Electric Supplementary information for

Argentivorous Molecules Bearing Three Aromatic-Side Arms: Selective Synthesis of Triple-Armed Cyclens and Their Complexing Property towards Ag^+

Yoichi Habata,[†,‡] Juli Kizaki,[†] Yasuhiro Hosoi,[†] Mari Ikeda,[‡,§] and Shunsuke Kuwahara[†,‡]*

[†]Department of Chemistry, Faculty of Science, and [‡]Research Center for Materials with Integrated Properties, Toho University, 2-2-1 Miyama, Funabashi, Chiba 274-8510, Japan

[§]Education Center, Faculty of Engineering, Chiba Institute of Technology, 2-1-1 Shibazono, Narashino, Chiba 275-0023, Japan

Table of Contents

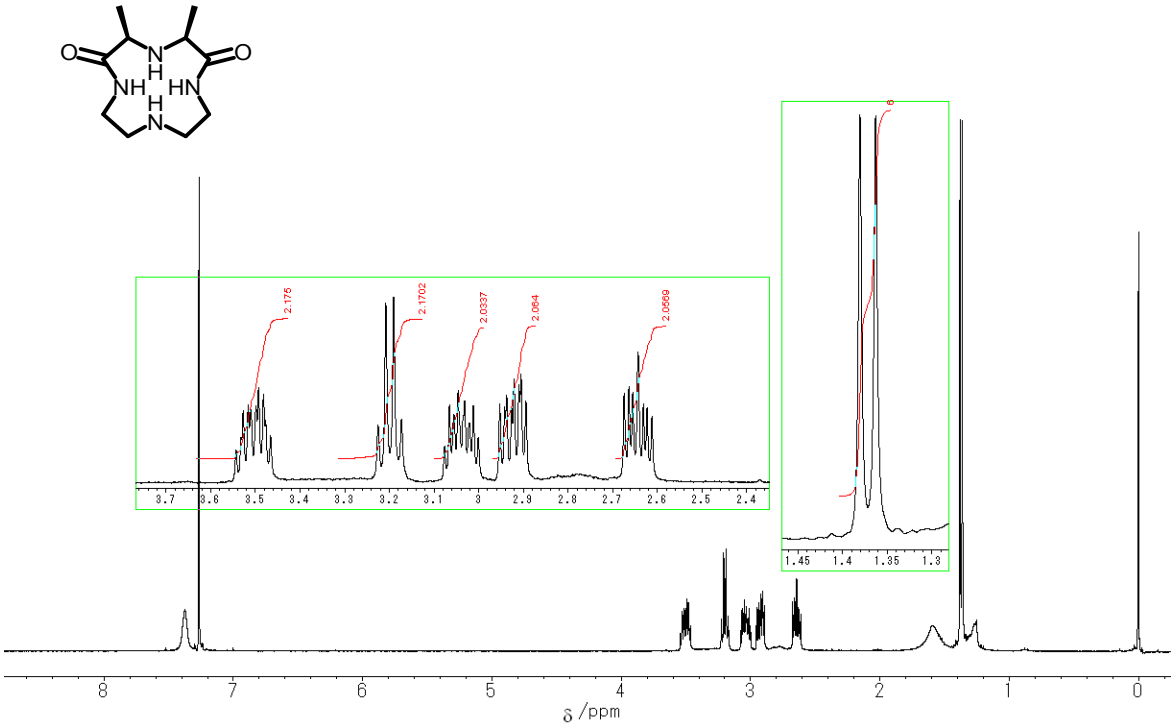


Figure S1. ^{1}H NMR spectra of *meso*-**6** in $CDCl_3$.

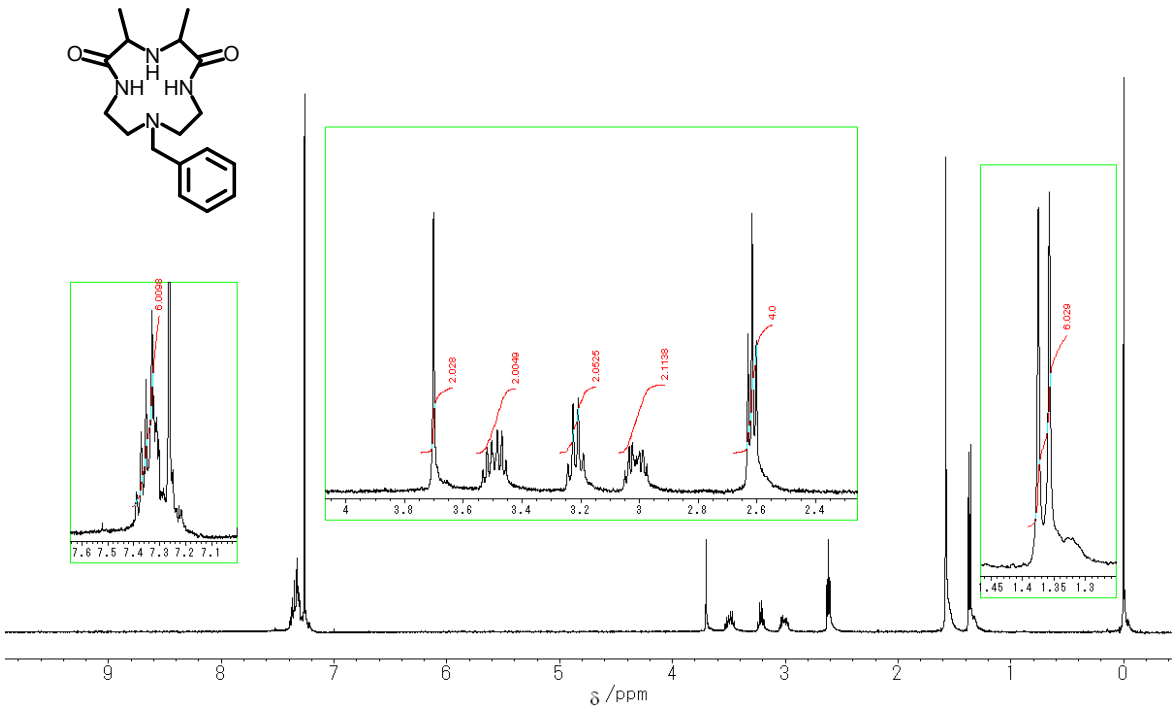


Figure S2. ^{1}H NMR spectra of *meso*-**7a** in $CDCl_3$.

