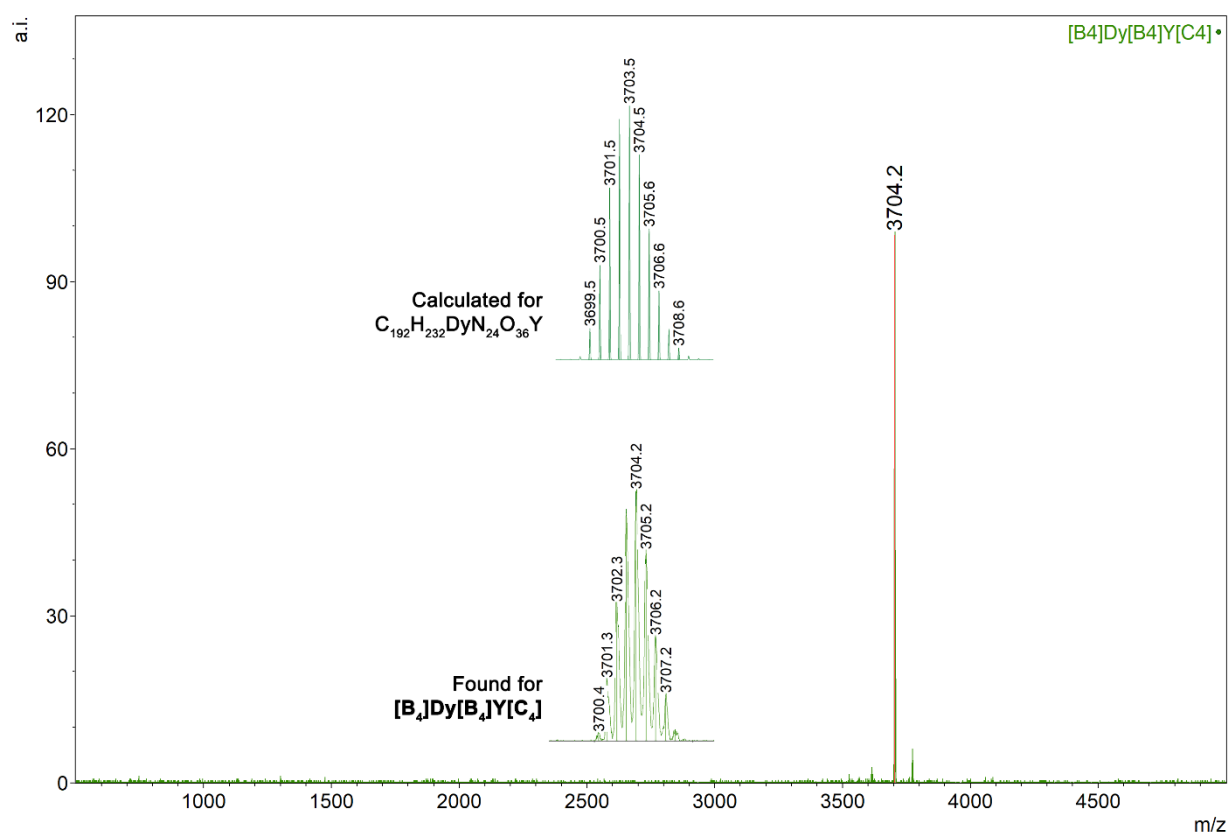
