Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

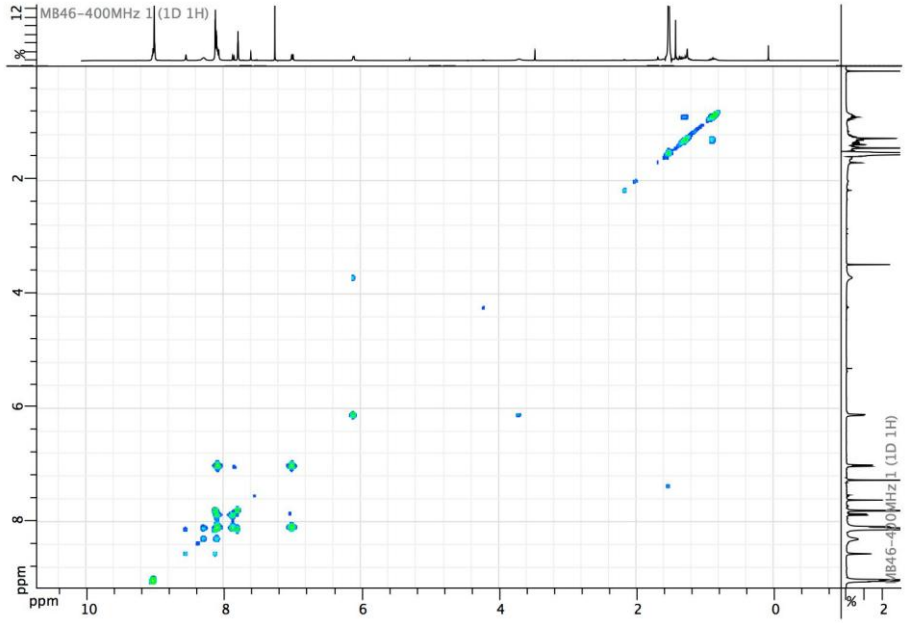


Figure SI-1. COSY spectrum (400MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **8** showing scalar couplings in the 0-8.6 ppm range.

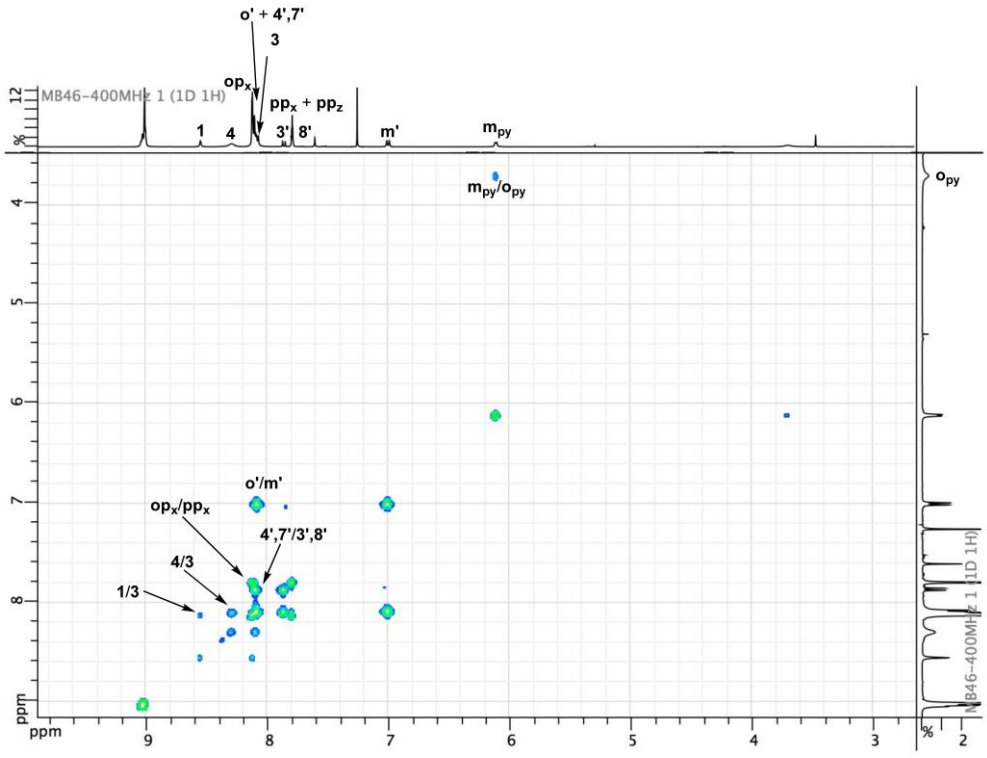


Figure SI-2. COSY spectrum (400 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **8** showing scalar couplings in the 4-9 ppm range.