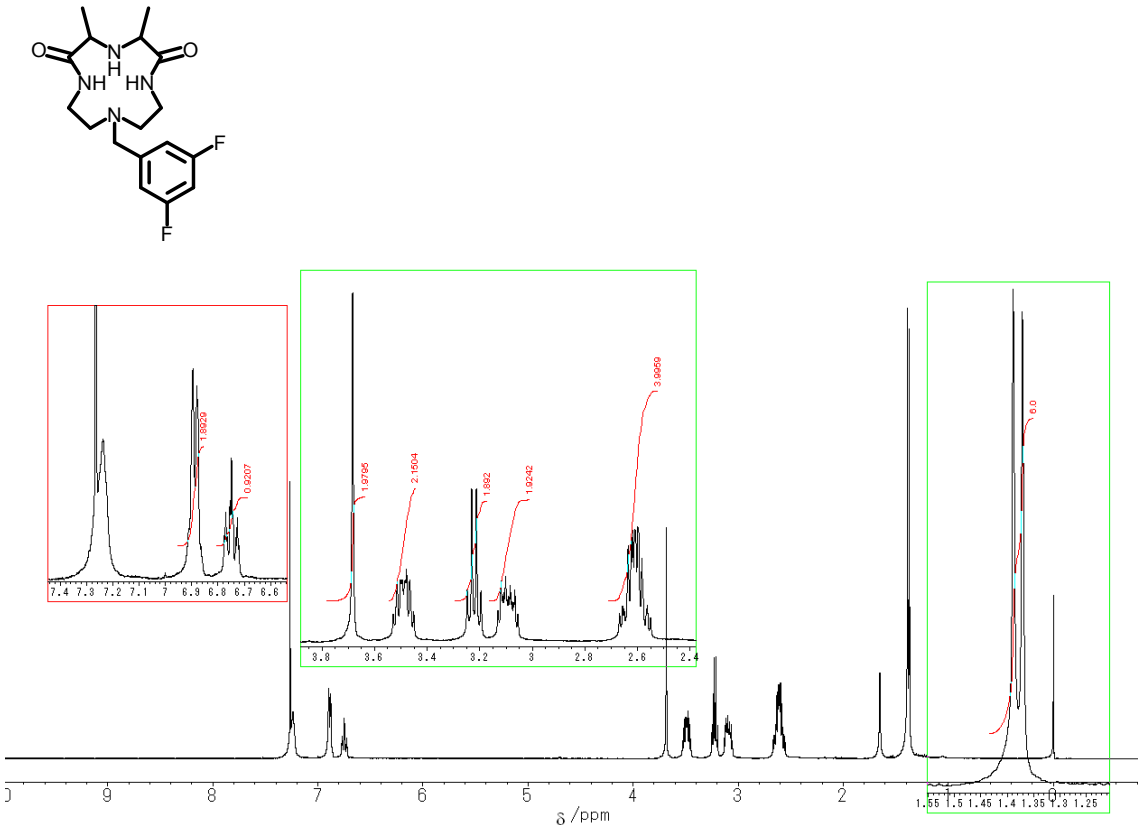


Figure S3. ^{1}H NMR spectra of *meso*-**7b** in $CDCl_3$.

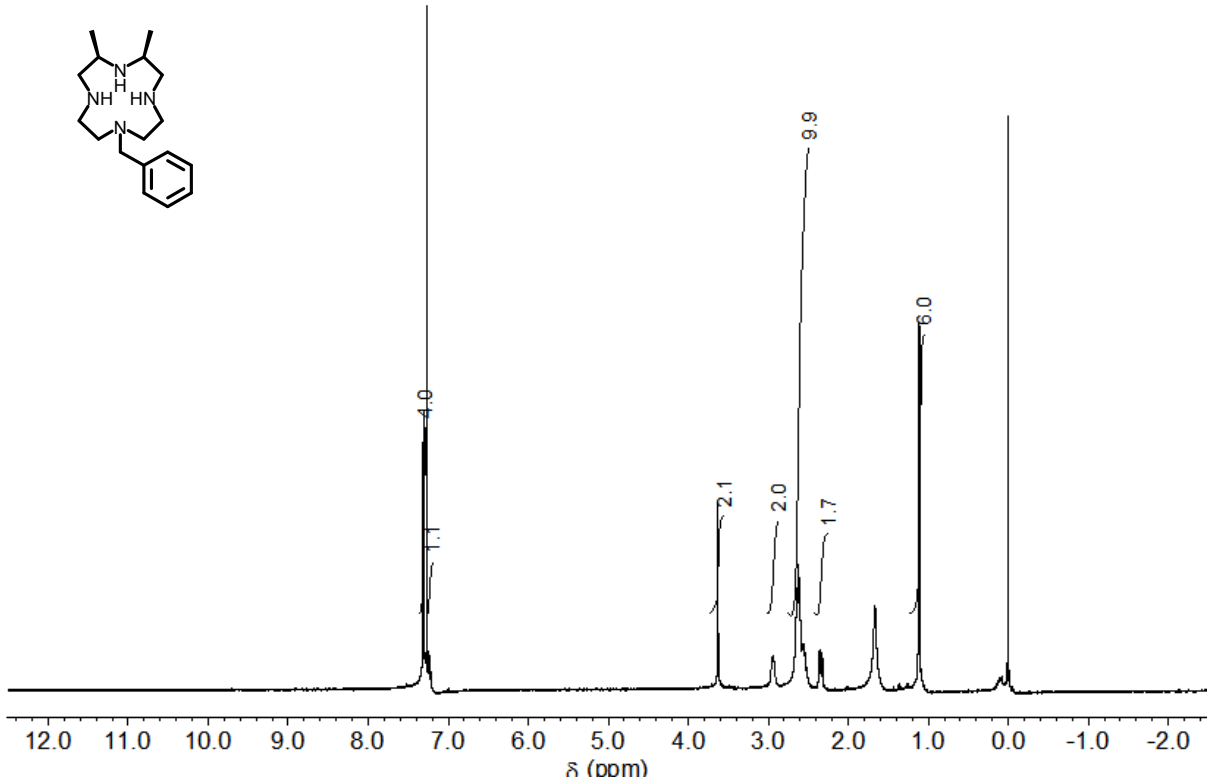


Figure S4. ^{1}H NMR spectra of *meso*-**8a** in $CDCl_3$.

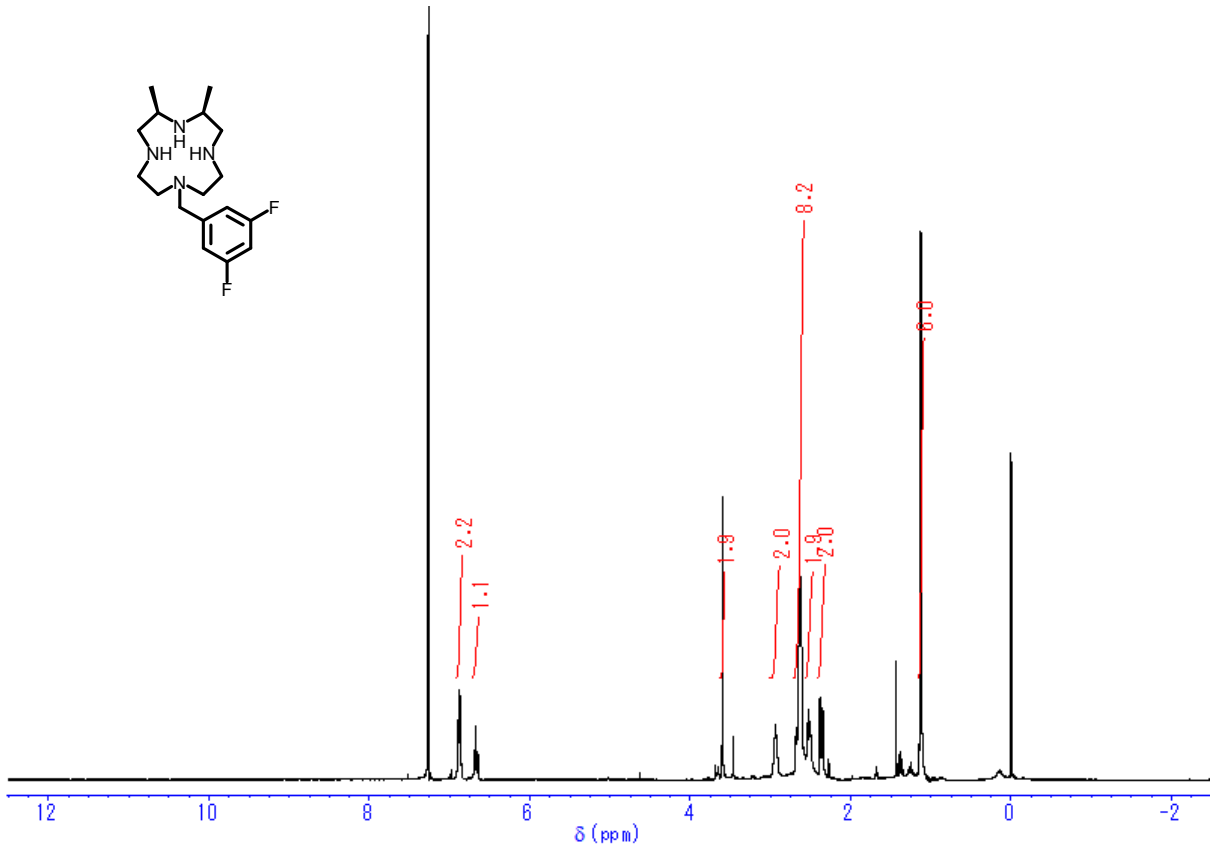


Figure S5. ^{1}H NMR spectra of *meso*-**8b** in $CDCl_3$.