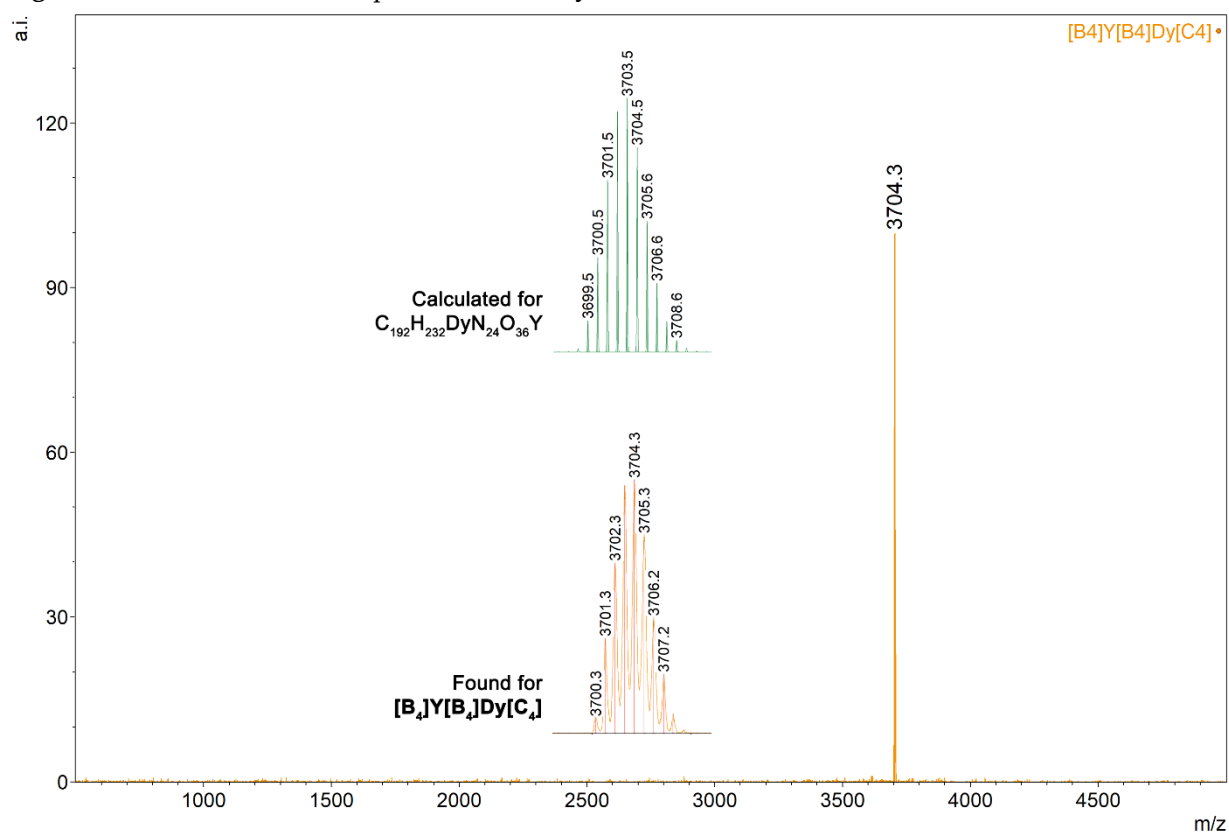
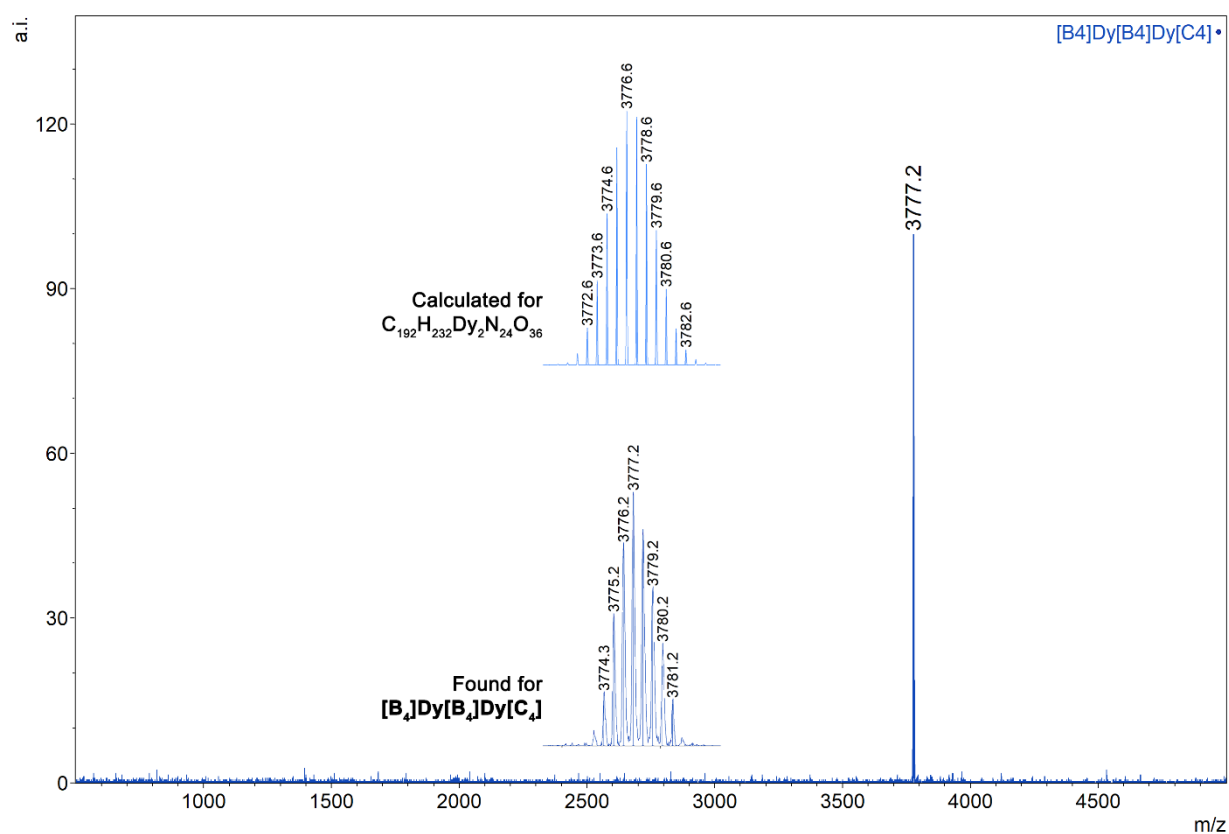