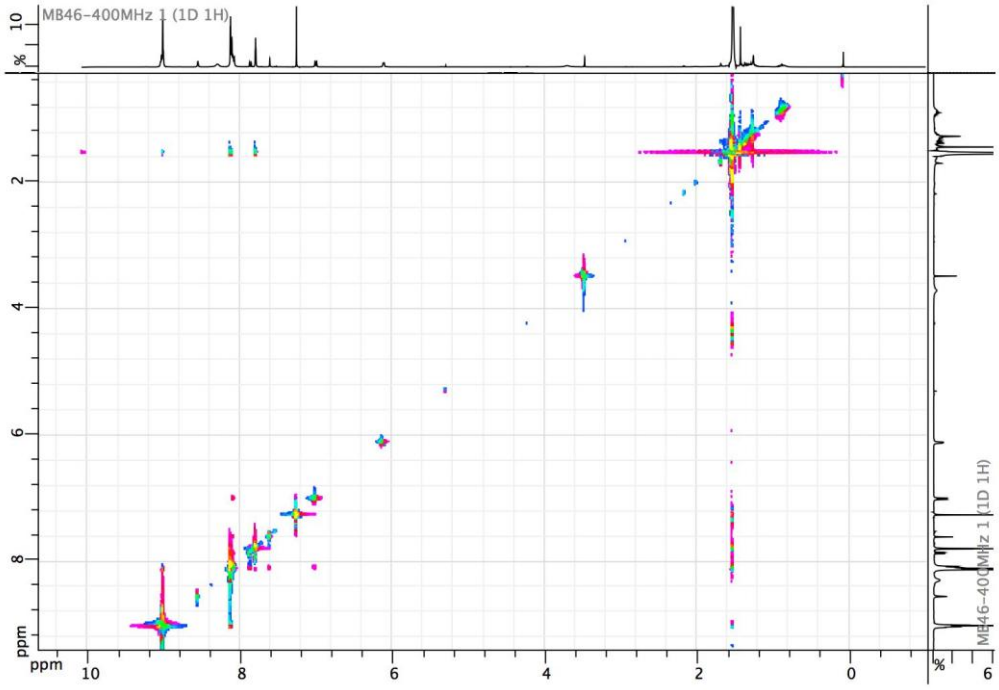


Figure SI-3. ROESY spectrum (400 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **8** showing dipolar couplings in the 0-9 ppm range.