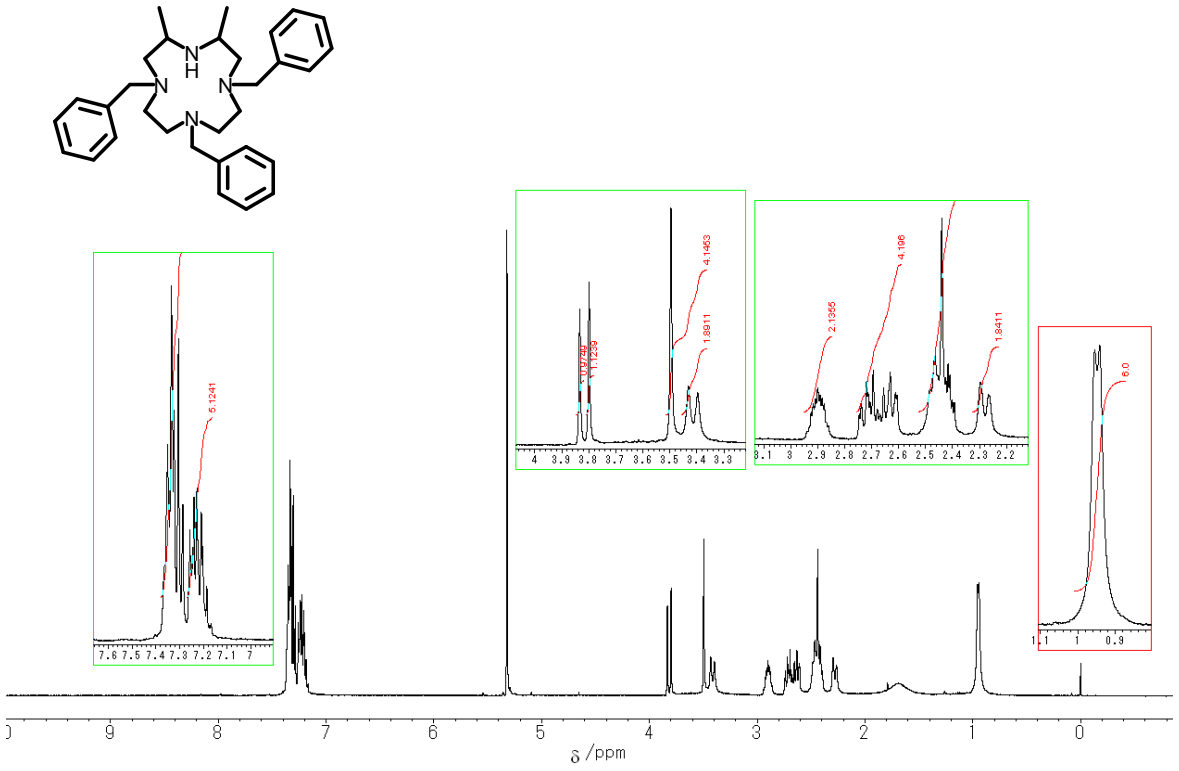


Figure S6. ^{1}H NMR spectra of *meso*-**9a** in CD_2Cl_2.

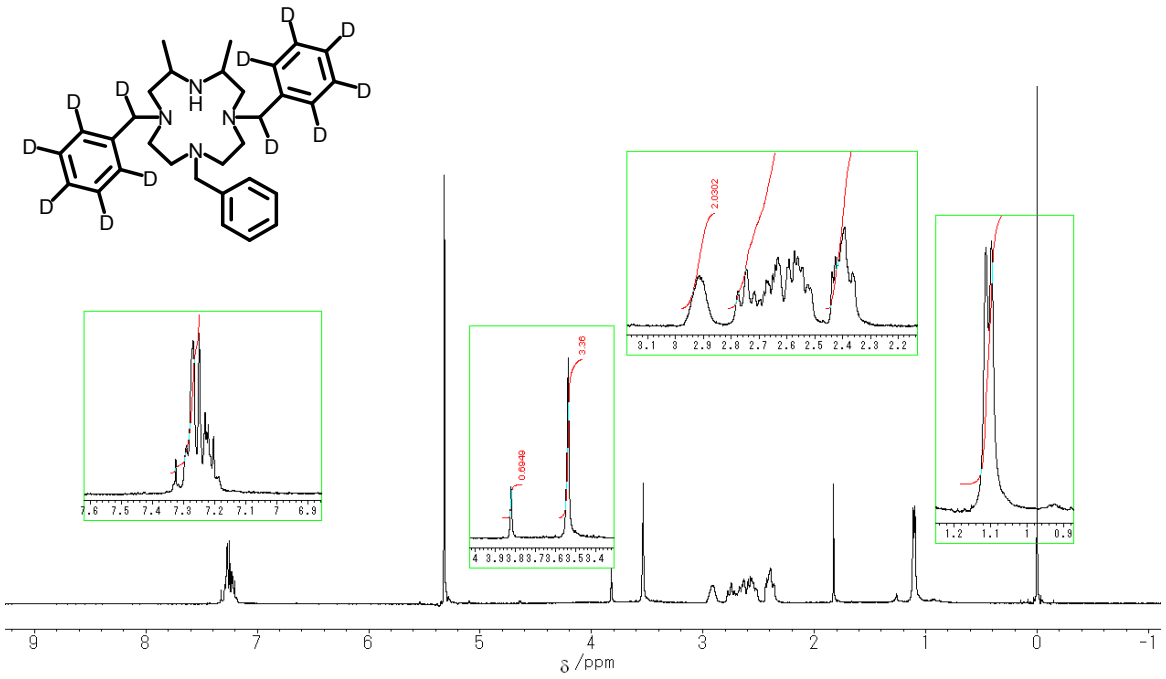


Figure S7. ^{1}H NMR spectra of *meso*-**9b** in CD_2Cl_2.

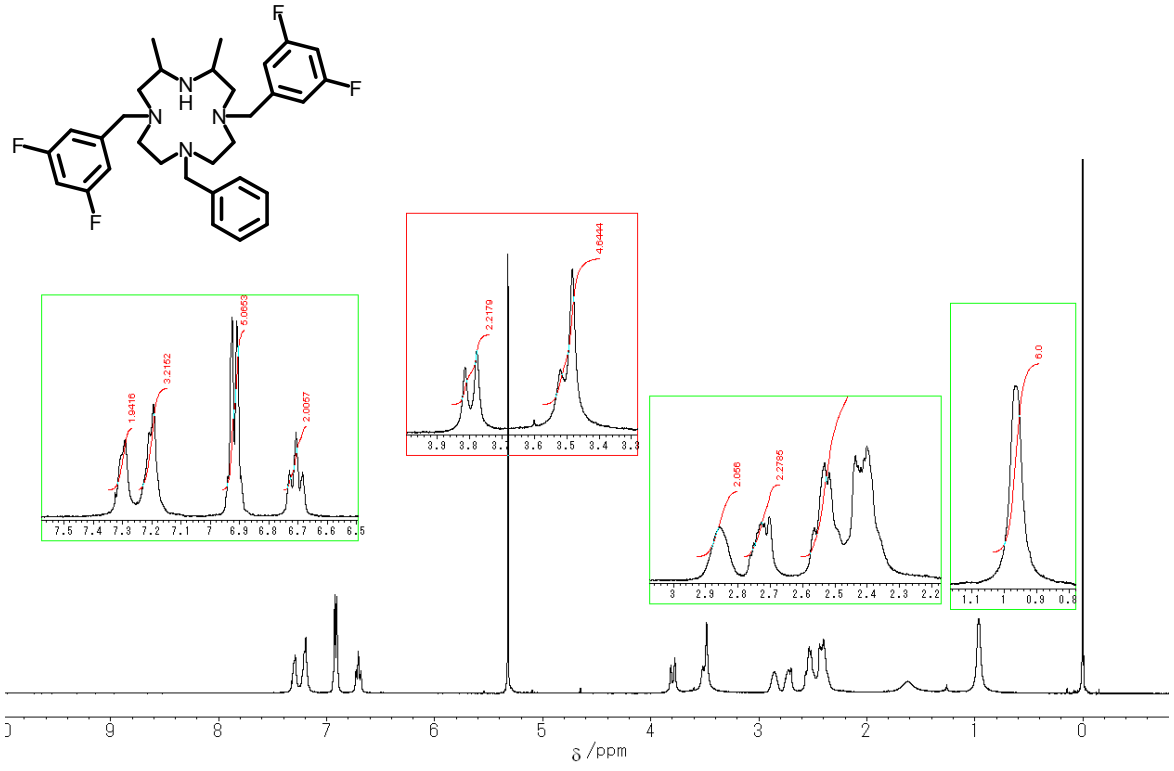


Figure S7. ^{1}H NMR spectra of *meso*-**9c** in CD_2Cl_2.