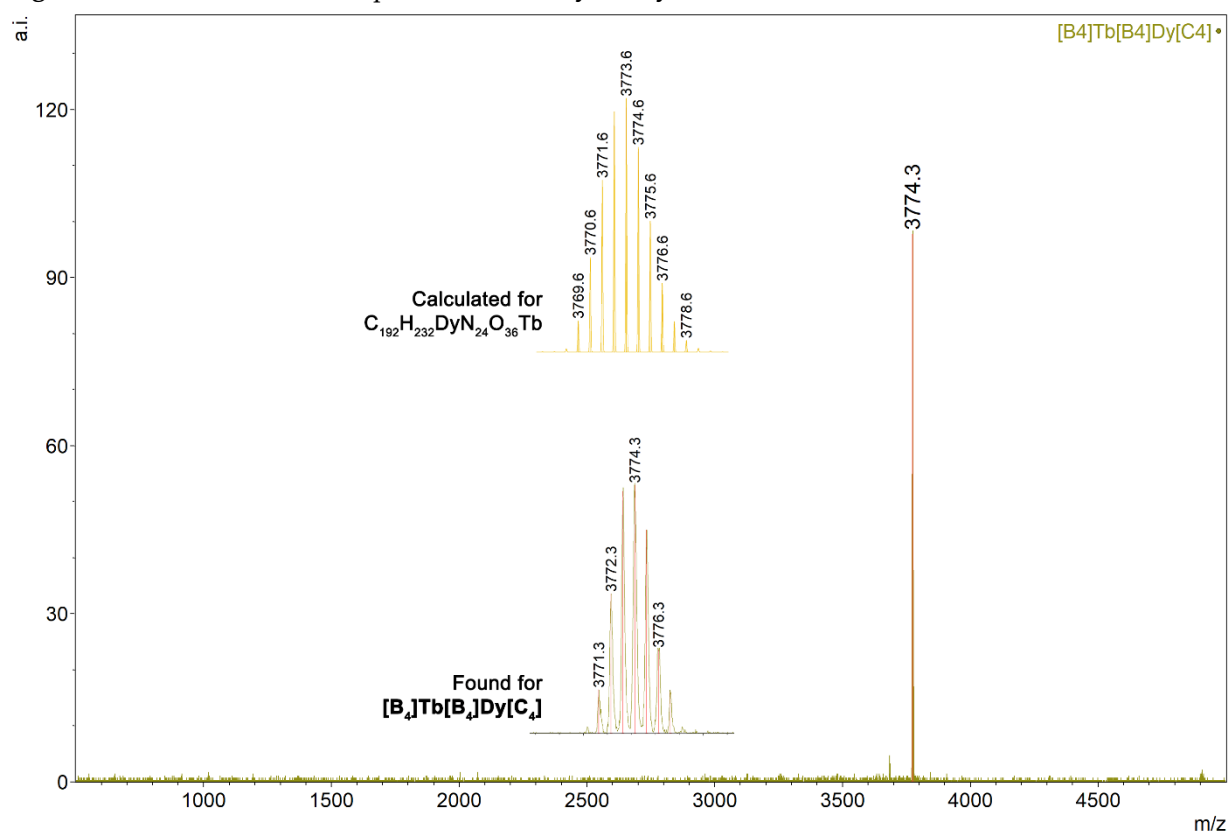