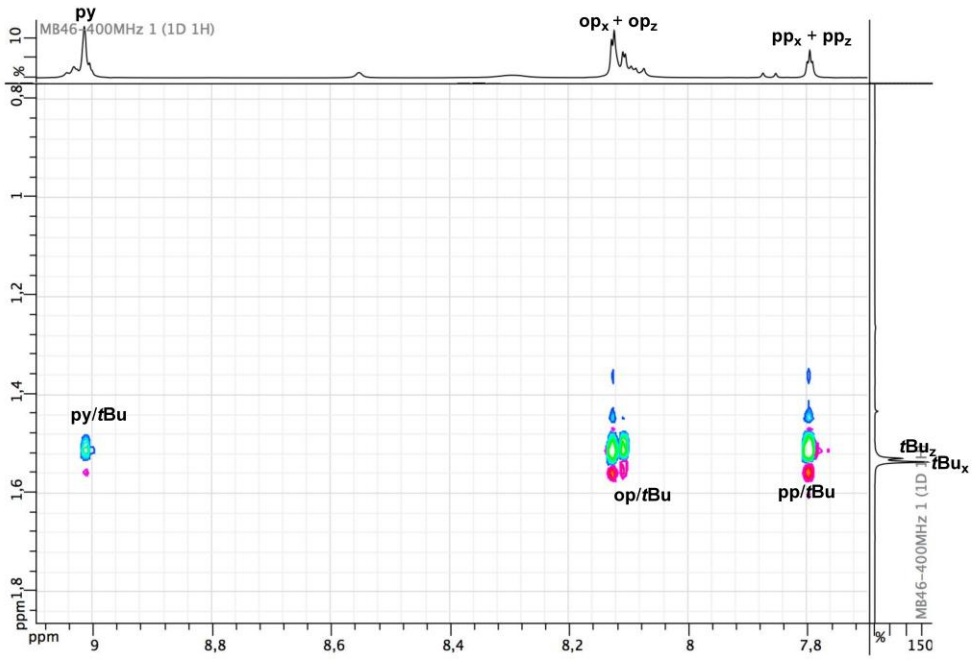


Fig SI-4. Zoom of the ROESY spectrum (400 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **8** showing specific dipolar couplings with the *t*Bu groups.