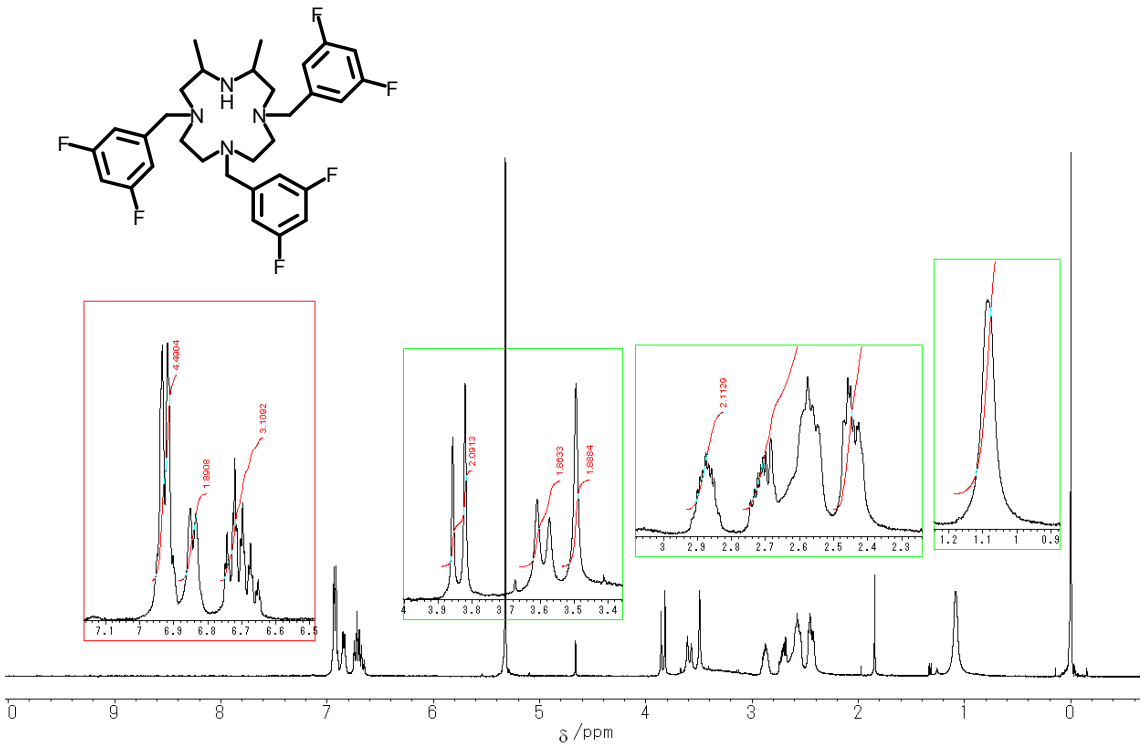


Figure S8. ^{1}H NMR spectra of *meso*-**9d** in CD_2Cl_2.