Magnetic Anisotropy of Homo- and Heteronuclear Terbium (III) and Dysprosium(III) Trisphthalocyaninates Derived from Paramagnetic ^1H -NMR Investigation

Ilya D. Kormschikov, Marina A. Polovkova, Gayane A. Kirakosyan ^{2,3}, Alexander G. Martynov ^{2,*}, Yulia G. Gorbunova ^{2,3} and Aslan Yu. Tsivadze ^{2,3}

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Figure S3. MALDI-TOF mass spectrum of $[B_4]Dy[B_4]Dy[C_4]$.Figure S4. MALDI-TOF mass spectrum of $[B_4]Tb[B_4]Dy[C_4]$.

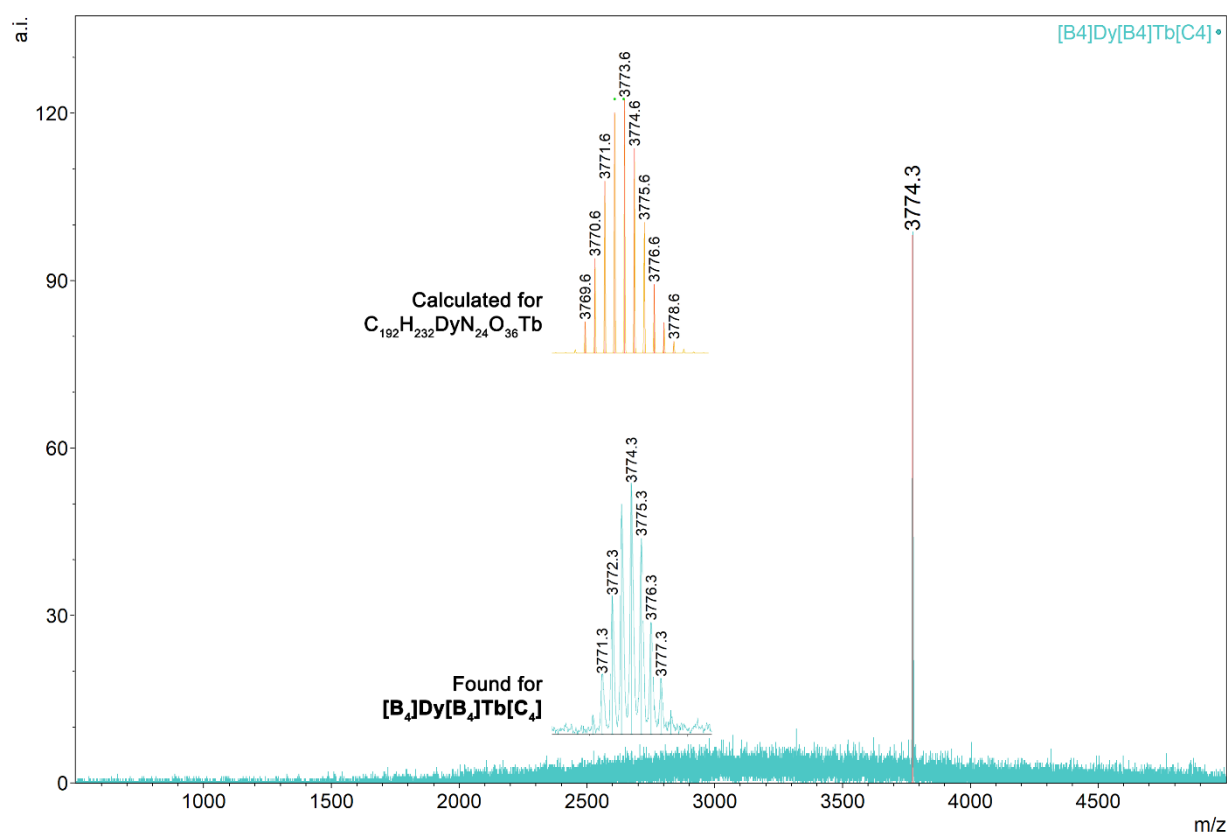


Figure S5. MALDI-TOF mass spectrum of $[B_4]Dy[B_4]Tb[C_4]$.