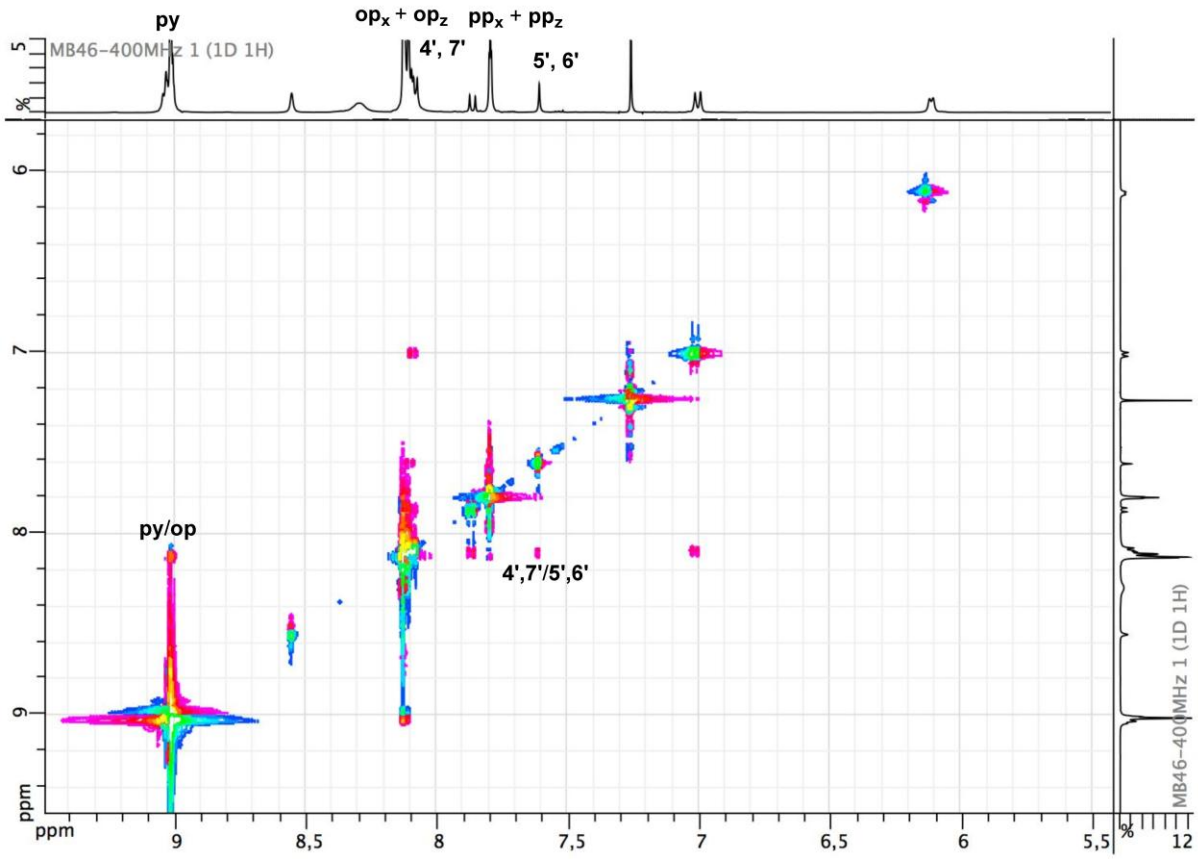
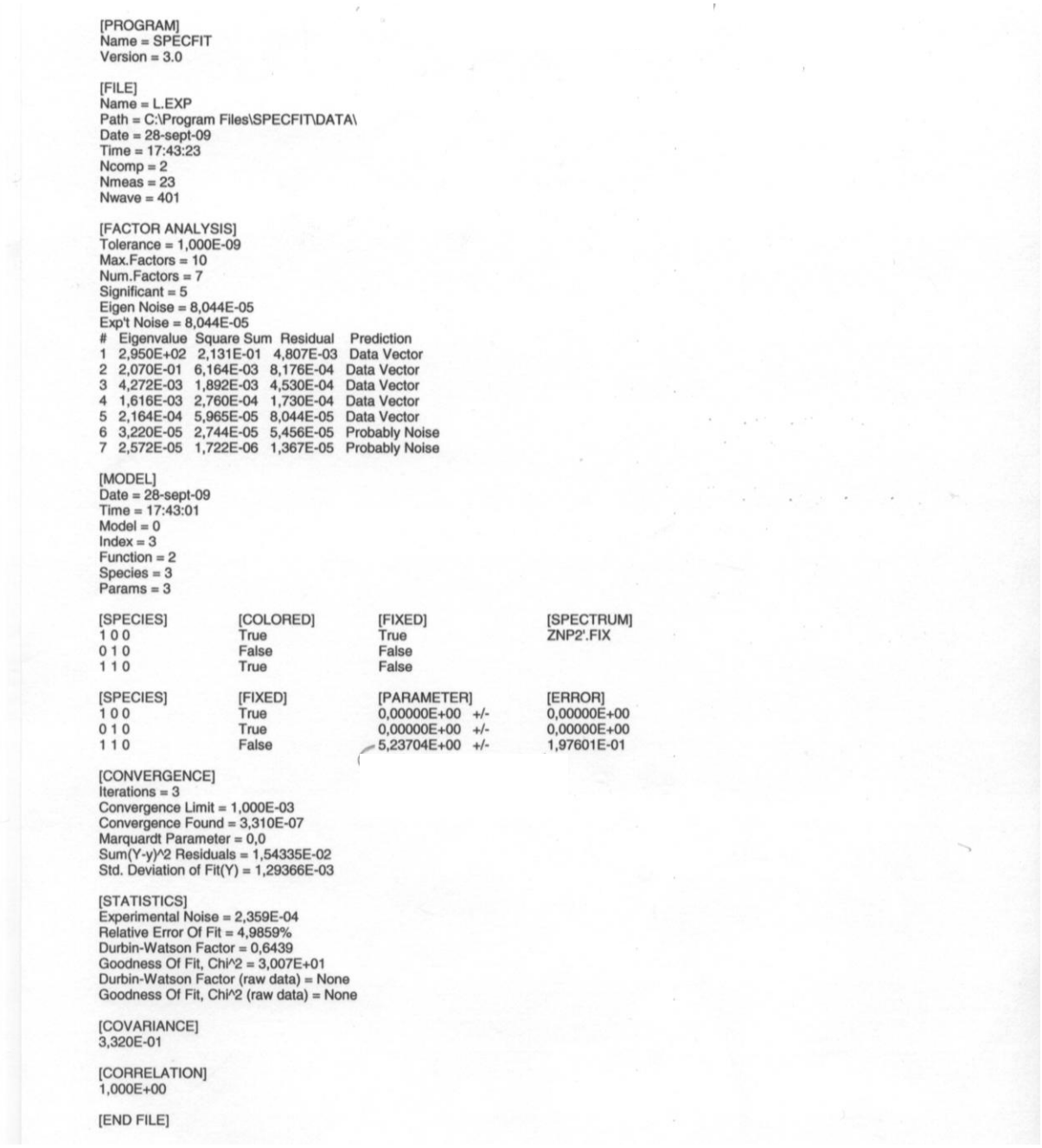


