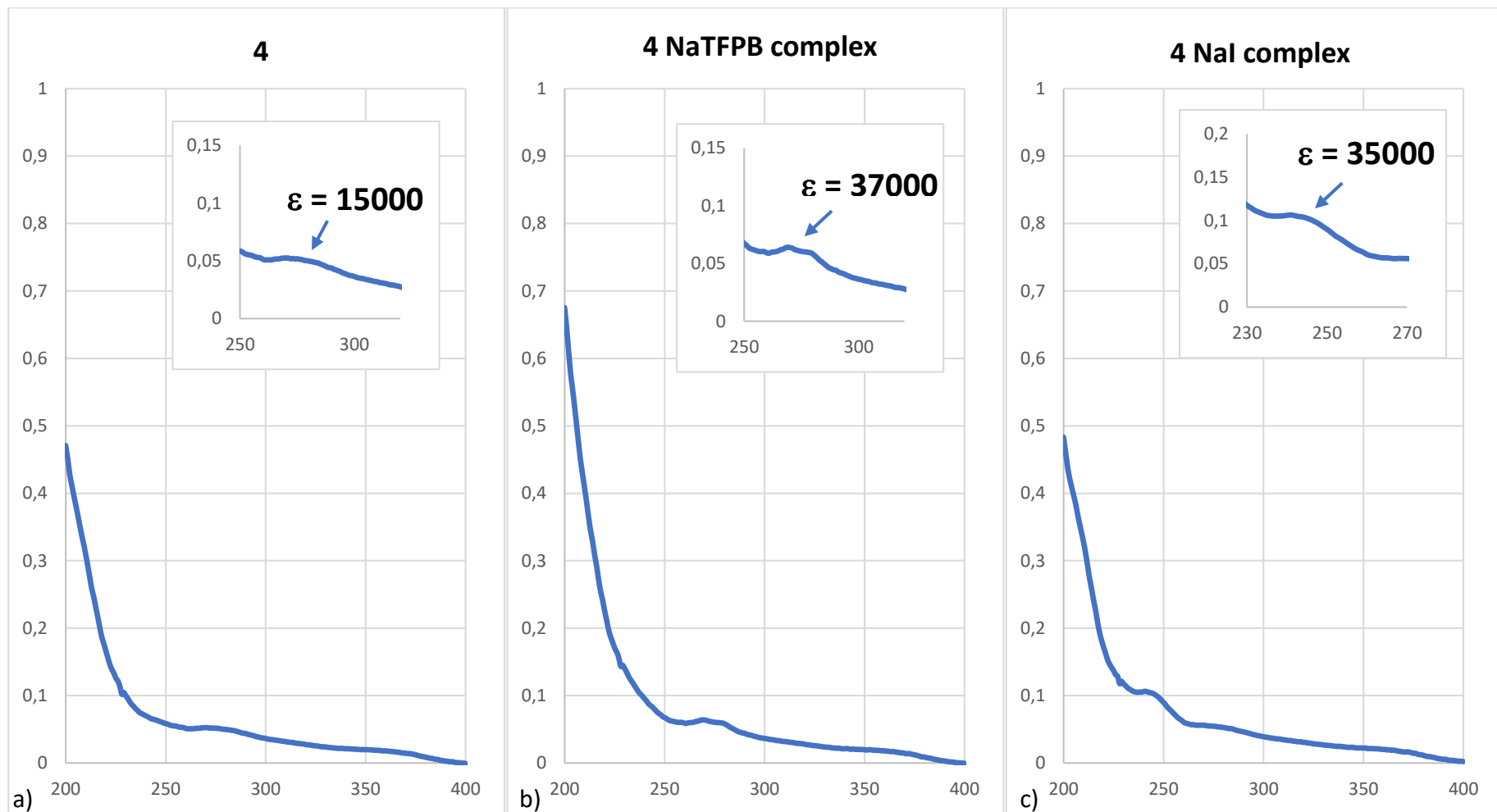


Figure S14. UV-Vis spectra of a) **4** (λ_{max} 271 nm, $\pi \rightarrow \pi^*$); b) **4** as NaTFPB complex (λ_{max} 269 nm, $\pi \rightarrow \pi^*$); c) **4** as NaI complex (λ_{max} 241 nm, $\pi \rightarrow \pi^*$).

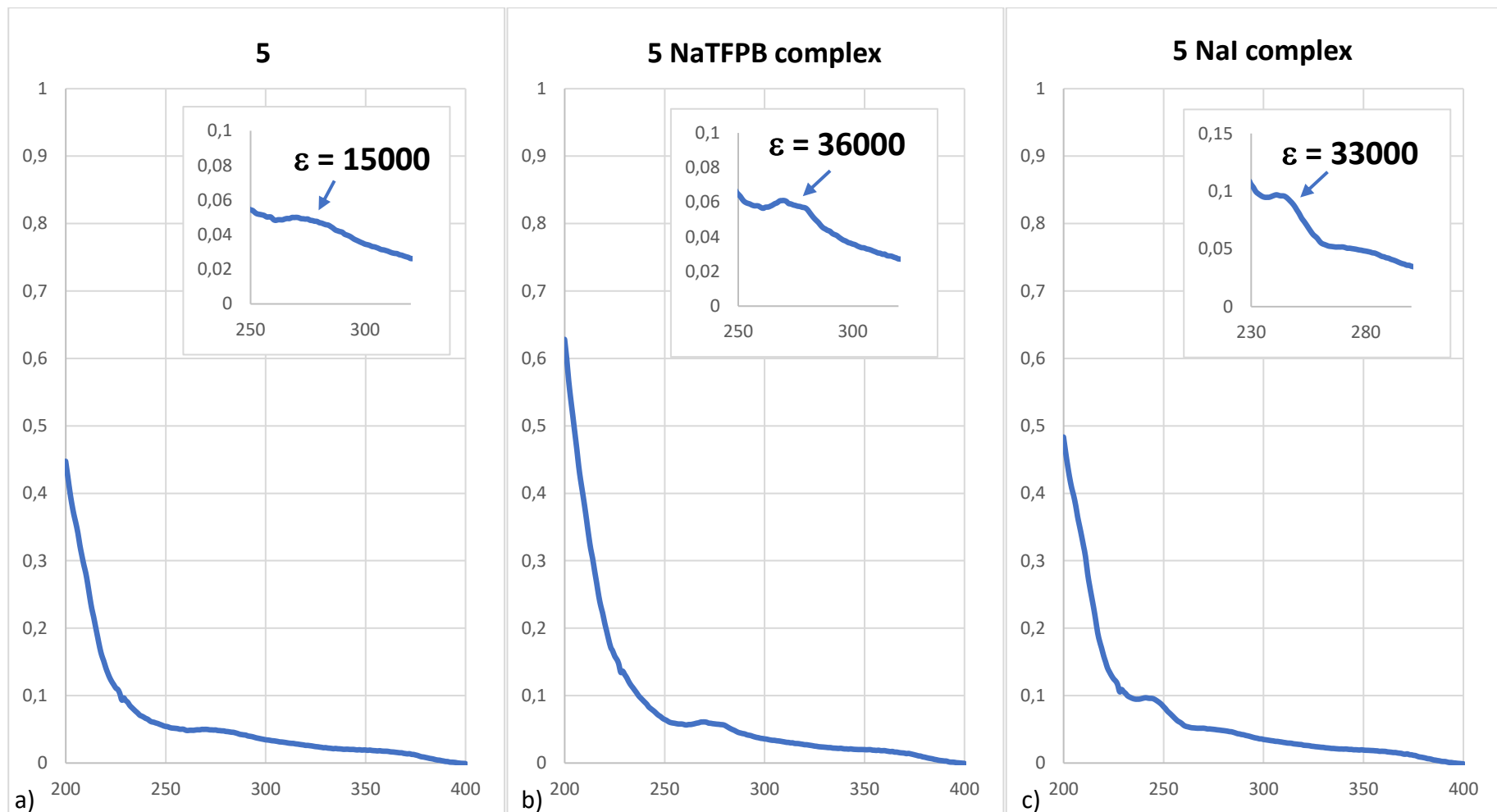


Figure S15. UV-Vis spectra of a) **5** (λ_{max} 270 nm, $\pi \rightarrow \pi^*$); b) **5** as NaTFPB complex (λ_{max} 270 nm, $\pi \rightarrow \pi^*$); c) **5** as NaI complex (λ_{max} 241 nm, $\pi \rightarrow \pi^*$).

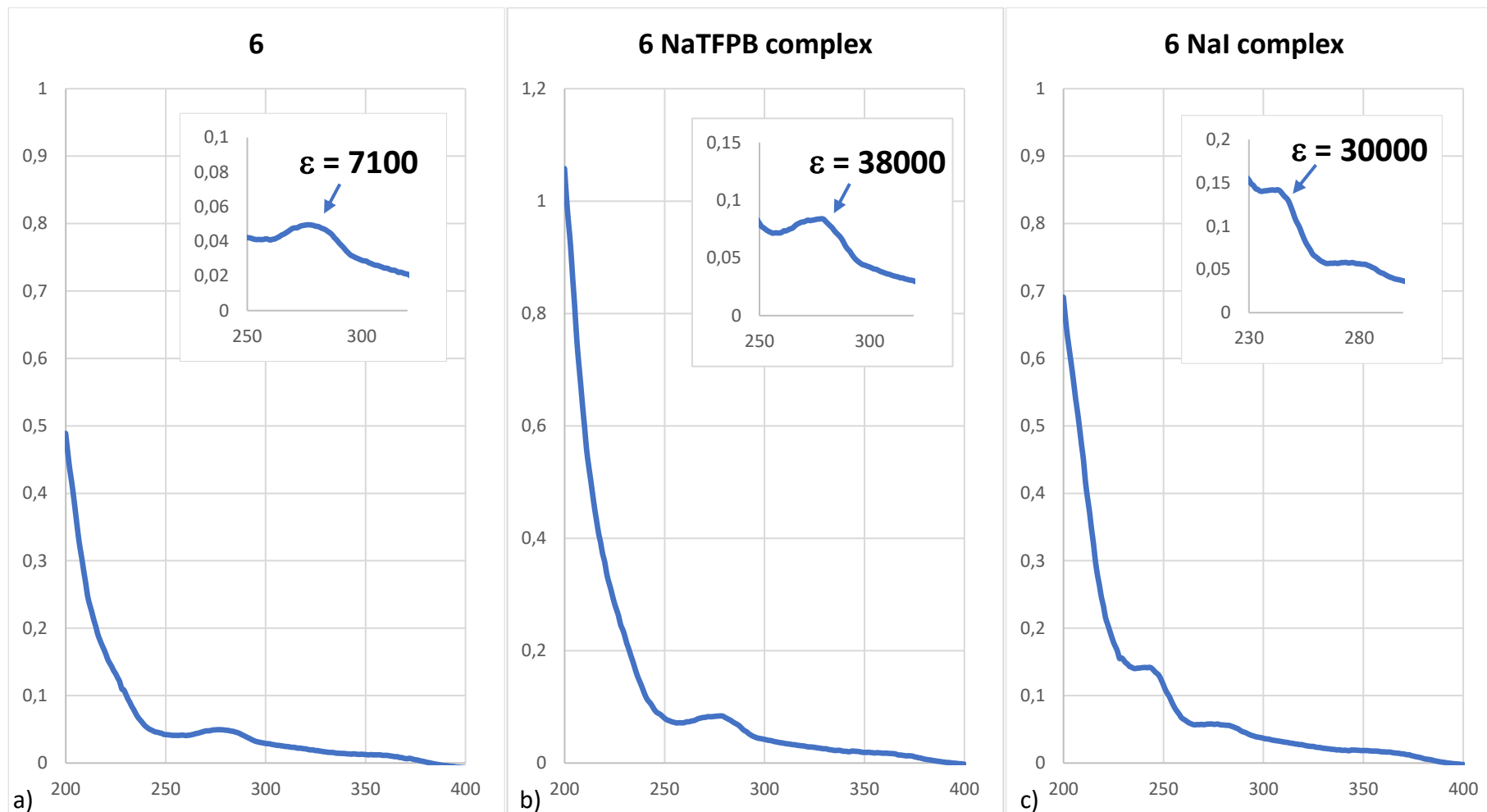


Figure S16. UV-Vis spectra of a) **6** (λ_{max} 277 nm, $\pi \rightarrow \pi^*$); b) **6** as NaTFPB complex (λ_{max} 278 nm, $\pi \rightarrow \pi^*$); c) **6** as NaI complex (λ_{max} 243 nm, $\pi \rightarrow \pi^*$).