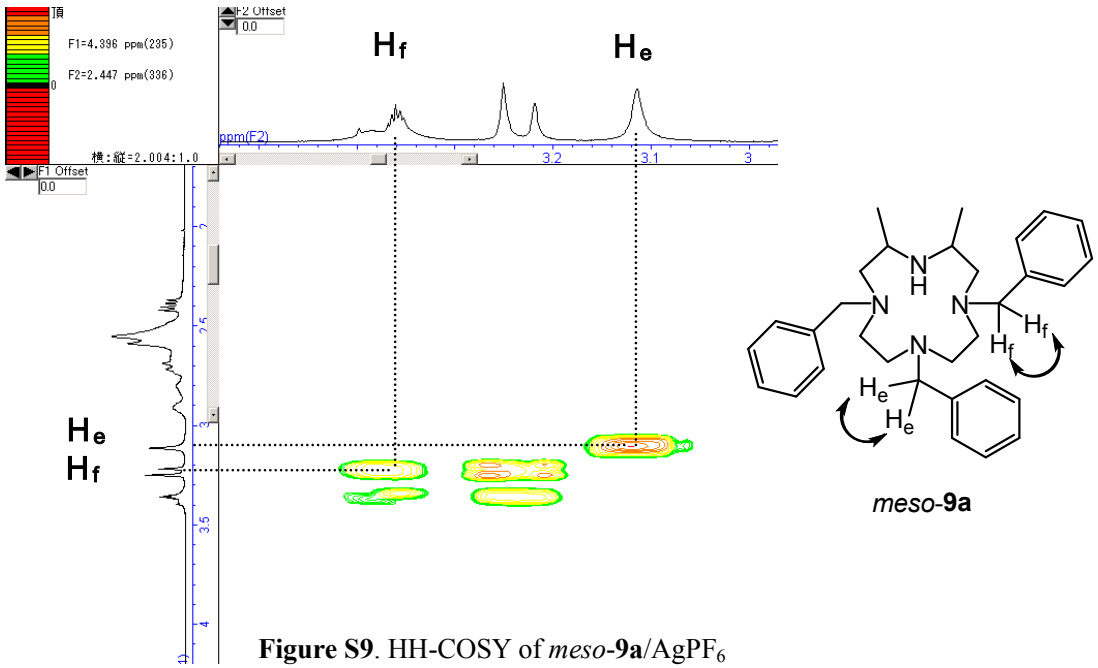


Figure S9. HH-COSY of *meso*-**9a**/$AgPF_6$

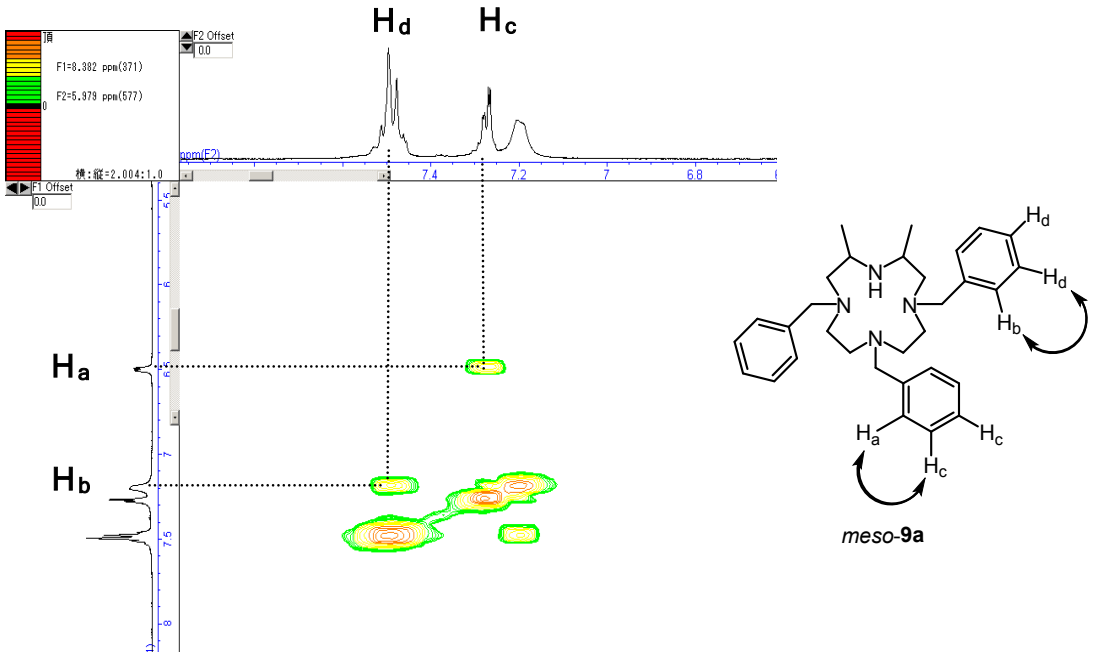


Figure S10. HH-COSY of *meso*-**9a**/$AgPF_6$

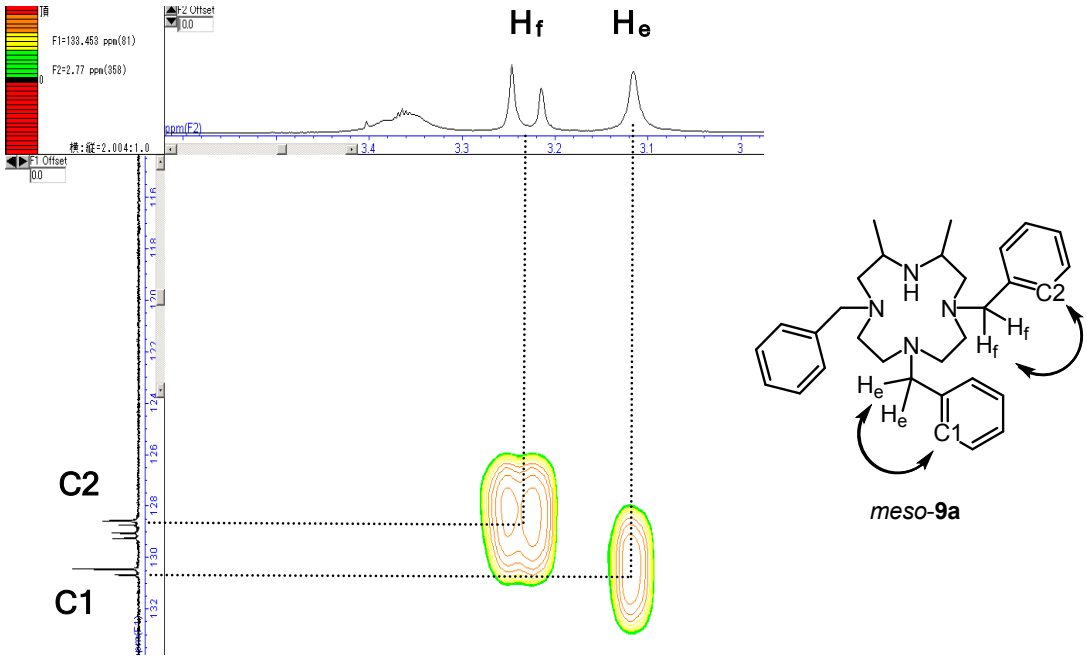


Figure S11. HMBC of *meso*-**9a**-$AgPF_6$

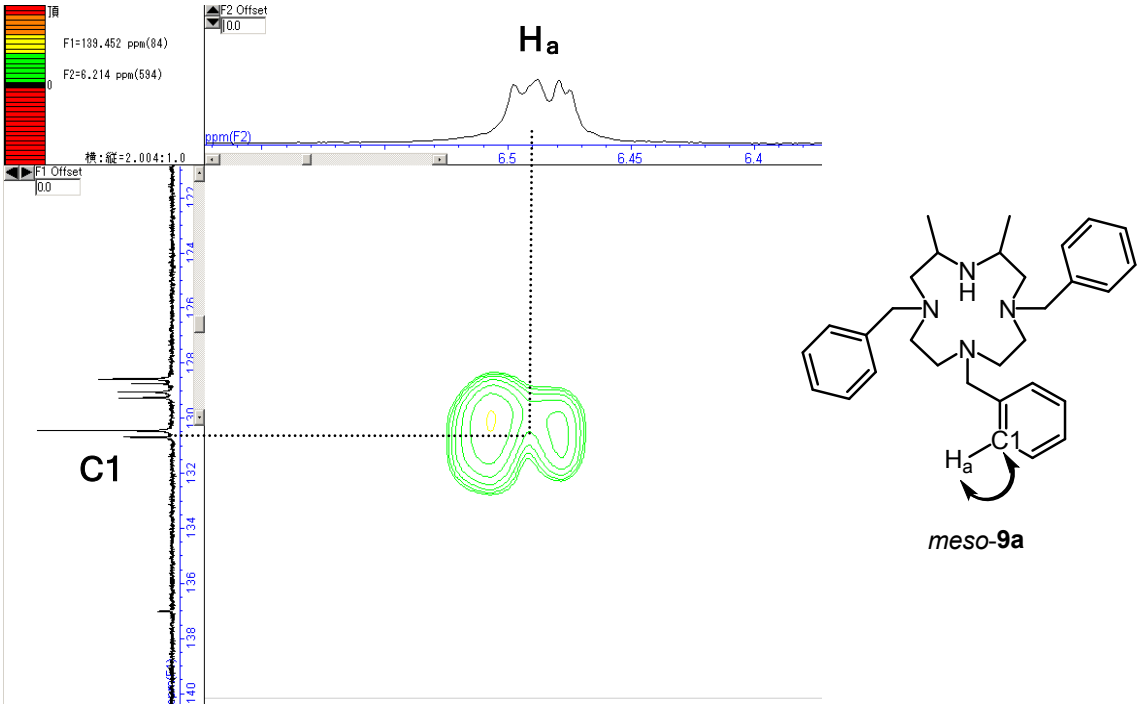


Figure S12a. HMQC of *meso*-**9a**-$AgPF_6$

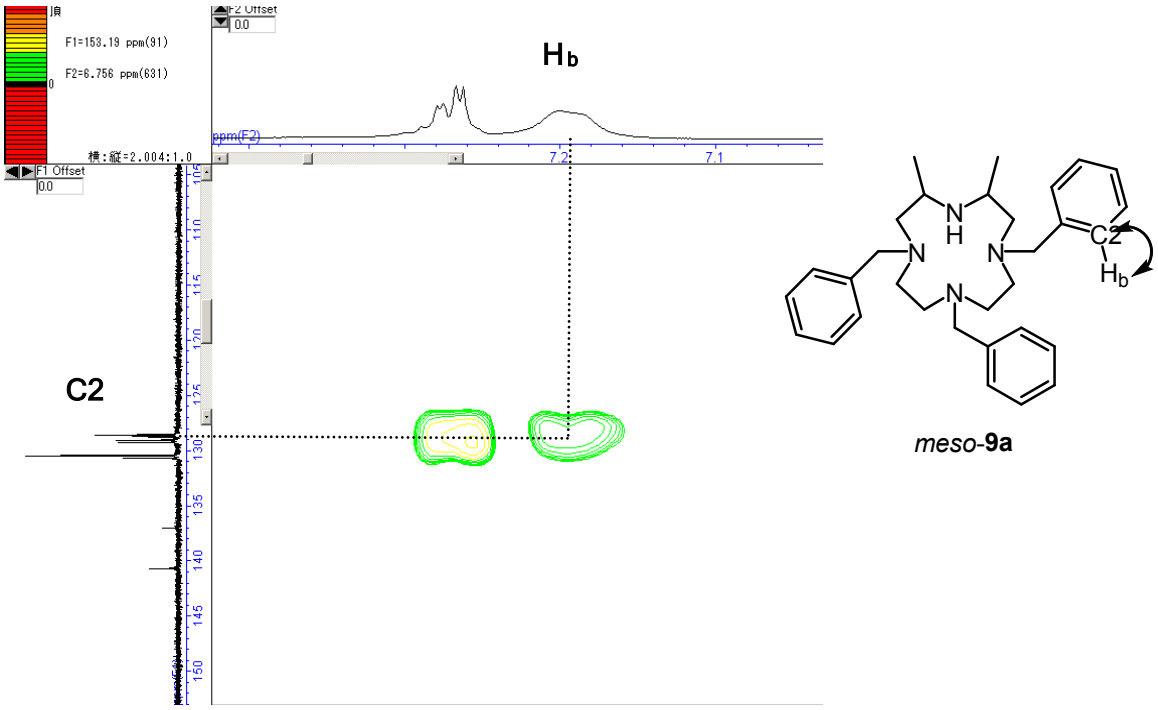


Figure S12b. HMQC of *meso*-**9a**-$AgPF_6$

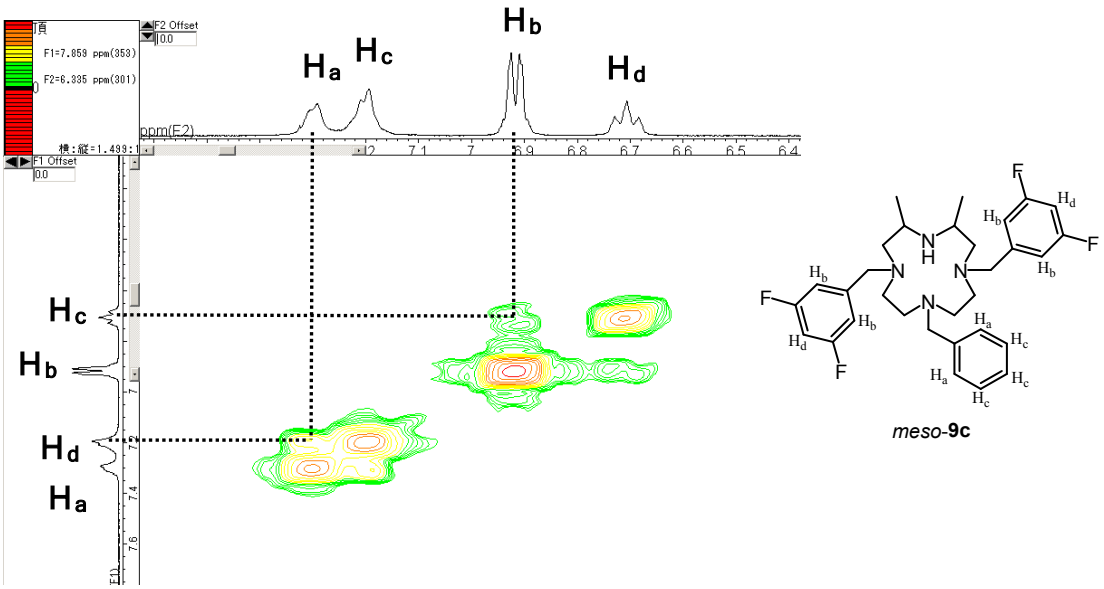