Figure SI-5. ROESY spectrum (400 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **8** showing dipolar couplings in the 5.5-9 ppm range.



```
[PROGRAM]
Name = SPECFIT
Version = 3.0

[FILE]
Name = L.EXP
Path = C:\Program Files\SPECFIT\DATA\
Date = 28-sept-09
Time = 17:43:23
Ncomp = 2
Nmeas = 23
Nwave = 401

[FACTOR ANALYSIS]
Tolerance = 1,000E-09
Max.Factors = 10
Num.Factors = 7
Significant = 5
Eigen Noise = 8,044E-05
Exp't Noise = 8,044E-05
#  Eigenvalue  Square Sum  Residual   Prediction
1  2,950E+02   2,131E-01  4,807E-03  Data Vector
2  2,070E-01   6,164E-03  8,176E-04  Data Vector
3  4,272E-03   1,892E-03  4,530E-04  Data Vector
4  1,616E-03   2,760E-04  1,730E-04  Data Vector
5  2,164E-04   5,965E-05  8,044E-05  Data Vector
6  3,220E-05   2,744E-05  5,456E-05  Probably Noise
7  2,572E-05   1,722E-06  1,367E-05  Probably Noise

[MODEL]
Date = 28-sept-09
Time = 17:43:01
Model = 0
Index = 3
Function = 2
Species = 3
Params = 3

[SPECIES]   [COLORED]   [FIXED]   [SPECTRUM]
1 0 0       True        True      ZNP2'.FIX
0 1 0       False       False
1 1 0       True        False

[SPECIES]   [FIXED]   [PARAMETER]          [ERROR]
1 0 0       True      0,00000E+00  +/-    0,00000E+00
0 1 0       True      0,00000E+00  +/-    0,00000E+00
1 1 0       False     5,23704E+00  +/-    1,97601E-01

[CONVERGENCE]
Iterations = 3
Convergence Limit = 1,000E-03
Convergence Found = 3,310E-07
Marquardt Parameter = 0,0
Sum(Y-y)^2 Residuals = 1,54335E-02
Std. Deviation of Fit(Y) = 1,29366E-03

[STATISTICS]
Experimental Noise = 2,359E-04
Relative Error Of Fit = 4,9859%
Durbin-Watson Factor = 0,6439
Goodness Of Fit, Chi^2 = 3,007E+01
Durbin-Watson Factor (raw data) = None
Goodness Of Fit, Chi^2 (raw data) = None

[COVARIANCE]
3,320E-01

[CORRELATION]
1,000E+00

[END FILE]
```

Figure SI-6. Fitting of the UV titration for macrocycle **8**. Addition of constant aliquots (10 μL) of a solution of bis(pyridine) **7** in toluene (c = 3.26 x 10^{-5} M) to a solution of bis-Zn porphyrin **4** in toluene (c = 1.09 x 10^{-6} M).