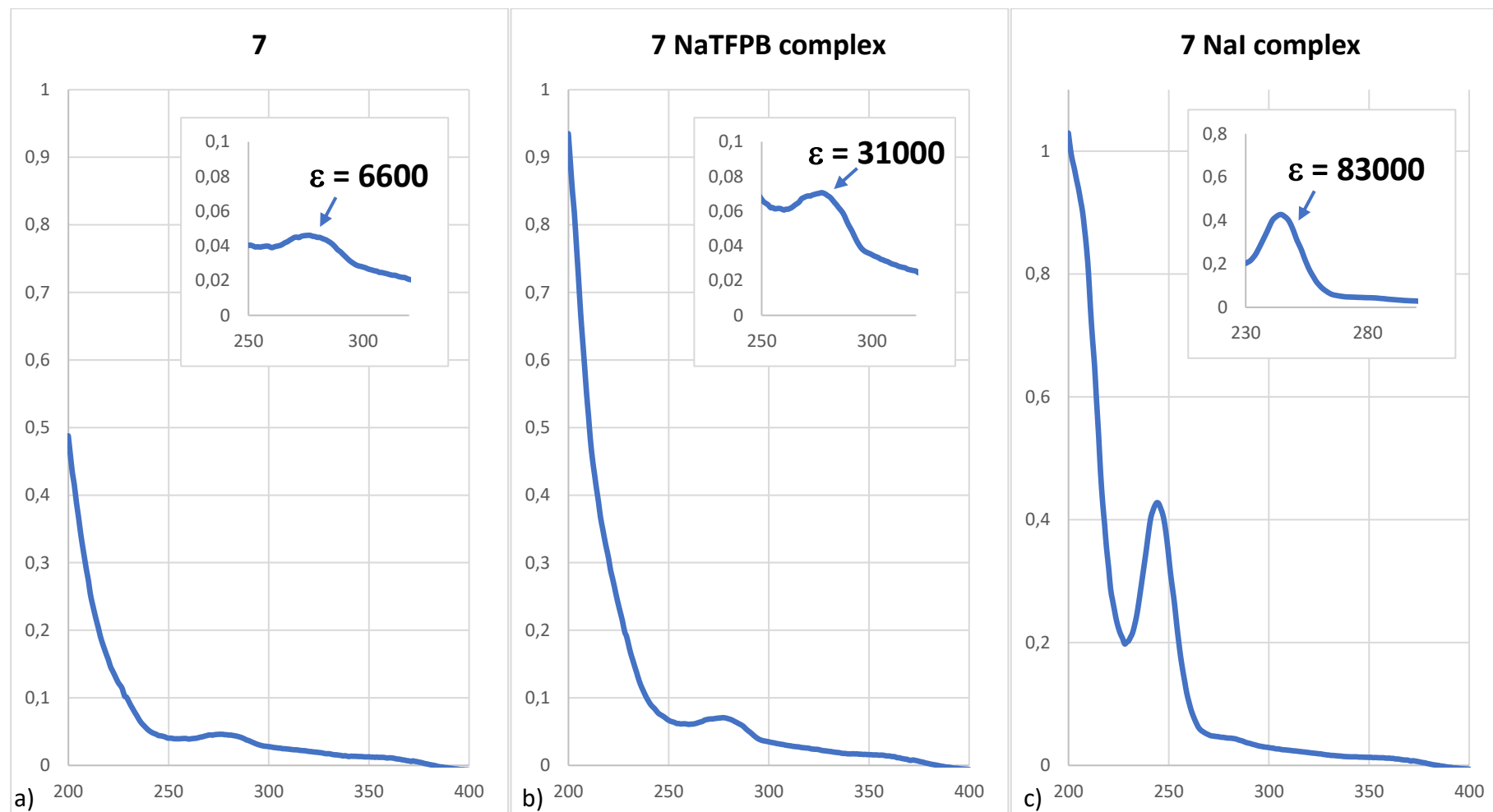


Figure S17. UV-Vis spectra of a) **7** (λ_{\max} 276 nm, $\pi \rightarrow \pi^*$); b) **7** as NaTFPB complex (λ_{\max} 277 nm, $\pi \rightarrow \pi^*$); c) **7** as NaI complex (λ_{\max} 244 nm, $\pi \rightarrow \pi^*$).

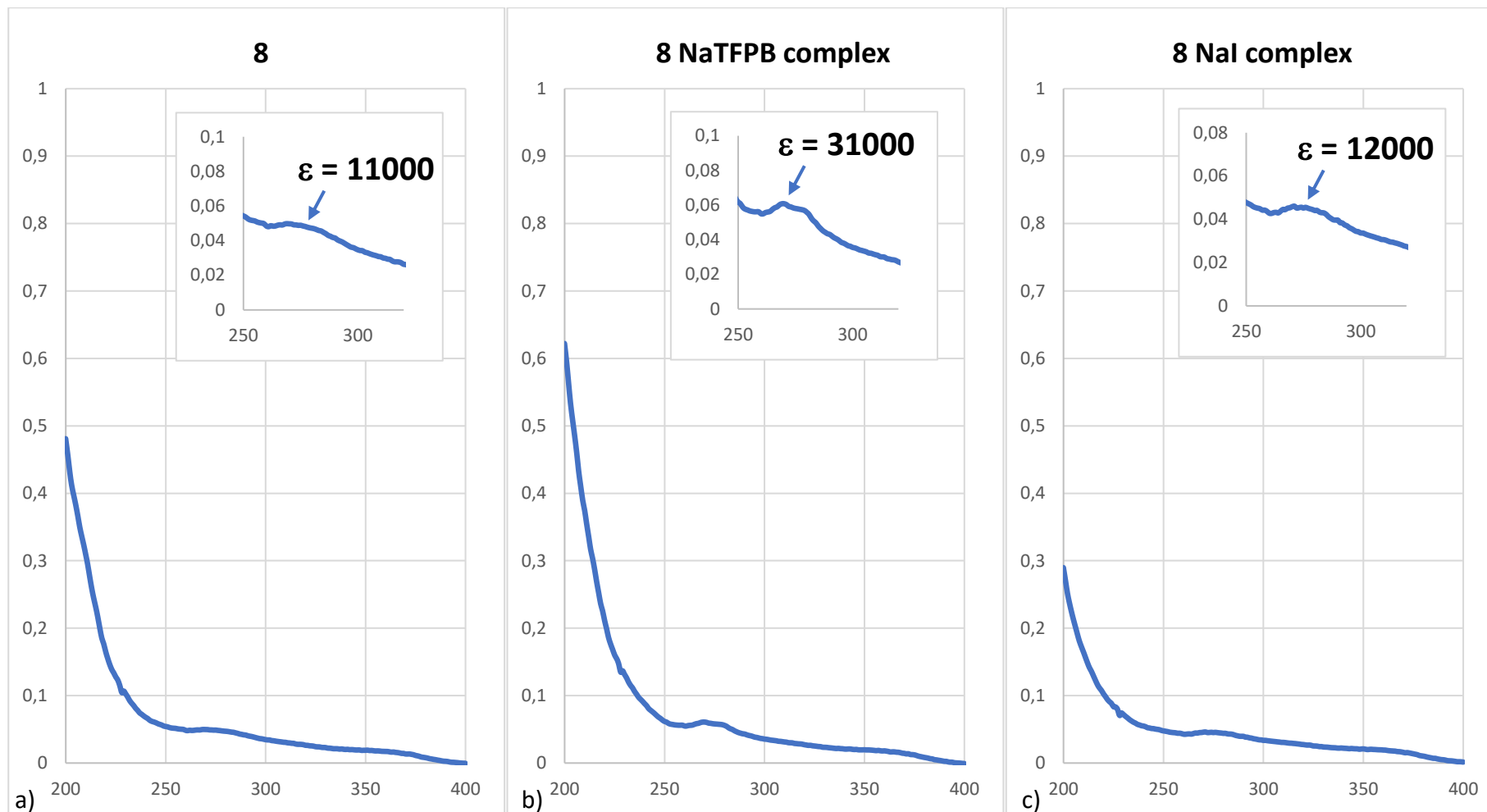


Figure S18. UV-Vis spectra of a) **8** (λ_{\max} 269 nm, $\pi \rightarrow \pi^*$); b) **8** as NaTFPB complex (λ_{\max} 270 nm, $\pi \rightarrow \pi^*$); c) **8** as NaI complex (λ_{\max} 271 nm, $\pi \rightarrow \pi^*$).

4.0 CD spectra (Figures S19-S26)

The spectra of the iodide salts were recorded in order to eliminate the possible influence of the large polyaromatic TFBP counterion.

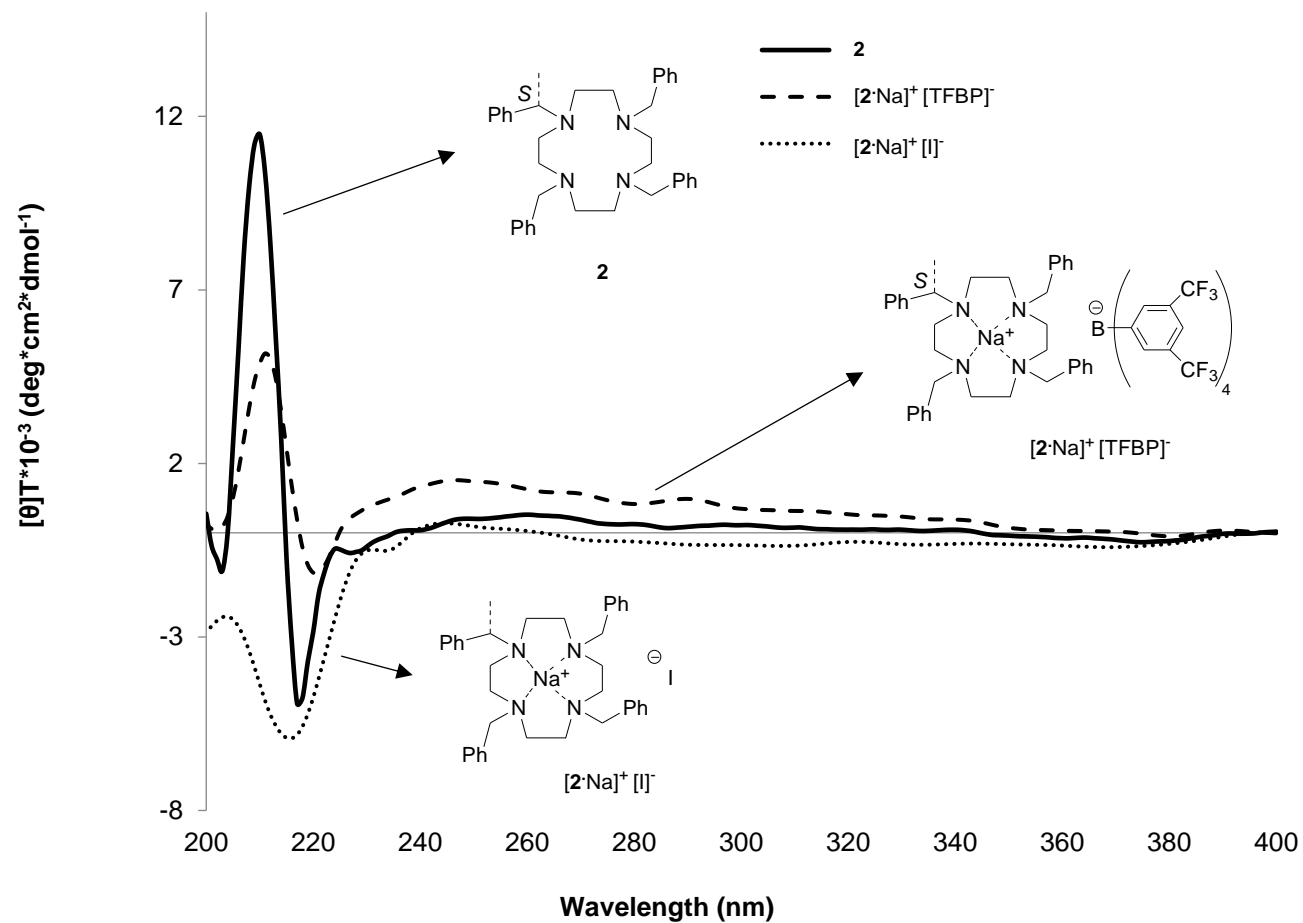


Figure S19. CD spectra of **2**, **2** in the presence of 1 equivalent NaTFBP, and **2** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