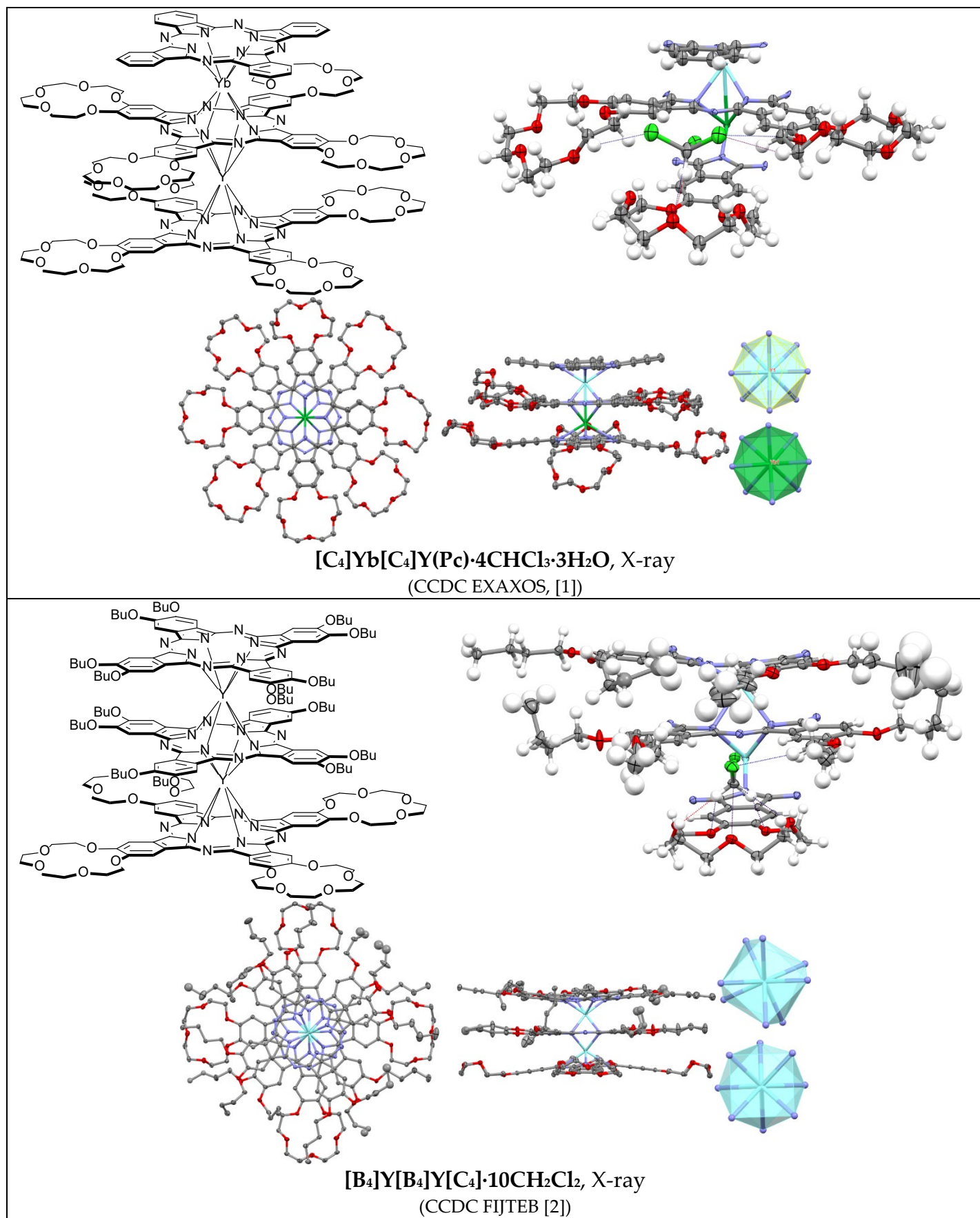


Figure S6. Fragments of X-ray structures of [C₄]Yb[C₄]Y(Pc)·4CHCl₃·3H₂O and [B₄]Y[B₄]Y[C₄]·10CH₂Cl₂, showing the analogy in localization of solvent molecules and contacts with substituents which stabilize staggered pairwise conformations.

In both cases chlorinated solvents are sitting atop the crown-ether rings forming weak CH...O contacts with oxygen atoms of crown-ether rings and CH...Cl contacts with the substituents of the neighboring ligands which stabilizes the pairwise staggered conformation.

1. Polovkova, M.A.; Martynov, A.G.; Birin, K.P.; Nefedov, S.E.; Gorbunova, Y.G.; Tsivadze, A.Y. Determination of the Structural Parameters of Heteronuclear (Phthalocyaninato)Bis(Crownphthalocyaninato)Lanthanide(III) Triple-Deckers in Solution by Simultaneous Analysis of NMR and Single-Crystal X-Ray Data. *Inorg. Chem.* **2016**, *55*, 9258–9269, doi:10.1021/acs.inorgchem.6b01292.
2. Martynov, A.G.; Sinelshchikova, A.A.; Dorovatovskii, P. V.; Polovkova, M.A.; Ovchenkova, A.E.; Birin, K.P.; Kirakosyan, G.A.; Gorbunova, Y.G.; Tsivadze, A.Y. Solvation-Induced Conformational Switching of Trisphthalocyanates for Control of Their Magnetic Properties. *Inorg. Chem.* **2023**, *62*, 10329–10342, doi:10.1021/acs.inorgchem.3c01169.