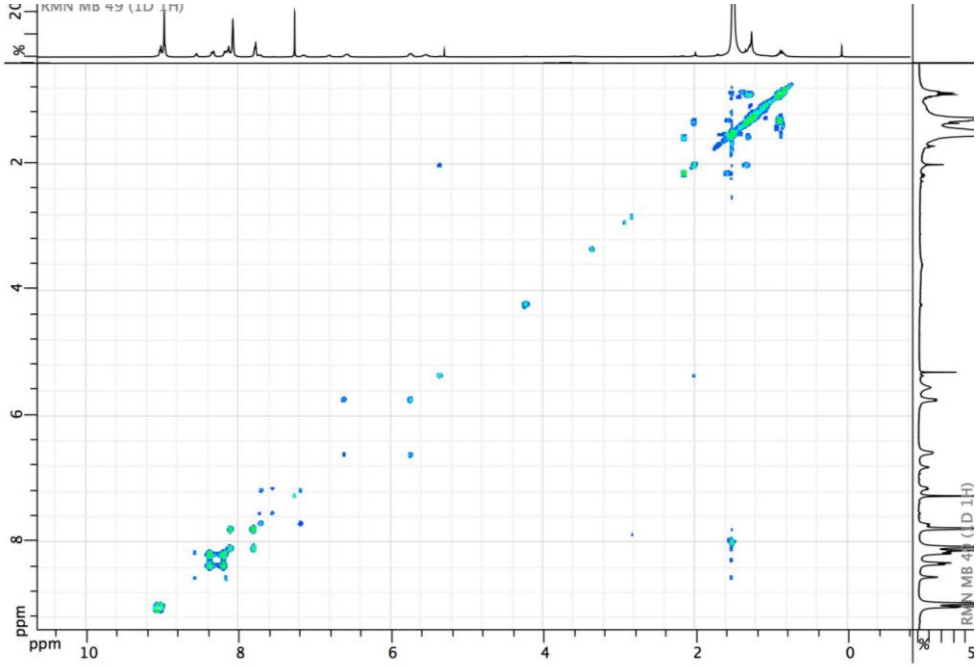


Figure SI-7. COSY spectrum (500 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **10.PF$_6$** showing scalar couplings in the 0-10 ppm range.

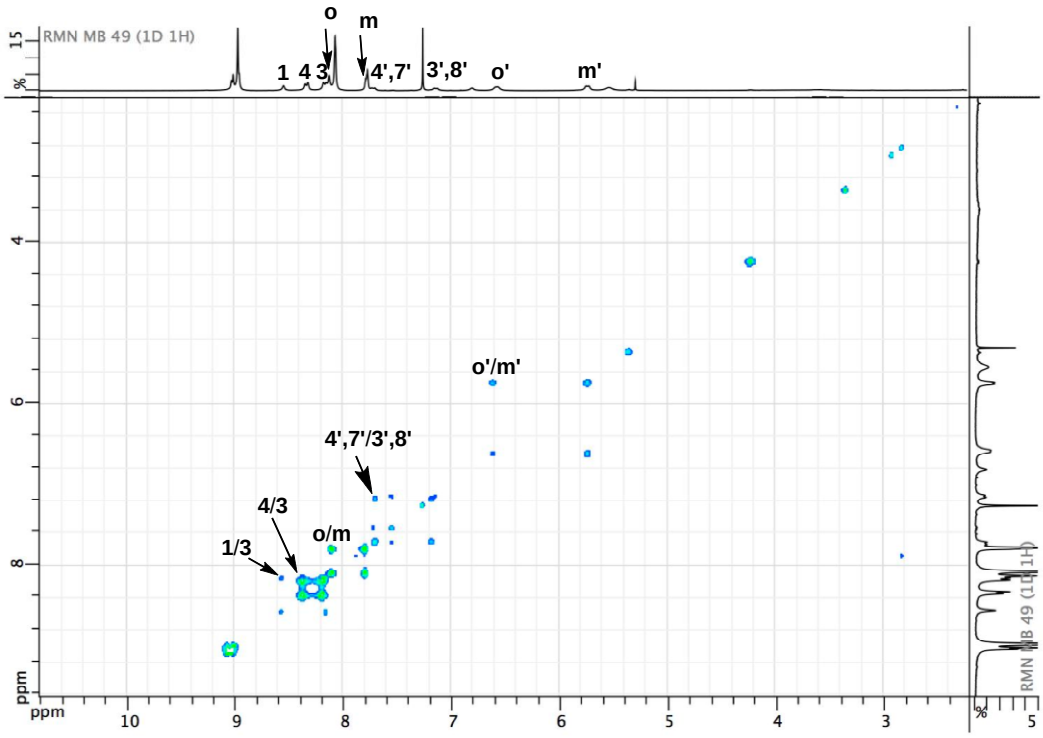


Figure SI-8. COSY spectrum (500 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **10.PF$_6$** showing scalar couplings in the 3-9 ppm range.