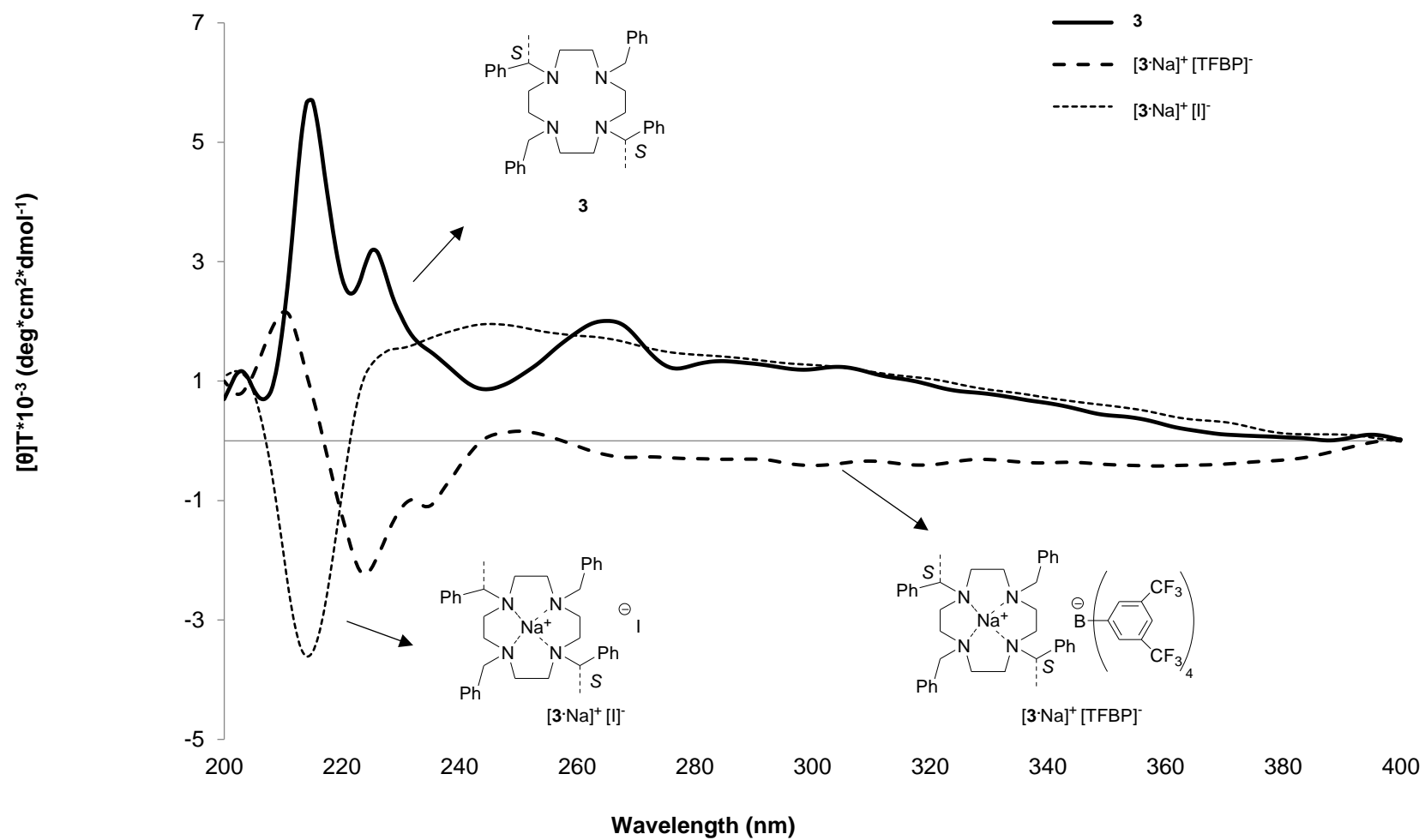


Figure S20. CD spectra of **3**, **3** in the presence of 1 equivalent NaTFPB, and **3** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

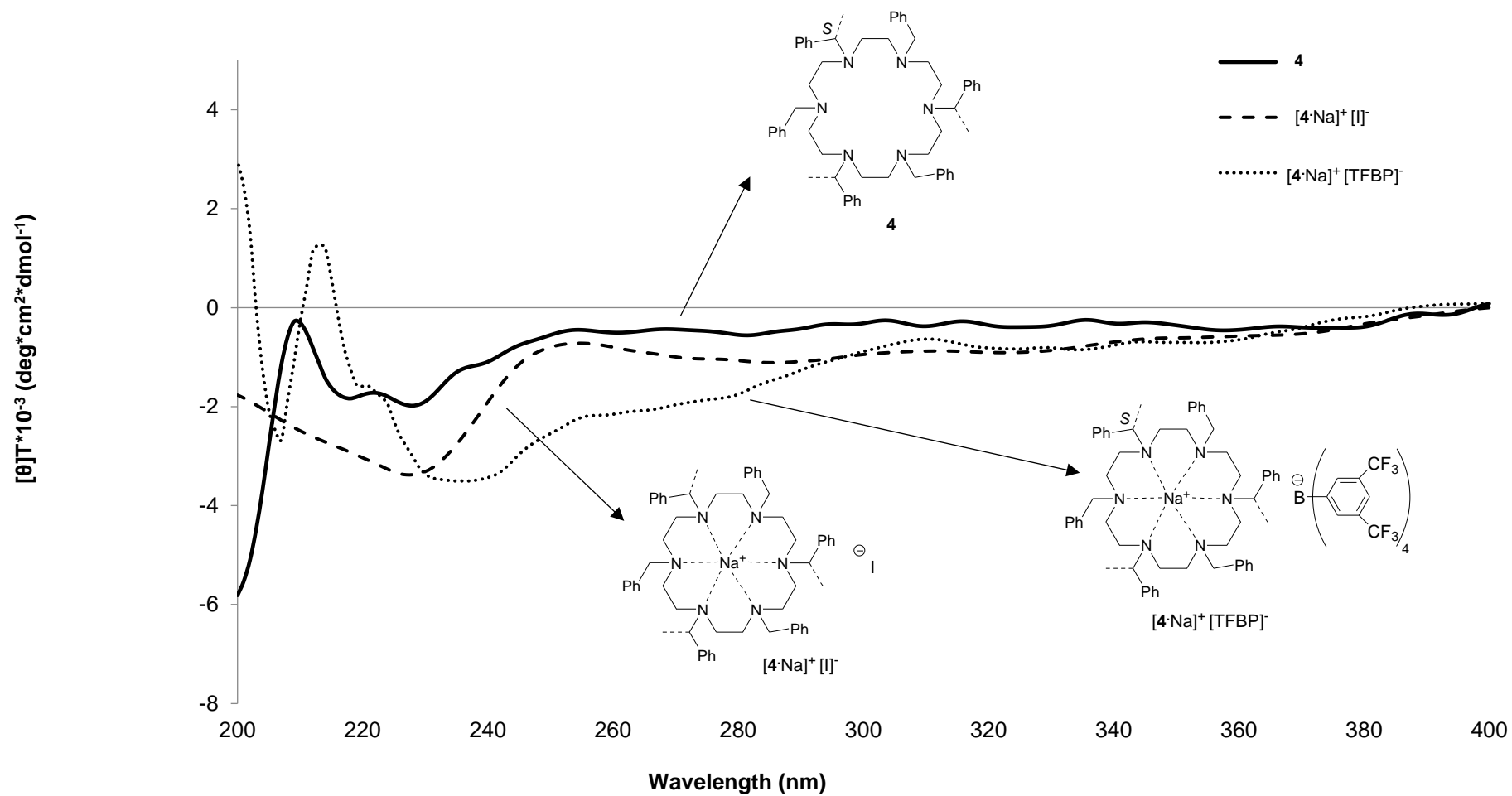


Figure S21. CD spectra of **4**, **4** in the presence of 1 equivalent NaIFPB, and **4** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

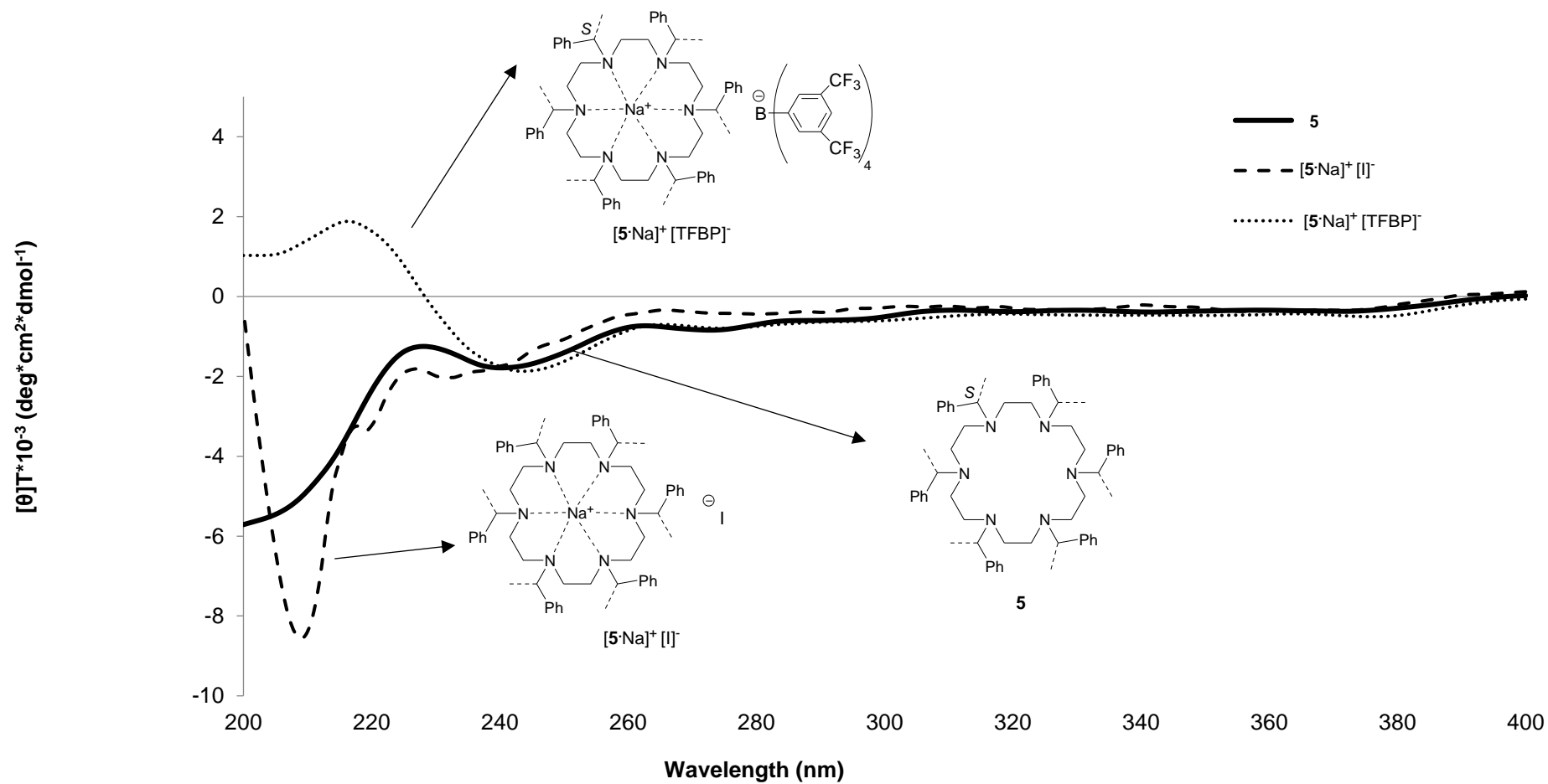


Figure S22. CD spectra of **5**, **5** in the presence of 1 equivalent NaTFPB, and **5** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