Figure13. HH-COSY of *meso*-**9c** in CD_2Cl_2

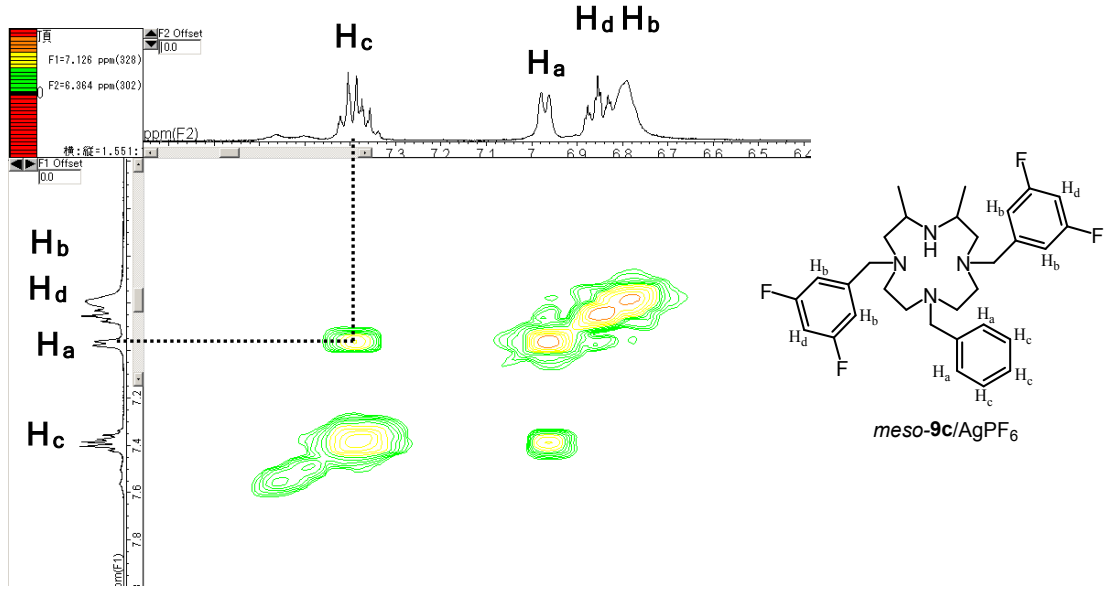


Figure14. HH-COSY of *meso*-**9c**/$AgPF_6$ in CD_2Cl_2

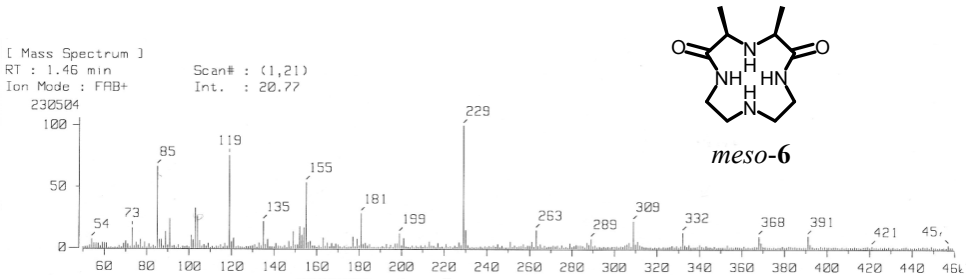


Figure S15. FAB-MS of *meso*-**6**.

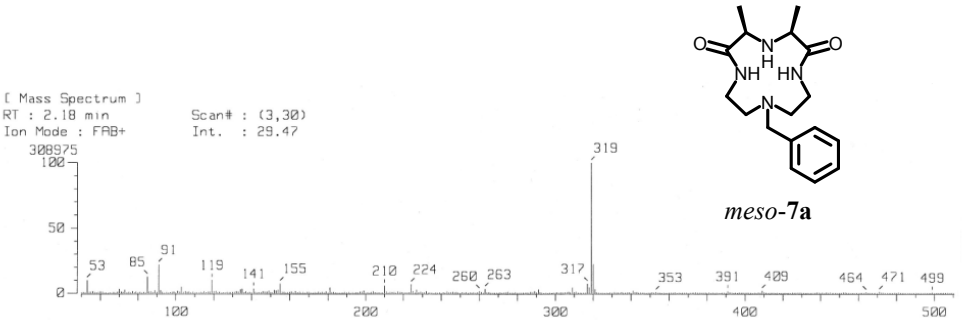


Figure S16. FAB-MS of *meso*-**7a**.

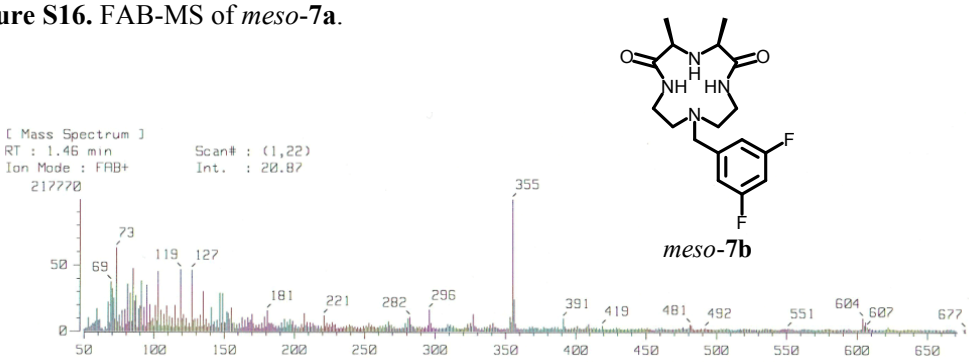


Figure S17. FAB-MS of *meso*-**7b**.

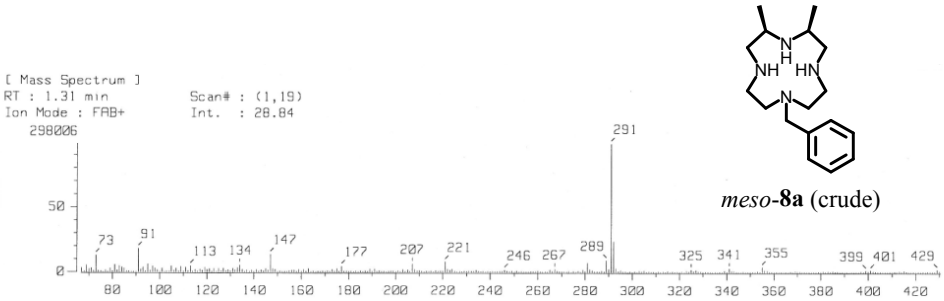


Figure S18. FAB-MS of *meso*-**8a**.