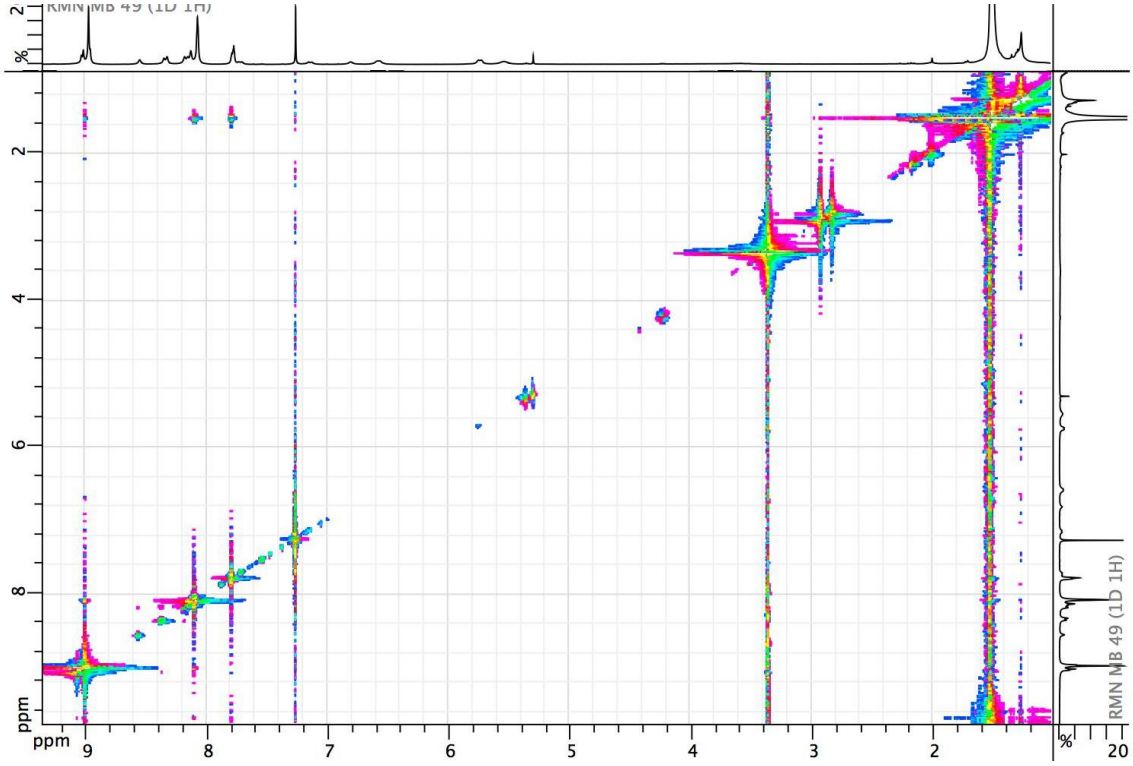


Figure SI-9. ROESY spectrum (500 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **10.PF$_6$** showing dipolar couplings in the 0-9 ppm range.