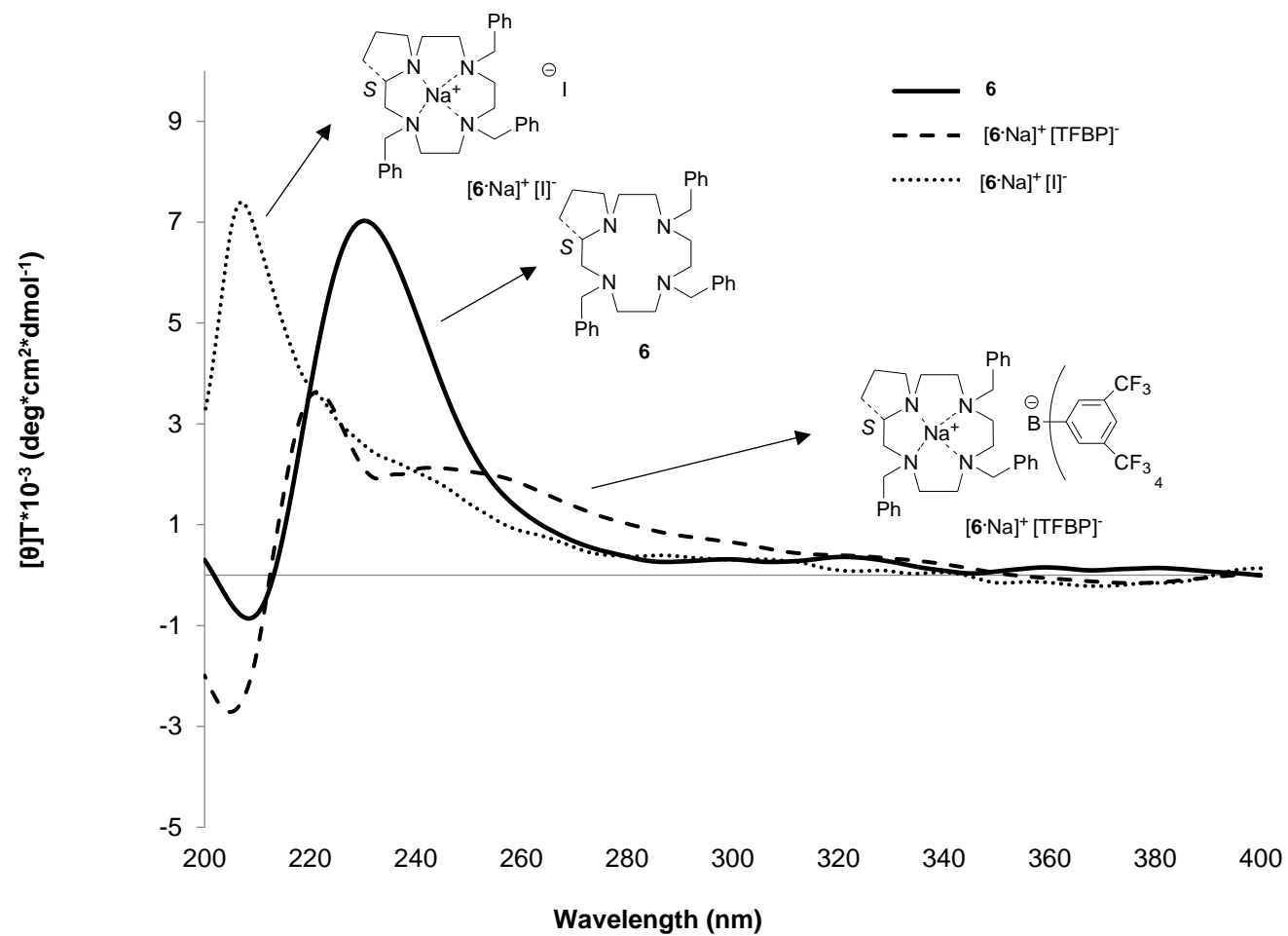


Figure S23. CD spectra of **6**, **6** in the presence of 1 equivalent NaTFPB, and **6** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

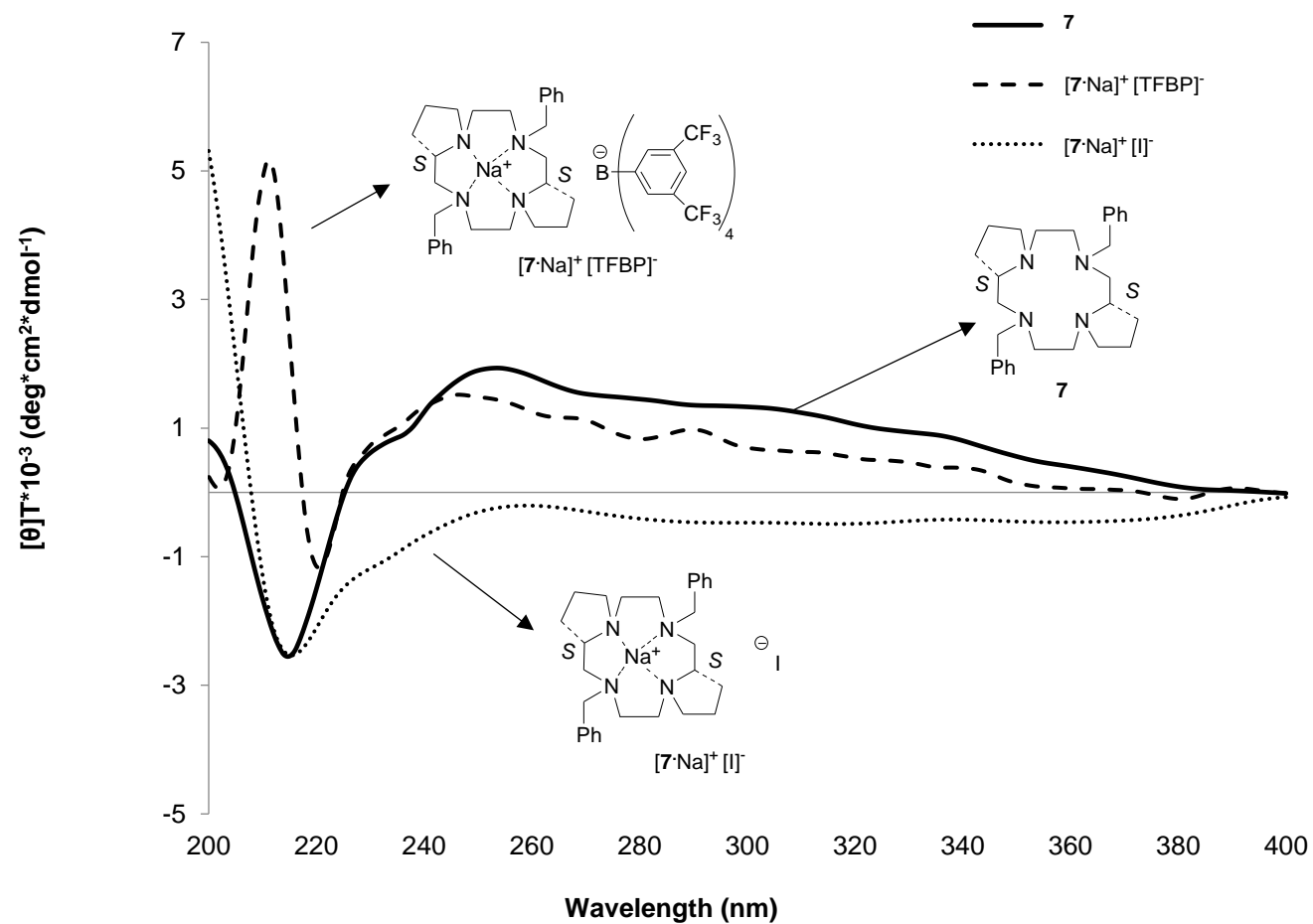


Figure S24. CD spectra of **7**, **7** in the presence of 1 equivalent NaTFPB, and **7** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

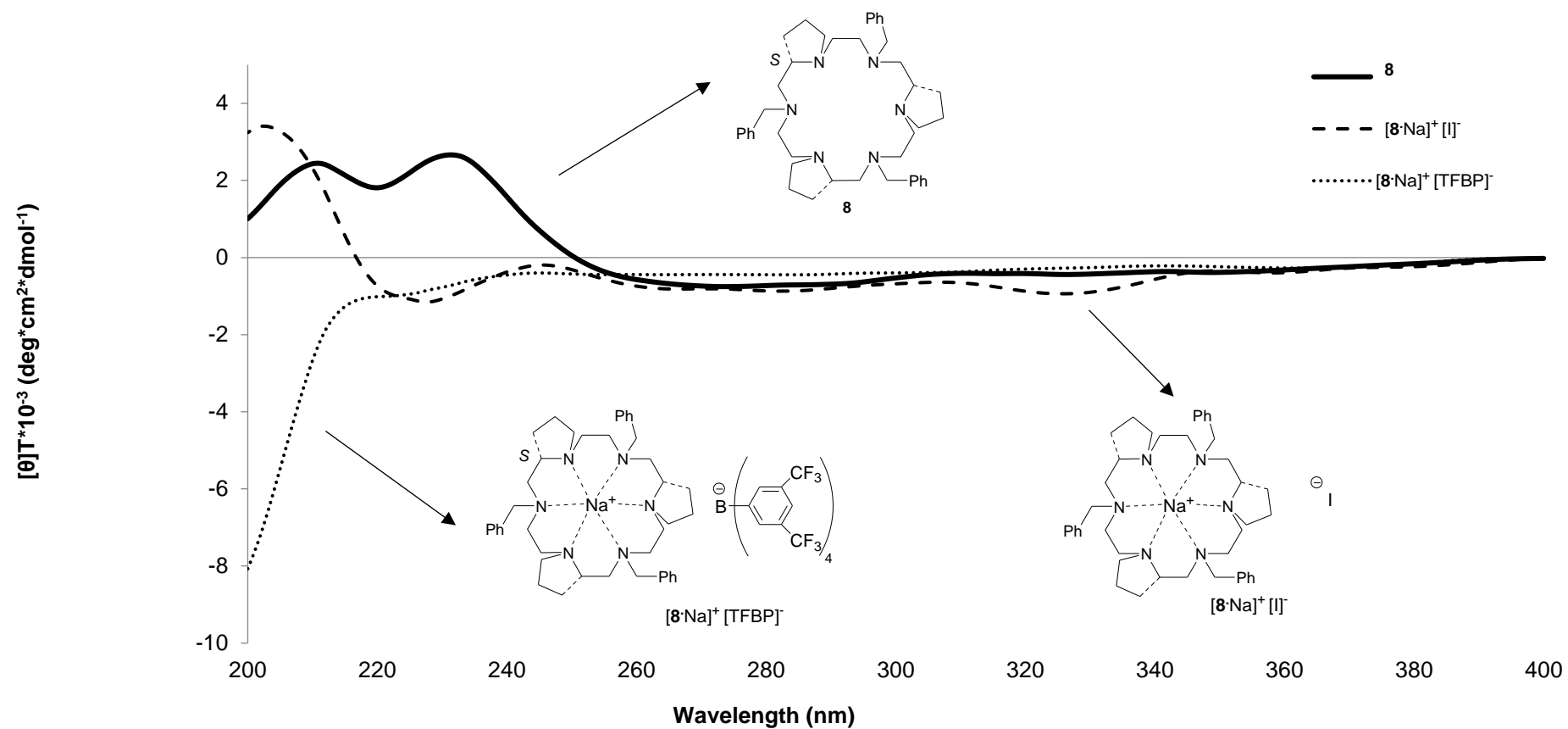


Figure S25. CD spectra of **8**, **8** in the presence of 1 equivalent NaTFPB, and **8** in the presence of 1 equivalent of NaI. Solvent: acetonitrile.

5.0 Computational Details

The DFT calculations were performed with the Gaussian09 set of programs,¹ using the BP86 functional of Becke and Perdew.² The electronic configuration of the molecular systems was described with the standard triple zeta valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O, Na (TZVP keyword in Gaussian).³ The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations. Solvent effects including contributions of non electrostatic terms have been estimated in single-point calculations on the gas phase optimized structures, based on the polarizable continuous solvation model PCM using CHCl₃ or Toluene as a solvent.⁴

¹ Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; N. Kudin, K.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

² a) Becke, A. *Phys. Rev. A* **1988**, *38*, 3098– 3100. b) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822– 8824. c) Perdew, J. P. *Phys. Rev. B* **1986**, *34*, 7406– 7406.

³ Schaefer, A., Horn, H. and Ahlrichs, R. *J. Chem. Phys.* **1994**, *100*, 5829– 5835.

⁴ a) Barone, V. and Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995– 2001. b) Tomasi, J. and Persico, M. *Chem. Rev.* **1994**, *94*, 2027– 2094.