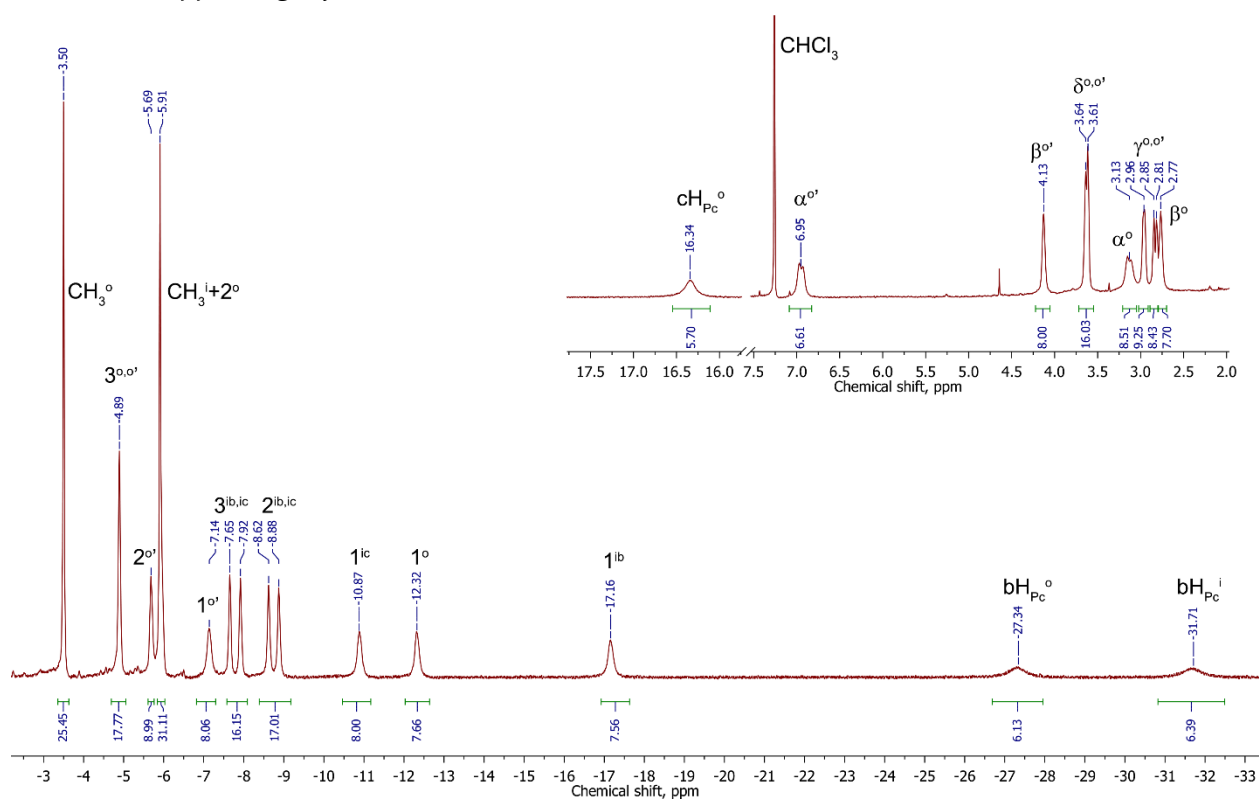


Figure S7. ^1H -NMR spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Y}[\text{C}_4]$ in CDCl_3 .