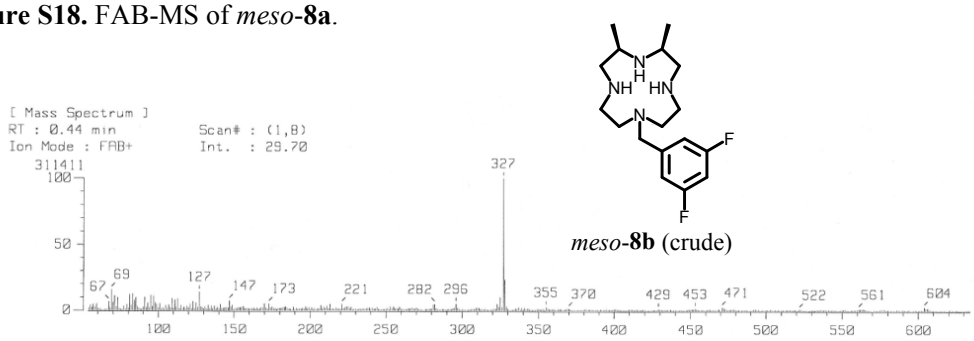


Figure S19. FAB-MS of *meso*-**8b**.

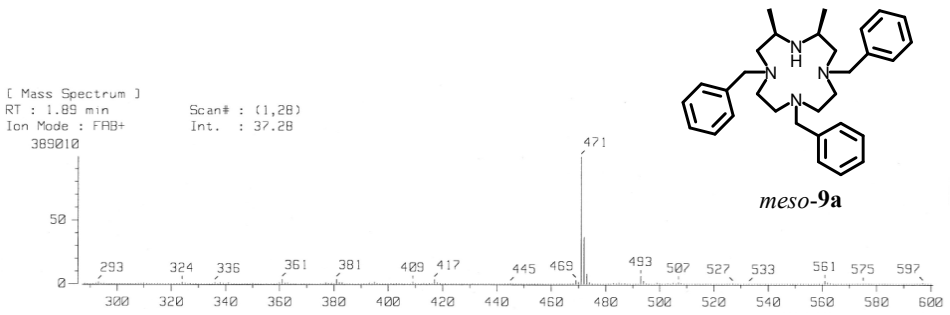


Figure S20. FAB-MS of *meso*-**9a**.

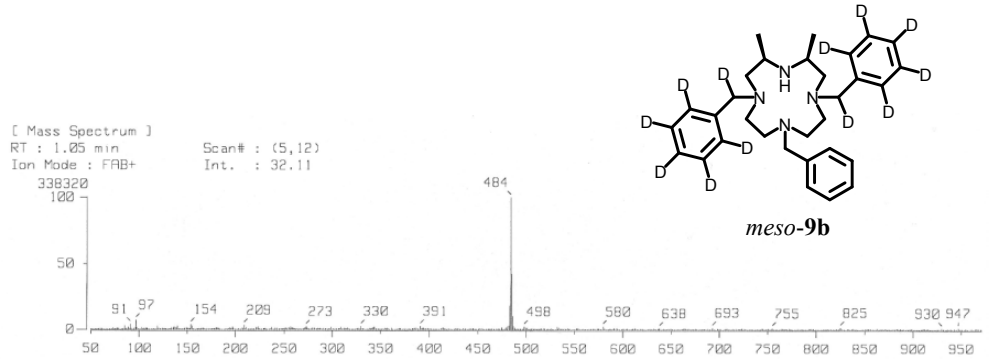


Figure S21. FAB-MS of *meso*-**9b**.

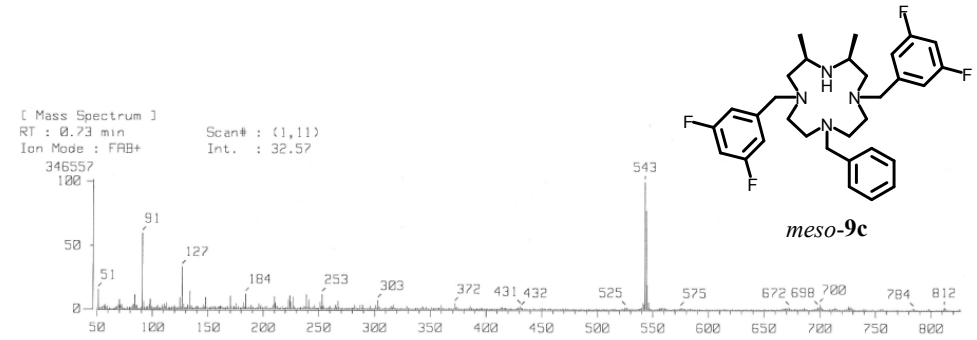


Figure S22. FAB-MS of *meso*-**9c**.

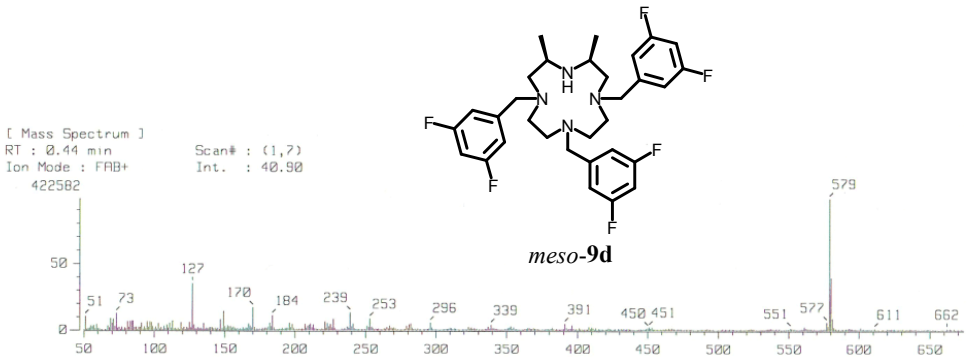
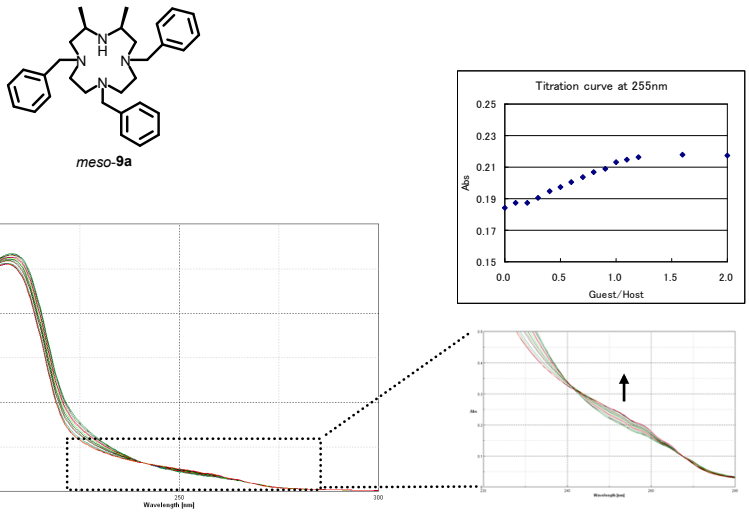
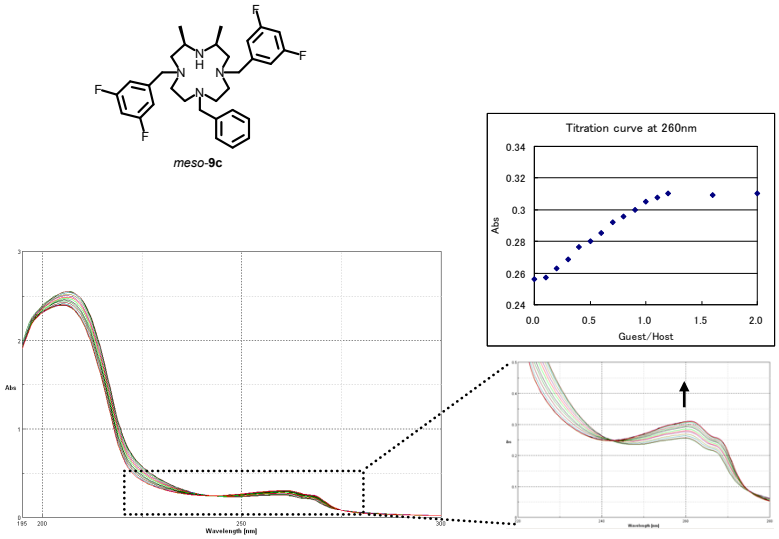


Figure S23. FAB-MS of *meso*-**9d**.