5.1 Cartesian Coordinates and energies of calculated structures

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13 E(gas)=-1760.39607517 E(CHCl3)=-1760.41146672

C	1.796215	-2.177652	0.279454
N	0.937741	-3.325260	-0.032205
N	2.084858	0.224838	-0.372965
N	-0.244640	2.211273	0.051586
N	-1.349998	-1.338933	0.442115
C	3.212675	-2.796905	0.177671
H	1.567986	-1.813608	1.291028
C	1.583770	-1.010061	-0.730568
C	1.653172	-4.370438	-0.798110
H	1.651211	-5.304695	-0.214009
H	1.133880	-4.570909	-1.746061
C	3.063418	-3.789238	-0.989225
H	3.837635	-4.568389	-0.982251
C	1.772308	1.397285	-1.201675
H	1.215147	1.040589	-2.078611
H	2.701262	1.874976	-1.543615
C	1.022829	2.493072	-0.407536
C	2.910283	0.496819	0.807901
H	2.862190	-0.363820	1.486526
H	2.458809	1.334665	1.363066
C	4.369353	0.817077	0.501634
C	4.994640	0.416876	-0.687751
H	4.414489	-0.099116	-1.456957
C	6.350619	0.688768	-0.907287
H	6.820576	0.375971	-1.842503
C	7.099109	1.361606	0.062737
H	8.156247	1.575457	-0.108381
C	6.480921	1.770473	1.250551
H	7.054031	2.307948	2.009368
C	5.125812	1.505550	1.463792
H	4.645480	1.841755	2.387058
C	-0.984583	1.007582	-0.278656
H	-0.653566	0.620352	-1.252491
H	-2.045528	1.285772	-0.389119
C	-0.823408	-0.115565	0.775831
C	-0.905374	3.167511	0.957492
H	-0.146149	3.923984	1.202132
H	-1.175571	2.633242	1.882146
C	-2.128324	3.822361	0.343178
C	-2.020022	4.555472	-0.851704
H	-1.044806	4.644771	-1.337139
C	-3.141588	5.174528	-1.409000
H	-3.042368	5.746480	-2.334504
C	-4.389653	5.071413	-0.780039
H	-5.265197	5.557430	-1.216122

C	-4.507836	4.345848	0.408804
H	-5.476918	4.261716	0.906064
C	-3.382444	3.723645	0.964374
H	-3.476477	3.158844	1.896550
C	-1.032445	-2.503887	1.272282
H	-1.954068	-2.967277	1.652172
H	-0.439646	-2.143133	2.124510
C	-0.307800	-3.598935	0.461745
C	-2.211095	-1.604940	-0.730849
H	-1.756075	-2.425501	-1.307168
H	-2.203781	-0.726105	-1.383619
C	-3.640675	-1.957701	-0.351948
C	-4.576005	-0.947766	-0.070649
H	-4.279740	0.103186	-0.135627
C	-5.889755	-1.270391	0.280654
H	-6.608087	-0.474313	0.489275
C	-6.285687	-2.611433	0.355345
H	-7.312880	-2.864560	0.627285
C	-5.362030	-3.623820	0.076616
H	-5.663913	-4.672078	0.132731
C	-4.046808	-3.299637	-0.276699
H	-3.321731	-4.092212	-0.481105
O	0.962907	-1.185356	-1.785358
O	1.581573	3.572087	-0.185812
O	-0.187646	0.075702	1.819970
O	-0.858195	-4.686578	0.244584
H	3.127895	-3.255441	-1.949172
H	4.002382	-2.051709	0.015561
H	3.434898	-3.329641	1.115990

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13a E(gas)=-1760.36268257 E(CHCl3)=-1760.37818581

H	2.408042	-0.924273	0.361312
H	0.959055	-0.632084	1.338512
C	0.803362	0.159808	-0.670965
C	1.679339	-3.001066	-0.959163
H	1.089437	-3.890397	-1.225466
H	1.827951	-2.403809	-1.873328
C	3.015022	-3.401598	-0.362929
C	3.078519	-4.076368	0.868704
H	2.153461	-4.291606	1.409424
C	4.307786	-4.476712	1.398301
H	4.341054	-5.004705	2.354191
C	5.494994	-4.211593	0.703142
H	6.455268	-4.527343	1.116798
C	5.443218	-3.541035	-0.522553
H	6.363901	-3.328458	-1.070838
C	4.210056	-3.135795	-1.048423
H	4.173286	-2.609532	-2.006607

C	0.160444	2.453234	-1.083228
H	-0.485837	1.889385	-1.774049
H	0.872689	3.027828	-1.694511
C	-0.656759	3.519529	-0.334696
C	1.698557	1.982198	0.837797
H	1.892530	1.167497	1.544468
H	1.111611	2.732841	1.388550
C	3.008043	2.580751	0.348293
C	4.180361	1.807416	0.322481
H	4.158043	0.775148	0.683215
C	5.384135	2.346674	-0.141931
H	6.287727	1.732934	-0.149280
C	5.430201	3.671891	-0.588349
H	6.369436	4.095989	-0.950399
C	4.270417	4.454040	-0.559396
H	4.301372	5.492029	-0.898188
C	3.067611	3.914915	-0.089951
H	2.166704	4.534718	-0.066554
C	-2.414302	1.912231	0.760144
C	-3.616286	2.110609	-0.189630
H	-2.847027	2.055345	1.770532
N	-1.668077	3.189060	0.556091
N	-1.859955	-0.581958	0.505315
C	-1.605610	0.629069	1.108404
C	-2.720429	4.218092	0.750471
C	-1.341179	-1.805644	1.146069
H	-2.191421	-2.458593	1.390706
H	-0.842478	-1.498700	2.074928
C	-0.427718	-2.682531	0.256616
C	-2.632510	-0.805296	-0.720874
H	-2.024053	-1.435625	-1.388065
H	-2.737010	0.151740	-1.243391
C	-3.997130	-1.446297	-0.509547
C	-4.726579	-1.282400	0.677134
H	-4.290748	-0.722371	1.508618
C	-5.999846	-1.846588	0.816976
H	-6.550785	-1.716030	1.751230
C	-6.563414	-2.578239	-0.232972
H	-7.556356	-3.019700	-0.124564
C	-5.840567	-2.752165	-1.418755
H	-6.266068	-3.334207	-2.239230
C	-4.565101	-2.196154	-1.551722
H	-3.997350	-2.352224	-2.473145
N	0.841441	-2.230290	-0.025334
N	0.844605	1.468841	-0.254537
O	0.287793	-0.178078	-1.742927
O	-0.407707	4.705541	-0.583998
O	-0.859959	0.715424	2.093671

O	-0.843646	-3.778496	-0.131977
C	1.307639	-0.901438	0.331140
C	-4.014942	3.572873	0.154498
H	-2.406138	5.137192	0.246601
H	-2.829652	4.423774	1.826222
H	-4.361771	4.115935	-0.735059
H	-4.831140	3.589197	0.891518
H	-4.432031	1.395549	-0.021085
H	-3.303640	2.043382	-1.242486

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13b E(gas)=-1760.37719057 E(CHCl3)=-1760.39724986

C	-1.408546	-1.680669	0.798229
C	-1.908898	0.495691	1.805425
C	-1.160204	1.841621	1.902746
C	-1.055364	-2.500156	-0.464358
C	0.837031	1.076035	0.542658
C	1.165618	-0.214048	1.322327
C	1.643817	-2.608866	1.229714
C	0.937217	-3.807850	0.579562
C	2.123267	-1.208635	-0.773512
C	3.644568	-1.069823	-0.796006
C	0.788573	3.300708	1.654805
C	1.008899	4.191341	0.447824
C	-0.785305	-4.921931	-0.730854
H	0.015024	-5.544068	-1.151339
C	-2.212944	0.235054	-0.643103
C	-3.730424	0.365644	-0.756375
H	-1.768726	1.238789	-0.765043
H	-2.968791	0.760389	1.936977
H	-1.600755	-0.108788	2.671154
C	-2.321122	-3.130548	-1.106929
H	-0.545929	-1.851371	-1.198164
H	0.310259	0.829752	-0.390472
H	1.773615	1.568335	0.236134
H	1.236677	-2.483879	2.243444
H	2.697906	-2.913510	1.322622
H	1.839160	-2.108224	-1.345187
H	1.677883	-0.353959	-1.305943
H	0.166709	3.809370	2.404175
H	1.753205	3.045674	2.123934
H	-1.264946	-5.501845	0.076357
C	-1.801499	-4.418950	-1.755847
H	-1.839061	-0.370944	-1.482052
N	0.083325	2.043606	1.328946
N	1.523007	-1.315078	0.556827
N	-0.206494	-3.675375	-0.177310
N	-1.726996	-0.336995	0.614176
O	1.033940	-0.267013	2.542139

O	1.428388	-4.925654	0.767913
O	-1.368492	-2.198284	1.911500
O	-1.709709	2.722848	2.570153
C	-4.264846	1.333716	-1.621624
C	-5.646845	1.453045	-1.793075
C	-6.515823	0.611747	-1.088910
C	-5.992175	-0.346055	-0.214987
C	-4.607639	-0.469750	-0.050868
H	-3.591967	2.004420	-2.164315
H	-6.046557	2.212328	-2.468896
H	-7.596243	0.709357	-1.213677
H	-6.663160	-0.997793	0.348924
H	-4.209802	-1.211194	0.645600
C	2.303134	4.499914	0.003161
C	2.501290	5.329184	-1.108501
C	1.401972	5.859993	-1.788766
C	0.104455	5.561058	-1.350649
C	-0.090390	4.734551	-0.241639
H	3.166960	4.093957	0.537959
H	3.516023	5.559807	-1.440777
H	1.552721	6.508454	-2.654636
H	-0.757919	5.984864	-1.870769
H	-1.102146	4.514881	0.109510
C	4.335603	-1.369357	-1.981301
C	5.721843	-1.211697	-2.058468
C	6.439581	-0.760089	-0.944531
C	5.760364	-0.469851	0.242209
C	4.370304	-0.622580	0.316190
H	3.783255	-1.733523	-2.852851
H	6.244570	-1.450952	-2.987234
H	7.523942	-0.643874	-1.000040
H	6.312956	-0.128419	1.120325
H	3.853262	-0.405721	1.253875
H	-1.305345	-4.197981	-2.714817
H	-2.600577	-5.148437	-1.947508
H	-2.818458	-2.445283	-1.806402
H	-3.039734	-3.379572	-0.310261

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(*S,S*)- $\Delta(\delta\delta\delta\delta)$ -[3·Na]⁺ E(gas)=-1858.60049697 E(CHCl₃)=-1858.64697181

C	-1.075101	1.898225	-2.765233
H	-1.732282	2.599611	-3.322388
H	-0.764949	1.139278	-3.498084
C	0.156038	2.681078	-2.289796
H	0.524583	3.271711	-3.153218
H	-0.150332	3.408285	-1.524138
C	-2.689500	2.230138	-0.986750
H	-2.042441	3.082329	-0.732753
H	-3.465595	2.609103	-1.685520

C	-3.350367	1.732493	0.280788
C	-2.631777	1.691146	1.488216
H	-1.592620	2.033647	1.514434
C	-3.247132	1.268183	2.671288
H	-2.682474	1.265251	3.606257
C	-4.591078	0.876012	2.664086
H	-5.073733	0.553728	3.588812
C	-5.319242	0.921358	1.470836
H	-6.372928	0.635214	1.461005
C	-4.702909	1.352113	0.290343
H	-5.287019	1.415205	-0.632116
C	1.961912	1.095509	-2.749099
H	2.703991	1.738281	-3.263911
H	1.239592	0.811935	-3.528548
C	2.701173	-0.152344	-2.251222
H	3.310708	-0.543576	-3.095018
H	3.414956	0.133519	-1.465051
C	2.166424	2.653896	-0.838552
C	2.792315	3.873477	-1.538797
H	2.988003	1.961077	-0.597712
C	1.511597	2.994185	0.499059
C	1.570905	2.053934	1.544606
H	2.051562	4.637628	-1.812570
C	1.016205	2.330973	2.798988
H	1.102731	1.597817	3.603932
C	0.383769	3.558153	3.030825
H	-0.037485	3.784910	4.012173
C	0.318394	4.503218	2.002353
H	-0.157771	5.470037	2.178156
C	0.881110	4.224720	0.750485
H	0.851586	4.995564	-0.022347
C	1.075113	-1.898338	-2.765171
H	1.732302	-2.599743	-3.322295
H	0.764970	-1.139417	-3.498051
C	-0.156031	-2.681179	-2.289725
H	-0.524569	-3.271835	-3.153135
H	0.150329	-3.408367	-1.524045
C	2.689484	-2.230187	-0.986650
H	3.465577	-2.609191	-1.685402
H	2.042420	-3.082362	-0.732611
C	3.350362	-1.732487	0.280859
C	4.702916	-1.352152	0.290391
H	5.287020	-1.415308	-0.632067
C	5.319266	-0.921353	1.470860
H	6.372962	-0.635245	1.461011
C	4.591107	-0.875920	2.664109
H	5.073775	-0.553604	3.588817
C	3.247147	-1.268044	2.671335