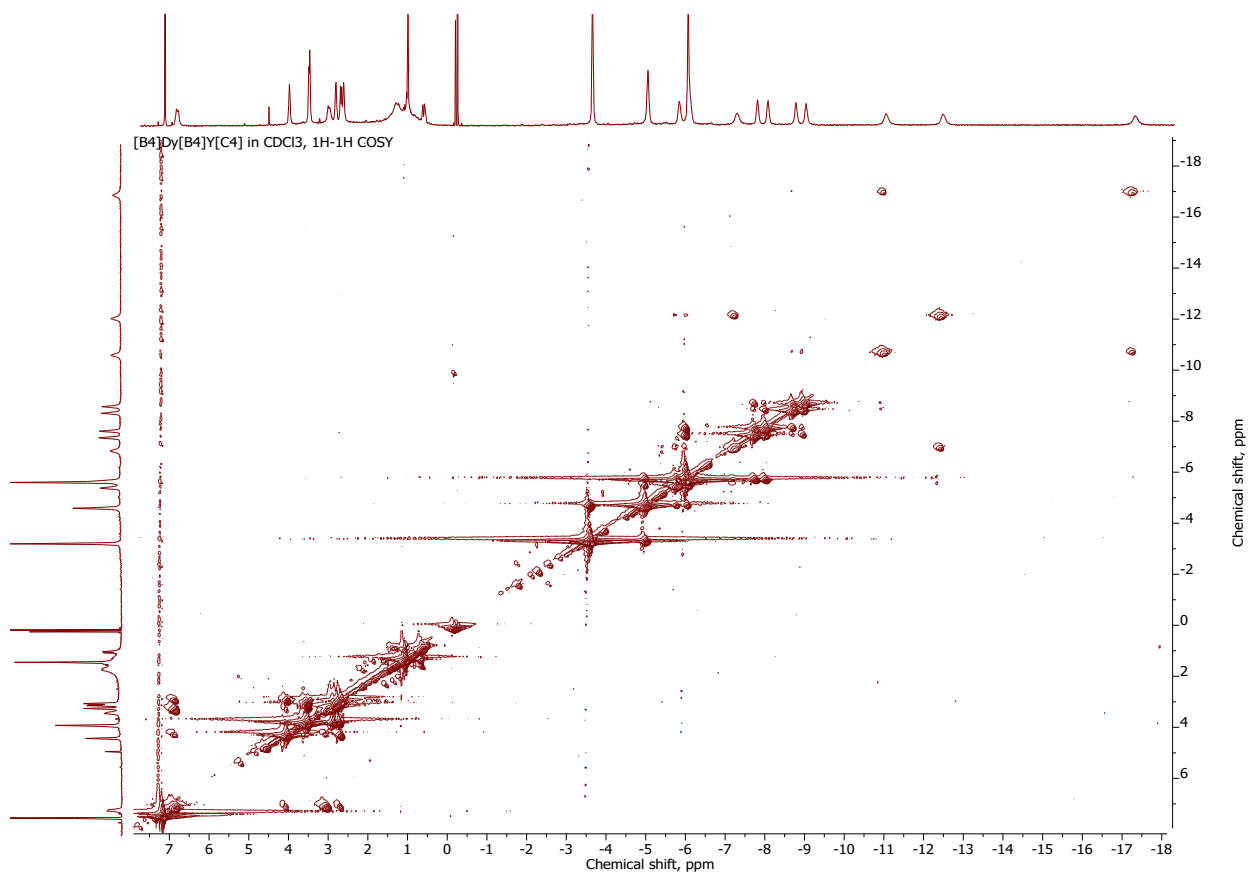


Figure S8. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Y}[\text{C}_4]$ in CDCl_3 .