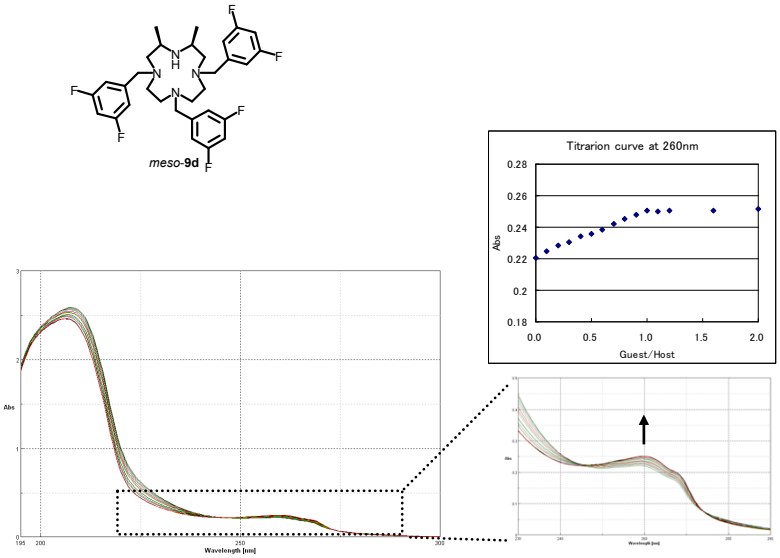

```
Hyperquad refinement output. Version number 1.1.33
Produced at 2014/06/17 20:02:05
from data stored in I:\Dropbox\0000_HyperSpec\001_Juli\Bz\Bz.HQD
Project title
</intro>
<iterations>
Initial Sigma =4.7008E-03
Iteration 1
              relative
Parameter     shift      new value
Log beta AB   0.0000     5.6335

New sigma =4.7008E-03
Change =563.3518%
</iterations>
<results>
HypSpec. Refinement concluded at 2014/06/17 20:02:06
Data from I:\Dropbox\0000_HyperSpec\001_Juli\Bz\Bz.HQD
Project title:
Converged in 1 iterations with sigma = 4.7008E-03

                     standard
Log beta   value     deviation
AB         5.6335    0.0369
AB2 was ignored
```

Figure S24. Ag^{+}-ion-induced UV-Vis spectral chngnes and log*K* calculation by *HyperSpec* of *meso*-**9a**.




```
Hyperquad refinement output. Version number 1.1.33
Produced at 2014/06/17 20:03:10
from data stored in I:\Dropbox\0000_HyperSpec\001_Juli\35F_Bz\35F_Bz.HQD
Project title
</intro>
<iterations>
Initial Sigma =2.5739E-04
Iteration 1
             relative
Parameter    shift     new value
Log beta AB  0.0000    6.5812

New sigma =2.5739E-04
Change =658.1167%
</iterations>
<results>
HypSpec. Refinement concluded at 2014/06/17 20:03:10
Data from I:\Dropbox\0000_HyperSpec\001_Juli\35F_Bz\35F_Bz.HQD
Project title:
Converged in 1 iterations with sigma = 2.5739E-04

                     standard
Log beta   value     deviation
AB         6.5812    0.0296
```

Figure S25. Ag^{+}-ion-induced UV-Vis spectral changes and log*K* calculation by *HyperSpec* of *meso*-**9c**.

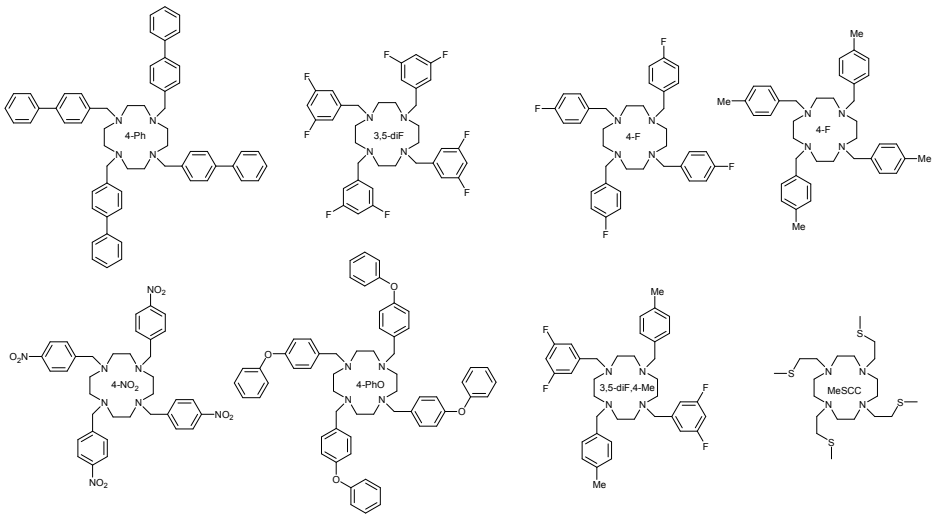



```
Hyperquad refinement output. Version number 1.1.33
Produced at 2014/06/17 20:05:39
from data stored in I:\Dropbox\0000_HyperSpec\001_Juli\35F\35F.HQD
Project title
</intro>
<iterations>
Initial Sigma =1.1186E-03
Iteration 1
             relative
Parameter    shift     new value
Log beta AB  0.0000    6.4916

New sigma =1.1186E-03
Change =649.1624%
</iterations>
<results>
HypSpec. Refinement concluded at 2014/06/17 20:05:39
Data from I:\Dropbox\0000_HyperSpec\001_Juli\35F\35F.HQD
Project title:
Converged in 1 iterations with sigma = 1.1186E-03

                     standard
Log beta   value     deviation
AB         6.4916    0.0198
```

Figure S26. Ag^{+}-ion-induced UV-Vis spectral changes and log*K* calculation by *HyperSpec* of *meso*-**9d**.

Table S1. Ag-N distances of Ag^+ complexes with **9a**, **9b**, **9c**, and tetra-armed cyclens previously reported.

	Ag-N distances (Å)				Mean Average Deviation	Ref #
9a/$AgClO_4$	2.402	2.52	2.193	2.428	0.073	
	2.515	2.491	2.466	2.389		
9b/$AgPF_6$	2.379	2.399	2.546	2.629	0.099	
9c/$AgClO_4$	2.49	2.495	2.424	2.375	0.047	
4-Ph	2.494	2.494	2.455	2.455	0.020	1
3,5-diF	2.495	2.457	2.404	2.426	0.031	1
4-F	2.473	2.467	2.432	2.442	0.017	1
4-Me	2.476	2.464	2.44	2.424	0.019	1
4-NO_2	2.474	2.476	2.441	2.418	0.023	1
4-PhO	2.429	2.47	2.441	2.471	0.018	1
3,5-diF,4-Me	2.459	2.428	2.463	2.463	0.013	2
MeS-CC	2.471	2.509	2.541	2.568	0.026	3
	2.566	2.51	2.554	2.529		



References

1) Y. Habata, M. Ikeda, S. Yamada, H. Takahashi, S. Ueno, T. Suzuki, and S. Kuwahara, *Org. Lett*., 2012, **14**, 4576–4579.

2) Y. Habata, Y. Oyama, M. Ikeda, and S. Kuwahara, *Dalton Trans*., 2013, **42**, 8212–8217.

3) T. Gyr, H. R. Macke, and M. Henning, *Angew. Chem. Int. Ed. Eng*., 1997, **36**, 2786–2788.