H	2.682491	-1.265043	3.606304
C	2.631775	-1.691049	1.488286
H	1.592607	-2.033516	1.514527
C	-1.961902	-1.095619	-2.749085
H	-2.703976	-1.738401	-3.263889
H	-1.239575	-0.812063	-3.528535
C	-2.701167	0.152247	-2.251246
H	-3.310701	0.543453	-3.095055
H	-3.414952	-0.133597	-1.465070
C	-2.166417	-2.653962	-0.838496
C	-2.792260	-3.873596	-1.538697
H	-2.988022	-1.961156	-0.597709
C	-1.511610	-2.994163	0.499146
C	-1.570986	-2.053864	1.544648
H	-3.323597	-3.581767	-2.456056
C	-1.016301	-2.330816	2.799055
H	-1.102879	-1.597625	3.603961
C	-0.383808	-3.557955	3.030964
H	0.037437	-3.784643	4.012331
C	-0.318365	-4.503064	2.002538
H	0.157844	-5.469852	2.178396
C	-0.881069	-4.224654	0.750644
H	-0.851485	-4.995532	-0.022152
N	-1.837430	1.219409	-1.688490
N	1.225984	1.841716	-1.700570
N	1.837426	-1.219485	-1.688442
N	-1.225982	-1.841802	-1.700531
Na	-0.000011	-0.000026	-0.439233
H	-3.526500	-4.346582	-0.871229
H	-2.051499	-4.637794	-1.812314
H	3.323767	3.581577	-2.456066
H	3.526464	4.346548	-0.871288
H	-2.111265	-1.112491	1.395435
H	2.111143	1.112529	1.395450

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(*S,S*)- $\Delta(\lambda\lambda\lambda\lambda)$ -[3Na]⁺ E(gas)=-1858.58693717 E(CHCl₃)=-1858.62972051

N	-1.726342	1.469228	-1.397444
N	-1.427049	-1.653507	-1.369720
N	1.726230	-1.469154	-1.397343
N	1.426973	1.653523	-1.369613
C	-2.212410	0.526756	-2.438770
H	-3.114112	0.938170	-2.939863
H	-1.443711	0.466147	-3.224608
C	-2.561640	-0.889937	-1.956723
H	-3.006784	-1.424281	-2.822867
H	-3.345191	-0.820791	-1.192665
C	-2.864040	2.163177	-0.712918
H	-3.473710	2.700336	-1.469904

H	-2.412225	2.925944	-0.059890
C	-3.778671	1.295158	0.124297
C	-5.074686	0.978025	-0.313133
H	-5.422525	1.351132	-1.280638
C	-5.928177	0.198521	0.476500
H	-6.933817	-0.035866	0.121394
C	-5.499390	-0.265088	1.724788
H	-6.167534	-0.863497	2.347223
C	-4.218223	0.065034	2.183699
H	-3.892313	-0.266626	3.172138
C	-3.368088	0.841984	1.389916
H	-2.385775	1.138802	1.770620
C	-0.517587	-2.103326	-2.451875
H	-0.959000	-2.941556	-3.026650
H	-0.439457	-1.274306	-3.171891
C	0.889407	-2.531655	-2.023370
H	1.396023	-2.950742	-2.919613
H	0.814378	-3.352617	-1.299313
C	-1.958944	-2.763550	-0.484854
H	-2.826019	-2.296250	0.008964
C	-2.492430	-3.990238	-1.240592
C	-1.001759	-3.107971	0.661879
C	-0.301170	-4.321238	0.748865
H	-3.225743	-3.690305	-2.003439
C	0.529360	-4.599230	1.842580
H	1.058901	-5.553181	1.889323
C	0.665172	-3.672938	2.880713
H	1.300477	-3.897389	3.739535
C	-0.046991	-2.468906	2.823151
H	0.013785	-1.758591	3.651113
C	-0.870841	-2.195177	1.726050
H	-1.483143	-1.286224	1.725108
C	2.212443	-0.526714	-2.438603
H	3.114195	-0.938137	-2.939595
H	1.443830	-0.466083	-3.224528
C	2.561624	0.889992	-1.956486
H	3.006880	1.424366	-2.822566
H	3.345056	0.820837	-1.192310
C	2.863843	-2.163143	-0.712671
H	2.411907	-2.925669	-0.059454
H	3.473349	-2.700585	-1.469577
C	3.778794	-1.295219	0.124314
C	3.368534	-0.842003	1.390026
H	2.386207	-1.138606	1.770869
C	4.218952	-0.065238	2.183683
H	3.893282	0.266438	3.172198
C	5.500100	0.264640	1.724552
H	6.168489	0.862883	2.346884

C	5.928568	-0.199003	0.476165
H	6.934175	0.035233	0.120870
C	5.074786	-0.978326	-0.313334
H	5.422401	-1.351503	-1.280894
C	0.517558	2.103266	-2.451832
H	0.959068	2.941378	-3.026712
H	0.439347	1.274165	-3.171740
C	-0.889404	2.531713	-2.023400
H	-1.395952	2.950901	-2.919635
H	-0.814368	3.352615	-1.299281
C	1.958695	2.763591	-0.484772
H	2.825861	2.296434	0.009033
C	2.492268	3.990521	-1.240608
C	1.001536	3.108074	0.661932
C	0.301049	4.321401	0.748923
H	3.225605	3.690593	-2.003425
C	-0.529491	4.599468	1.842608
H	-1.058922	5.553481	1.889348
C	-0.665461	3.673155	2.880706
H	-1.300757	3.897655	3.739523
C	0.046573	2.469052	2.823137
H	-0.014360	1.758703	3.651060
C	0.870457	2.195270	1.726082
H	1.482587	1.286201	1.725103
Na	-0.000047	-0.000027	-0.198684
H	1.706105	4.572781	-1.742129
H	3.003676	4.664932	-0.538977
H	-1.706286	-4.572492	-1.742154
H	-3.003895	-4.664734	-0.539077
H	0.410804	5.075690	-0.033098
H	-0.410843	-5.075511	-0.033185

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(S,S)- Λ ($\delta\delta\delta\delta$)-[3 \cdot Na]⁺ E(gas)=-1858.57997014 E(CHCl₃)=-1858.62655292

N	-1.135250	1.862823	-1.362476
N	2.001494	1.188343	-1.356148
N	1.135040	-1.862878	-1.362707
N	-2.001702	-1.188361	-1.355957
C	-0.131066	2.157126	-2.417107
H	-0.426282	3.072775	-2.973614
H	-0.170802	1.340759	-3.153815
C	1.310617	2.374227	-1.942095
H	1.884748	2.770359	-2.808232
H	1.299742	3.162588	-1.183306
C	-1.508464	3.096944	-0.604946
H	-1.556763	3.965217	-1.292792
H	-2.530786	2.939061	-0.228273
C	-0.639558	3.451809	0.587623
C	-0.013932	4.704950	0.673761

H	-0.102717	5.408252	-0.159261
C	0.702963	5.074627	1.818395
H	1.175309	6.057794	1.868572
C	0.805903	4.192423	2.898227
H	1.357970	4.481898	3.794312
C	0.178290	2.942142	2.831236
H	0.227349	2.262093	3.684809
C	-0.540966	2.580577	1.687470
H	-1.097917	1.637957	1.675737
C	2.241307	0.179225	-2.429840
H	3.167764	0.428282	-2.988249
H	1.430116	0.266551	-3.166628
C	2.358503	-1.286106	-1.988624
H	2.657018	-1.875029	-2.882262
H	3.173240	-1.378028	-1.263607
C	3.330681	1.629681	-0.774571
C	3.227722	2.851239	0.155673
H	3.977750	1.917713	-1.631794
C	4.052577	0.507437	-0.038257
C	5.282533	0.027410	-0.514222
H	2.457871	2.714888	0.929034
C	5.981643	-0.971371	0.174236
H	6.936402	-1.331880	-0.214193
C	5.461928	-1.499583	1.360011
H	6.006661	-2.274686	1.902467
C	4.247069	-1.012442	1.859026
H	3.848592	-1.403995	2.797659
C	3.552905	-0.014954	1.167246
H	2.623652	0.383069	1.585391
C	0.130702	-2.156997	-2.417257
H	0.425868	-3.072527	-2.973980
H	0.170314	-1.340489	-3.153809
C	-1.310908	-2.374202	-1.942102
H	-1.885148	-2.770226	-2.808214
H	-1.299967	-3.162659	-1.183408
C	1.508293	-3.097173	-0.605484
H	2.530811	-2.939595	-0.229215
H	1.556077	-3.965385	-1.293435
C	0.639759	-3.451878	0.587402
C	0.541543	-2.580526	1.687193
H	1.098577	-1.637961	1.675185
C	-0.177379	-2.941940	2.831214
H	-0.226144	-2.261798	3.684733
C	-0.805033	-4.192186	2.898527
H	-1.356847	-4.481540	3.794806
C	-0.702462	-5.074501	1.818753
H	-1.174840	-6.057641	1.869173
C	0.014097	-4.704976	0.673858

H	0.102573	-5.408366	-0.159123
C	-2.241730	-0.179182	-2.429575
H	-3.168309	-0.428206	-2.987792
H	-1.430696	-0.266494	-3.166537
C	-2.358809	1.286128	-1.988273
H	-2.657408	1.875105	-2.881846
H	-3.173470	1.378054	-1.263171
C	-3.330743	-1.629817	-0.774168
C	-3.227367	-2.851230	0.156253
H	-3.977841	-1.918117	-1.631275
C	-4.052720	-0.507552	-0.037990
C	-5.282700	-0.027629	-0.513999
H	-3.018653	-3.783445	-0.384362
C	-5.981822	0.971231	0.174331
H	-6.936602	1.331653	-0.214126
C	-5.462097	1.499631	1.360022
H	-6.006835	2.274813	1.902361
C	-4.247220	1.012592	1.859084
H	-3.848730	1.404289	2.797652
C	-3.553043	0.015024	1.167431
H	-2.623776	-0.382907	1.585629
Na	-0.000283	-0.000097	-0.205441
H	-4.192010	-2.981361	0.666196
H	-2.456928	-2.714890	0.929028
H	3.018471	3.783317	-0.384953
H	4.192713	2.981606	0.664901
H	-5.697989	-0.439915	-1.437990
H	5.697819	0.439540	-1.438285

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(S,S)-Λ(λλλλ)-[3·Na]⁺ SS-III-Lambda E(gas)=-1858.59209289 E(CHCl₃)=-1858.63830389

C	-1.176702	-1.742269	-2.751605
H	-1.872829	-2.359497	-3.359883
H	-0.768815	-0.987859	-3.440974
C	-0.051661	-2.658230	-2.259453
H	0.277980	-3.281252	-3.118191
H	-0.455127	-3.358983	-1.515500
C	-2.826238	-1.988730	-0.980469
H	-2.221727	-2.856656	-0.679333
H	-3.596676	-2.358788	-1.689693
C	-3.502035	-1.418348	0.248093
C	-2.789928	-1.273299	1.451296
H	-1.752446	-1.618064	1.510512
C	-3.413026	-0.759508	2.593529
H	-2.853667	-0.673351	3.527781
C	-4.761670	-0.385065	2.550409
H	-5.250735	0.007900	3.443853
C	-5.485172	-0.540303	1.363823
H	-6.542342	-0.269579	1.327519