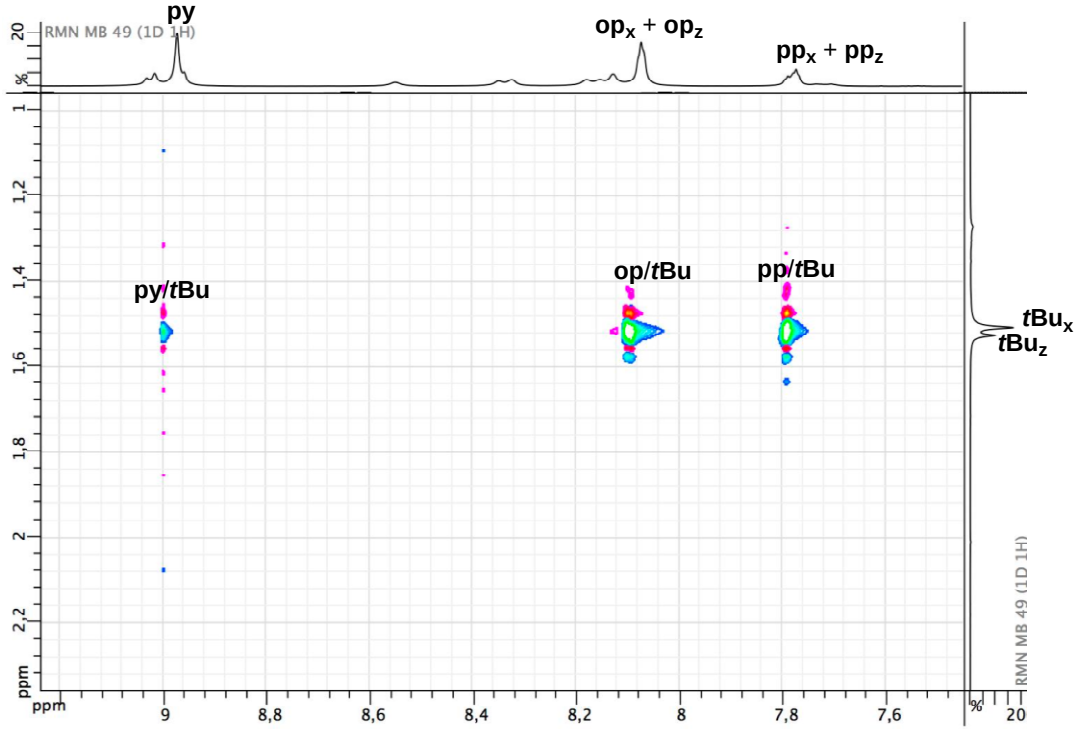


Figure SI-10. Zoom of the ROESY spectrum (500 MHz, $CDCl_3$, c = 1 x 10^{-3} M) of **10.PF$_6$** showing specific dipolar couplings with the *t*Bu groups.

```
[PROGRAM]
Name = SPECFIT
Version = 3.0

[FILE]
Name = L.EXP
Path = C:\Program Files\SPECFIT\DATA\
Date = 29-sept-09
Time = 19:19:42
Ncomp = 2
Nmeas = 27
Nwave = 341

[FACTOR ANALYSIS]
Tolerance = 1,000E-09
Max.Factors = 10
Num.Factors = 6
Significant = 3
Eigen Noise = 4,268E-04
Exp't Noise = 4,268E-04
#  Eigenvalue  Square Sum  Residual   Prediction
1  3,473E+02   3,201E-01  5,897E-03  Data Vector
2  3,128E-01   7,362E-03  8,943E-04  Data Vector
3  5,686E-03   1,676E-03  4,268E-04  Data Vector
4  8,939E-04   7,823E-04  2,916E-04  Probably Noise
5  4,939E-04   2,883E-04  1,770E-04  Probably Noise
6  2,532E-04   3,510E-05  6,177E-05  Probably Noise

[MODEL]
Date = 29-sept-09
Time = 19:19:40
Model = 0
Index = 3
Function = 2
Species = 3
Params = 3

[SPECIES]   [COLORED]   [FIXED]    [SPECTRUM]
1 0 0       True        True       ZNP2'.FIX
0 1 0       True        True       MB48.FIX
2 1 0       True        False

[SPECIES]   [FIXED]     [PARAMETER]          [ERROR]
1 0 0       True        0,00000E+00  +/-     0,00000E+00
0 1 0       True        0,00000E+00  +/-     0,00000E+00
2 1 0       False       1,09399E+01  +/-     9,91649E-02

[CONVERGENCE]
Iterations = 6
Convergence Limit = 1,000E-03
Convergence Found = 1,429E-05
Marquardt Parameter = 0,0
Sum(Y-y)^2 Residuals = 1,60010E-02
Std. Deviation of Fit(Y) = 1,31837E-03

[STATISTICS]
Experimental Noise = 1,996E-04
Relative Error Of Fit = 6,4393%
Durbin-Watson Factor = 0,1680
Goodness Of Fit, Chi^2 = 4,362E+01
Durbin-Watson Factor (raw data) = None
Goodness Of Fit, Chi^2 (raw data) = None

[COVARIANCE]
6,580E-02

[CORRELATION]
1,000E+00

[END FILE]
```

Figure SI-11. Fitting of the UV titration for [2]catenane **10.PF$_6$**. Addition of constant aliquots (10 μL) of a solution of **9.PF$_6$** in toluene (c = 3.26 x 10^{-5} M) to a solution of bis-Zn porphyrin **4** in toluene (c = 1.09 x 10^{-6} M).

Electronic Supplementary Material (ESI) for New Journal of Chemistry