C	-4.858250	-1.054679	0.222905
H	-5.434817	-1.189739	-0.696443
C	1.926967	-1.316853	-2.695443
H	2.636489	-2.028780	-3.163287
H	1.238180	-1.032976	-3.505110
C	2.722445	-0.077689	-2.257538
H	3.299466	0.278141	-3.139478
H	3.458010	-0.362969	-1.498426
C	1.884230	-3.042318	-0.871835
H	1.920593	-3.947189	-1.515937
C	3.338816	-2.691848	-0.529846
C	1.133590	-3.420497	0.402308
C	1.078357	-2.538043	1.496713
H	3.954784	-2.537619	-1.426477
C	0.444043	-2.911447	2.686505
H	0.434644	-2.224917	3.536316
C	-0.155225	-4.171993	2.800923
H	-0.644983	-4.465237	3.731380
C	-0.105001	-5.058953	1.721905
H	-0.556811	-6.049518	1.805203
C	0.538735	-4.684837	0.535564
H	0.594338	-5.394468	-0.295213
C	1.176594	1.741528	-2.751672
H	1.872710	2.358692	-3.360029
H	0.768675	0.987067	-3.440966
C	0.051588	2.657560	-2.259572
H	-0.278076	3.280485	-3.118371
H	0.455077	3.358394	-1.515710
C	2.826215	1.988126	-0.980653
H	3.596576	2.358151	-1.689980
H	2.221715	2.856060	-0.679527
C	3.502168	1.417881	0.247888
C	4.858356	1.054121	0.222538
H	5.434783	1.188997	-0.696925
C	5.485438	0.539904	1.363440
H	6.542583	0.269106	1.327005
C	4.762128	0.384930	2.550178
H	5.251318	-0.007902	3.443611
C	3.413517	0.759476	2.593461
H	2.854316	0.673531	3.527827
C	2.790258	1.273095	1.451238
H	1.752807	1.617934	1.510551
C	-1.927049	1.316163	-2.695419
H	-2.636582	2.028076	-3.163266
H	-1.238268	1.032266	-3.505081
C	-2.722519	0.077006	-2.257499
H	-3.299537	-0.278828	-3.139441
H	-3.458092	0.362287	-1.498400

C	-1.884431	3.041900	-0.872239
H	-1.921314	3.946391	-1.516845
C	-3.338873	2.690979	-0.529665
C	-1.133697	3.421074	0.401538
C	-1.077745	2.539147	1.496327
H	-3.955177	2.536892	-1.426091
C	-0.443458	2.913462	2.685842
H	-0.433491	2.227323	3.535962
C	0.155060	4.174425	2.799592
H	0.644796	4.468383	3.729836
C	0.104138	5.060860	1.720175
H	0.555378	6.051729	1.802946
C	-0.539574	4.685827	0.534111
H	-0.595732	5.395034	-0.296992
N	-1.916962	-1.029220	-1.682637
N	1.120510	-1.978336	-1.635121
N	1.916895	1.028548	-1.682682
N	-1.120594	1.977760	-1.635125
Na	-0.000087	-0.000342	-0.460517
H	-3.419884	1.806387	0.117550
H	-3.772241	3.539540	0.018551
H	3.420373	-1.807492	0.117623
H	3.772249	-3.540687	0.017895
H	1.587797	-1.569993	1.444919
H	-1.586582	1.570758	1.445019

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(1R,2S,4S,7R,8S,10S)-(δδδδ)- [7·Na]⁺ E(gas)=-1472.60310273 E(Toluene)=-1472.64083526

C	1.982868	-0.823051	-0.795028
H	2.922614	-0.971042	-1.363544
H	1.262639	-0.392676	-1.508049
C	1.478383	-2.199002	-0.341147
H	1.512307	-2.868654	-1.223239
H	2.177427	-2.625995	0.393817
C	3.328500	-0.178302	1.192605
H	3.119389	-1.155880	1.654767
C	4.705785	-0.211926	0.550194
H	3.319943	0.565418	2.005895
C	5.490959	0.951147	0.461012
C	6.750162	0.922156	-0.146258
C	7.248676	-0.275454	-0.670748
C	6.488110	-1.445145	-0.572636
C	5.229211	-1.411290	0.036014
H	5.124365	1.887402	0.890937
H	7.349620	1.833354	-0.198929
H	8.234455	-0.300169	-1.139176
H	6.880623	-2.387655	-0.959907
H	4.656693	-2.338338	0.133126
C	-0.953982	-2.156308	-0.742838

C	-1.202846	-3.647223	-1.152382
H	-0.595573	-1.569691	-1.601260
C	-2.266443	-1.539983	-0.213954
H	-3.021117	-1.620612	-1.021931
H	-2.636134	-2.168875	0.612300
C	-0.125116	-3.457125	1.022865
C	-0.513866	-4.495792	-0.051206
H	-0.960108	-3.298647	1.724488
H	0.753561	-3.738221	1.620060
H	-0.788393	-3.862400	-2.146433
H	0.382326	-4.996483	-0.445202
H	-2.281672	-3.854228	-1.211719
C	-1.982538	0.822915	-0.794541
H	-2.922020	0.970445	-1.363607
H	-1.261775	0.392592	-1.507054
C	-1.478464	2.198949	-0.340623
H	-1.512579	2.868693	-1.222621
H	-2.177477	2.625695	0.394506
C	-3.328559	0.178195	1.192903
C	-4.705734	0.211820	0.550276
H	-3.119523	1.155754	1.655127
H	-3.320129	-0.565524	2.006198
C	-5.490908	-0.951244	0.460985
C	-6.750014	-0.922254	-0.146488
C	-7.248436	0.275351	-0.671077
C	-6.487872	1.445035	-0.572867
C	-5.229065	1.411176	0.035975
H	-5.124393	-1.887494	0.890991
H	-7.349469	-1.833449	-0.199240
H	-8.234142	0.300066	-1.139660
H	-6.880314	2.387544	-0.960212
H	-4.656559	2.338224	0.133150
C	0.953865	2.156484	-0.742743
C	1.203066	3.647490	-1.152037
H	0.595007	1.570109	-1.601136
C	2.266389	1.539922	-0.214287
H	3.020895	1.620676	-1.022406
H	2.636244	2.168699	0.611980
C	0.124952	3.457619	1.022798
C	0.512662	4.495998	-0.051782
H	0.960369	3.299718	1.724055
H	-0.753537	3.738500	1.620378
H	0.790116	3.862633	-2.146714
H	2.281970	3.854552	-1.209794
N	2.166714	0.155708	0.302544
N	0.130256	-2.180349	0.294356
N	-2.166651	-0.155830	0.303025
N	-0.130213	2.180538	0.294788

Na	0.000147	-0.000188	1.416663
H	1.166719	5.281265	0.350657
H	-0.384087	4.995227	-0.446472
H	-1.169097	-5.279875	0.351682

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(1*S*,2*S*,4*R*,7*S*,8*S*,10*R*)-(δδδδ)-[7·Na]⁺ E(gas)=-1472.59507243 E(Toluene)=-1472.63315873

C	-2.219567	0.897904	-0.714412
H	-3.243731	1.095513	-1.084489
H	-1.636198	0.616058	-1.603596
C	-1.669836	2.184485	-0.100169
C	-1.893701	3.484147	-0.906132
H	-2.175462	2.322936	0.873696
C	-3.361456	-0.199337	1.199531
H	-3.269624	0.732798	1.780083
C	-4.759202	-0.275956	0.608286
H	-3.209963	-1.030555	1.906791
C	-5.372732	-1.513854	0.346327
C	-6.651833	-1.575946	-0.214755
C	-7.343719	-0.397720	-0.517016
C	-6.755552	0.841321	-0.243699
C	-5.475666	0.898575	0.317736
H	-4.855971	-2.442434	0.603885
H	-7.116100	-2.546124	-0.403439
H	-8.345424	-0.445832	-0.948361
H	-7.299188	1.764207	-0.456095
H	-5.037529	1.871868	0.558032
C	0.695264	1.907773	-0.904573
H	0.755418	2.770884	-1.594689
H	0.278232	1.078104	-1.493894
C	2.121578	1.549138	-0.462027
H	2.789853	1.589759	-1.344250
H	2.482657	2.323519	0.231367
C	-0.031690	3.594743	0.699525
H	1.031266	3.869734	0.714505
H	-0.405190	3.677546	1.731941
H	-2.934590	3.829945	-0.839958
H	-1.674951	3.321698	-1.973268
C	2.219722	-0.896961	-0.714596
H	3.244157	-1.094626	-1.083914
H	1.636976	-0.615102	-1.604183
C	1.669880	-2.183657	-0.100606
C	1.893941	-3.483063	-0.906895
H	2.175546	-2.322235	0.873222
C	3.361165	0.200121	1.199573
C	4.759119	0.275584	0.608485
H	3.268820	-0.731803	1.780393
H	3.210020	1.031599	1.906601
C	5.372517	1.512860	0.343273

C	6.651655	1.573571	-0.217865
C	7.343704	0.394617	-0.516922
C	6.755666	-0.843754	-0.240346
C	5.475720	-0.899632	0.321094
H	4.855712	2.442084	0.598357
H	7.115835	2.543288	-0.409120
H	8.345437	0.441704	-0.948316
H	7.299408	-1.767147	-0.450250
H	5.037545	-1.872320	0.563823
C	-0.695199	-1.906235	-0.904683
H	-0.754959	-2.768537	-1.595854
H	-0.278324	-1.075793	-1.493047
C	-2.121603	-1.548132	-0.461988
H	-2.789945	-1.588798	-1.344158
H	-2.482507	-2.322632	0.231365
C	0.031617	-3.594340	0.698303
H	2.934692	-3.829102	-0.840019
C	-0.886651	4.476901	-0.263643
C	0.886341	-4.475946	-0.265550
H	-1.031362	-3.869216	0.713203
H	0.405285	-3.677822	1.730600
H	0.263002	-4.963430	-1.027741
H	1.393148	-5.277111	0.289430
H	-1.393975	5.277190	0.292086
H	-0.263411	4.965525	-1.025229
H	1.676100	-3.320206	-1.974155
N	-2.208625	-0.244375	0.238463
N	-0.204994	2.180442	0.251546
N	2.208489	0.245327	0.238342
N	0.205054	-2.179770	0.251171
Na	0.000266	0.000024	1.380408

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(1R,2S,4S,7R,8S,10S)-(λλλλ)-[7·Na]⁺ E(gas)=-1472.59793642 E(Toluene)=-1472.63540379

C	2.240140	0.986569	-0.827324
H	3.256080	1.253126	-1.174196
H	1.709452	0.653657	-1.732463
C	1.559741	2.280903	-0.335528
H	1.635981	2.985715	-1.195254
C	2.149075	2.981718	0.895487
C	3.518855	-0.163833	0.986525
H	3.489907	0.747885	1.597788
C	4.867613	-0.245801	0.289622
H	3.408186	-1.015441	1.676869
C	5.448968	-1.484936	-0.033889
C	6.686634	-1.550978	-0.680996
C	7.370351	-0.375388	-1.010526
C	6.816753	0.864624	-0.676611
C	5.578450	0.925390	-0.028722

H	4.941608	-2.412857	0.243633
H	7.125519	-2.522791	-0.916320
H	8.339729	-0.426851	-1.509993
H	7.355545	1.785526	-0.908975
H	5.170933	1.898722	0.258651
C	-0.782771	1.843436	-1.069783
H	-0.869411	2.730982	-1.733891
H	-0.347983	1.039780	-1.684712
C	-2.199544	1.454860	-0.628246
H	-2.854565	1.457279	-1.520838
H	-2.585939	2.243154	0.034481
C	-0.252968	3.374133	0.786874
H	-0.924193	3.136439	1.627065
C	1.073255	4.020260	1.255804
H	2.270164	2.263272	1.721034
H	3.131129	3.431027	0.693894
C	-2.240128	-0.986478	-0.827346
H	-3.256090	-1.252998	-1.174166
H	-1.709452	-0.653541	-1.732478
C	-1.559742	-2.280828	-0.335588
H	-1.635986	-2.985617	-1.195336
C	-2.149102	-2.981667	0.895377
C	-3.518828	0.163954	0.986497
C	-4.867618	0.245786	0.289613
H	-3.489831	-0.747710	1.597846
H	-3.408239	1.015606	1.676805
C	-5.448982	1.484873	-0.034101
C	-6.686664	1.550804	-0.681180
C	-7.370405	0.375155	-1.010463
C	-6.816809	-0.864794	-0.676333
C	-5.578475	-0.925450	-0.028485
H	-4.941622	2.412840	0.243255
H	-7.125552	2.522574	-0.916675
H	-8.339802	0.426532	-1.509902
H	-7.355620	-1.785735	-0.908501
H	-5.170929	-1.898731	0.259019
C	0.782825	-1.843391	-1.069777
H	0.869519	-2.730957	-1.733850
H	0.348034	-1.039767	-1.684744
C	2.199563	-1.454778	-0.628168
H	2.854653	-1.457280	-1.520710
H	2.585907	-2.243027	0.034647
C	0.252948	-3.373899	0.787076
H	-3.131211	-3.430874	0.693813
H	0.923758	-3.136009	1.627553
C	-1.073329	-4.020320	1.255510
H	-2.270073	-2.263298	1.721011
H	-1.250642	-4.957611	0.709126

H	-1.066252	-4.266165	2.325621
H	-0.804821	4.058279	0.114550
N	2.289251	-0.166688	0.113877
N	0.126330	2.122007	0.055514
N	-2.289221	0.166822	0.113887
N	-0.126353	-2.121944	0.055471
Na	0.000114	-0.000132	1.209289
H	0.805280	-4.058011	0.115095
H	1.065987	4.265612	2.326024
H	1.250702	4.957799	0.709886

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(S,S,S)-(δλδλδλ)-[4Na]⁺ E(gas)=-2706.76999929

N	1.352274	-2.480068	0.439012
N	-1.565314	-2.576349	-0.549581
N	-2.864728	0.091460	0.408053
N	-1.427410	2.648168	-0.590166
N	1.530689	2.422440	0.369759
N	3.068739	-0.093081	-0.591967
C	-1.378686	2.917857	-2.080549
C	-2.117865	4.179472	-2.532873
C	-1.748195	1.695709	-2.932967
H	-0.311435	3.100415	-2.275872
C	-2.790242	2.595564	-0.007858
H	-3.437366	3.404344	-0.400276
H	-2.681618	2.812893	1.065226
C	-0.660372	3.681682	0.153587
H	-0.878091	3.530861	1.221459
H	-1.019421	4.704616	-0.082906
C	0.849543	3.666285	-0.049250
H	1.088354	3.817675	-1.112767
H	1.262193	4.552744	0.475978
C	1.525915	2.244270	1.855522
C	2.187357	3.325212	2.700353
H	1.999315	1.272279	2.066218
H	0.472535	2.150017	2.166093
C	2.893190	2.433618	-0.206659
H	3.510970	3.244819	0.235061
H	2.778842	2.685452	-1.269307
C	3.690999	1.139625	-0.057947
H	4.695785	1.315032	-0.490031
H	3.872121	0.965707	1.012942
C	3.560567	-1.245797	0.201247
H	3.535900	-0.938858	1.257351
H	4.624484	-1.475377	-0.018069
C	3.275429	-0.324634	-2.071548
C	4.739818	-0.395984	-2.514554
C	2.448060	0.627007	-2.946279
H	2.857507	-1.328845	-2.241538

Na	-0.115106	-0.014545	-0.174065
C	1.168252	-2.273465	1.908467
C	1.756777	-3.306331	2.860236
H	1.595733	-1.286704	2.150186
H	0.083469	-2.196820	2.086817
C	2.776676	-2.544595	0.048357
H	3.319520	-3.324445	0.622539
H	2.802679	-2.878802	-0.999853
C	0.685258	-3.701430	-0.059558
H	0.981717	-3.813981	-1.110743
H	1.058115	-4.609425	0.460951
C	-0.836515	-3.713491	0.062856
H	-1.098185	-3.712969	1.131634
H	-1.198690	-4.687711	-0.319564
C	-1.792790	-2.693291	-2.044001
C	-2.529733	-3.958778	-2.488240
H	-2.467183	-1.853486	-2.270852
C	-0.524362	-2.440838	-2.870435
C	-2.861872	-2.432443	0.164504
H	-3.563663	-3.251594	-0.094740
H	-2.651168	-2.550991	1.237509
C	-3.591511	-1.113140	-0.052054
H	-4.585249	-1.197358	0.434033
H	-3.798208	-0.969196	-1.123256
C	-3.544304	1.278567	-0.159924
H	-3.716845	1.063259	-1.222374
H	-4.549927	1.421013	0.288841
C	-2.748675	0.151292	1.902368
C	-4.039202	0.173631	2.707973
H	-2.146500	-0.716821	2.214362
H	-2.152779	1.045061	2.144325
C	5.371791	-1.648322	-2.619378
C	6.715077	-1.758319	-2.993380
C	7.458587	-0.607649	-3.272647
C	6.844598	0.646244	-3.188296
C	5.499528	0.749964	-2.817319
H	4.796716	-2.558350	-2.425164
H	7.178376	-2.744053	-3.073719
H	8.506500	-0.687443	-3.568477
H	7.412553	1.549366	-3.422251
H	5.040425	1.740851	-2.787199
H	2.411575	0.238507	-3.974447
H	1.416215	0.708361	-2.571565
H	2.866427	1.639962	-3.002673
C	-1.410937	5.385997	-2.683703
C	-2.056735	6.562818	-3.077439
C	-3.431842	6.554574	-3.330655
C	-4.149871	5.361459	-3.198480

C	-3.498353	4.187108	-2.807171
H	-0.330785	5.402283	-2.511599
H	-1.483107	7.484722	-3.194310
H	-3.939487	7.469724	-3.641707
H	-5.221131	5.341952	-3.410125
H	-4.078258	3.263937	-2.737168
H	-1.440896	1.875989	-3.973499
H	-1.229710	0.789666	-2.582719
H	-2.824196	1.482142	-2.951628
C	-3.922994	-3.919602	-2.678823
C	-4.637256	-5.057989	-3.066536
C	-3.966238	-6.267191	-3.272409
C	-2.579124	-6.323231	-3.100725
C	-1.869208	-5.180333	-2.717400
H	-4.458286	-2.975345	-2.542272
H	-5.717489	-4.997805	-3.215379
H	-4.518414	-7.158005	-3.578197
H	-2.044132	-7.259050	-3.276122
H	-0.783123	-5.247363	-2.620554
H	-0.806337	-2.255312	-3.917181
H	0.024842	-1.559635	-2.504591
H	0.171380	-3.289505	-2.873587
C	-4.680268	1.386561	3.017761
C	-5.875600	1.405324	3.743671
C	-6.449759	0.206640	4.180126
C	-5.816148	-1.007615	3.896016
C	-4.621641	-1.020635	3.168608
H	-4.231196	2.333784	2.706660
H	-6.353996	2.358628	3.978217
H	-7.379932	0.219781	4.751598
H	-6.247718	-1.946469	4.249595
H	-4.125659	-1.975877	2.974569
C	1.025173	-4.446436	3.238466
C	1.572947	-5.402183	4.100224
C	2.866054	-5.231409	4.605701
C	3.602077	-4.095663	4.252202
C	3.049755	-3.144143	3.388754
H	0.003483	-4.583198	2.873807
H	0.984937	-6.277213	4.385483
H	3.293449	-5.974450	5.281856
H	4.605736	-3.945882	4.655845
H	3.629431	-2.251080	3.138802
C	3.559853	3.278560	3.003753
C	4.163685	4.281310	3.769461
C	3.401541	5.350744	4.251370
C	2.032048	5.405111	3.971983
C	1.433875	4.399891	3.205345
H	4.165592	2.437429	2.656258

H	5.229899	4.222259	3.998398
H	3.870569	6.131863	4.852892
H	1.426404	6.227252	4.359245
H	0.358043	4.443808	3.013332

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(1R,2S,4R,7R,8S,10R,13R,14S,16R)-(δλδλδλ)-[8·Na]⁺ E(gas)=-2127.80417872

N	2.182027	1.934402	-1.385291
N	2.731440	-0.959951	-0.520489
N	0.577483	-2.871582	-1.363097
N	-2.199306	-1.892046	-0.513960
N	-2.758770	0.923280	-1.392086
N	-0.540459	2.848085	-0.508267
C	2.337763	2.078409	-2.860634
C	3.067262	3.427761	-3.115853
H	1.334552	2.094483	-3.314638
H	2.864999	1.212073	-3.281929
C	1.921111	3.332983	-0.939239
C	2.828554	4.246478	-1.818682
H	2.194807	3.406543	0.123464
C	3.436604	1.459350	-0.753703
H	3.343794	1.643890	0.327769
H	4.320941	2.041206	-1.088098
C	3.752374	-0.009126	-1.006005
H	3.856807	-0.176099	-2.089549
H	4.752245	-0.220612	-0.573007
C	2.654488	-1.006821	0.973457
C	3.910037	-1.422915	1.727790
H	1.827765	-1.687405	1.231074
H	2.349864	-0.004112	1.313327
C	3.007449	-2.277101	-1.123172
H	3.964211	-2.705311	-0.756562
H	3.146109	-2.110337	-2.204291
C	1.924332	-3.339684	-0.923088
C	2.255431	-4.594991	-1.787136
H	1.862138	-3.597460	0.144732
C	-0.453580	-3.708562	-0.700497
H	-0.241160	-3.684108	0.379735
H	-0.382241	-4.773996	-1.002649
C	0.606910	-3.108783	-2.834281
C	1.391159	-4.429555	-3.067516
H	1.128850	-2.264138	-3.311331
H	-0.411731	-3.125650	-3.244037
Na	0.015415	-0.031418	-1.022714
C	-2.219088	-1.763465	0.976725
C	-3.208613	-2.630207	1.742272
H	-1.200639	-1.987964	1.332682
H	-2.404269	-0.702009	1.205237
C	-1.886463	-3.264240	-0.960775

H	-2.565160	-4.012501	-0.501584
H	-2.087493	-3.304167	-2.042865
C	-3.463539	-1.477640	-1.149604
H	-3.362976	-1.694158	-2.226349
H	-4.321378	-2.089496	-0.798000
C	-3.848042	-0.007041	-0.978013
H	-4.077314	0.189537	0.079356
C	-5.075281	0.323116	-1.886257
C	-2.936719	1.012041	-2.868468
C	-4.464877	1.001730	-3.142583
H	-2.426497	1.898117	-3.268981
H	-2.458945	0.132646	-3.329559
C	-2.982533	2.234973	-0.737222
H	-3.935488	2.708399	-1.054936
H	-3.091655	2.040715	0.341119
C	-1.879926	3.257667	-0.974437
H	-2.201688	4.216319	-0.516969
H	-1.797355	3.456592	-2.054392
C	0.457166	3.744148	-1.119050
H	0.230223	3.784094	-2.197359
H	0.357953	4.786690	-0.749018
C	-0.440499	2.787576	0.982400
C	-0.702938	4.073768	1.752913
H	-1.148438	2.014733	1.322736
H	0.568182	2.414652	1.218747
H	-4.850187	2.023772	-3.264665
H	-4.701746	0.461388	-4.069383
H	-5.773401	0.996875	-1.370695
H	-5.641622	-0.586184	-2.136239
H	0.706330	-5.279912	-3.193530
H	1.999782	-4.375283	-3.980576
H	1.996088	-5.518331	-1.251097
H	3.330437	-4.652217	-2.012332
H	4.140294	3.271768	-3.294136
H	2.669465	3.931142	-4.007816
H	3.776386	4.464373	-1.307134
H	2.348039	5.215577	-2.017189
C	0.331528	4.989960	2.013419
C	0.082923	6.184775	2.696676
C	-1.210020	6.483023	3.139580
C	-2.247229	5.574214	2.906437
C	-1.992589	4.381511	2.221337
H	1.352800	4.759696	1.698353
H	0.902368	6.879464	2.892909
H	-1.405434	7.413086	3.676887
H	-3.255317	5.789769	3.266885
H	-2.808485	3.669321	2.068281
C	-2.828179	-3.890781	2.236224

C	-3.735798	-4.701389	2.925461
C	-5.046866	-4.261736	3.137635
C	-5.437999	-3.003935	2.667252
C	-4.525424	-2.197523	1.979718
H	-1.799756	-4.238148	2.101432
H	-3.416136	-5.673993	3.305598
H	-5.756260	-4.890631	3.679017
H	-6.453697	-2.644479	2.845575
H	-4.841280	-1.206842	1.641936
C	4.172296	-2.774425	2.013862
C	5.333515	-3.156610	2.693026
C	6.255603	-2.188575	3.104723
C	6.002934	-0.837980	2.843365
C	4.840014	-0.461929	2.163206
H	3.449545	-3.541222	1.722165
H	5.513880	-4.211425	2.910773
H	7.160492	-2.484587	3.638986
H	6.708461	-0.074455	3.177826
H	4.643946	0.599775	1.988893