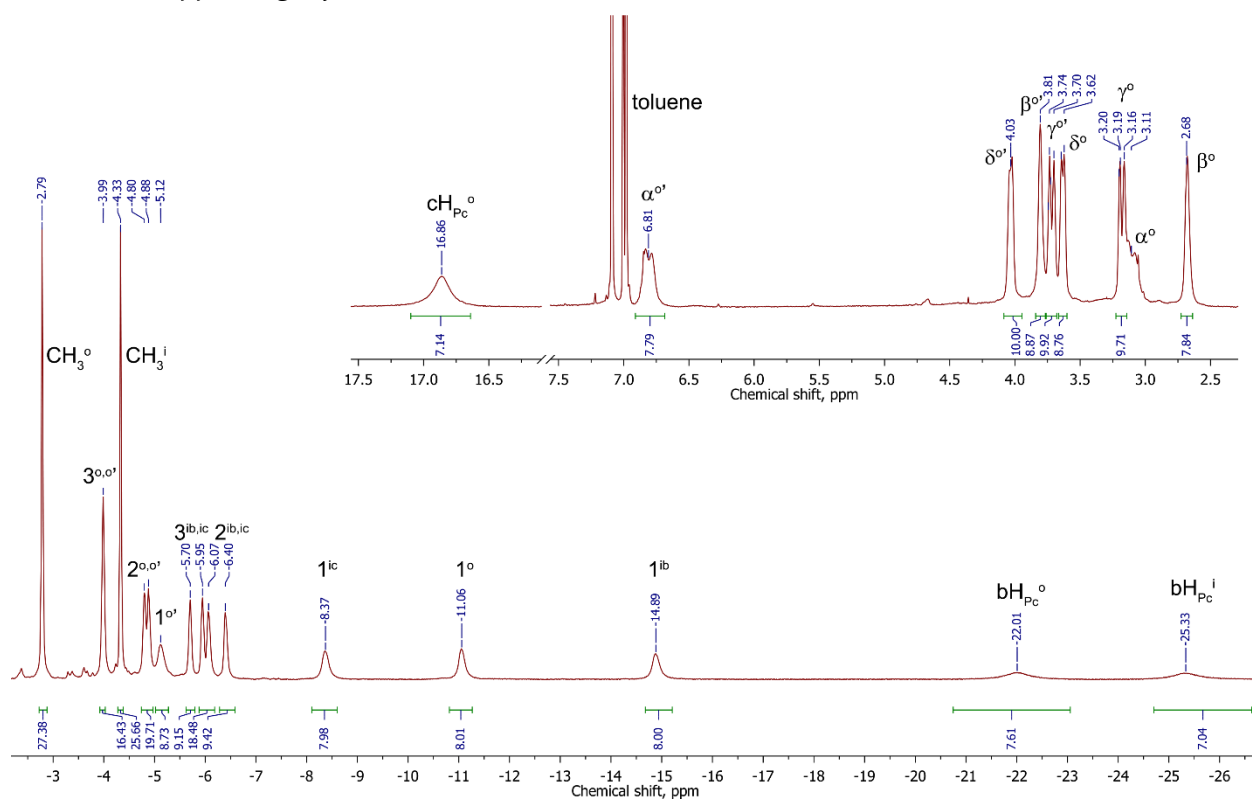


Figure S9. ^1H -NMR spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Y}[\text{C}_4]$ in toluene-d_8 .

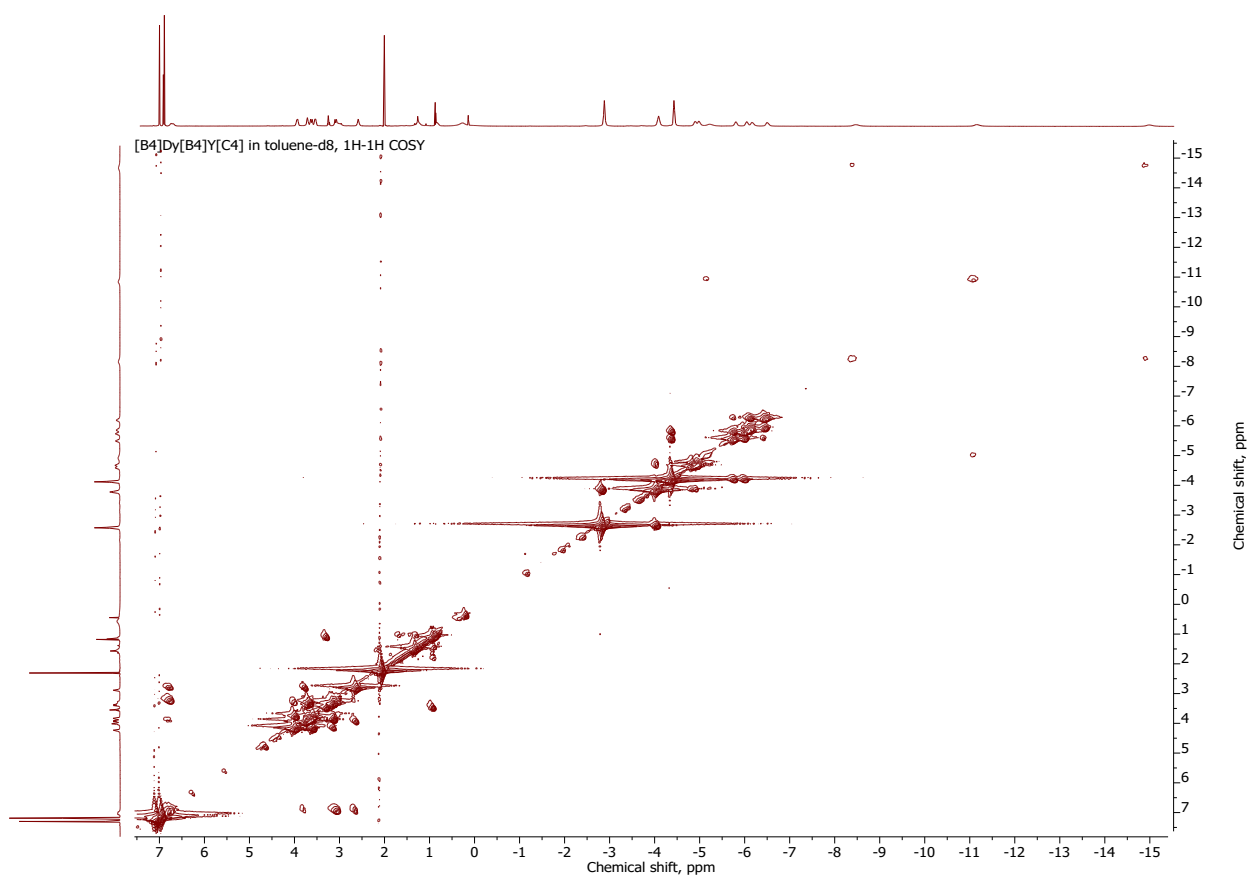


Figure S10. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Y}[\text{C}_4]$ in toluene-d_8 .

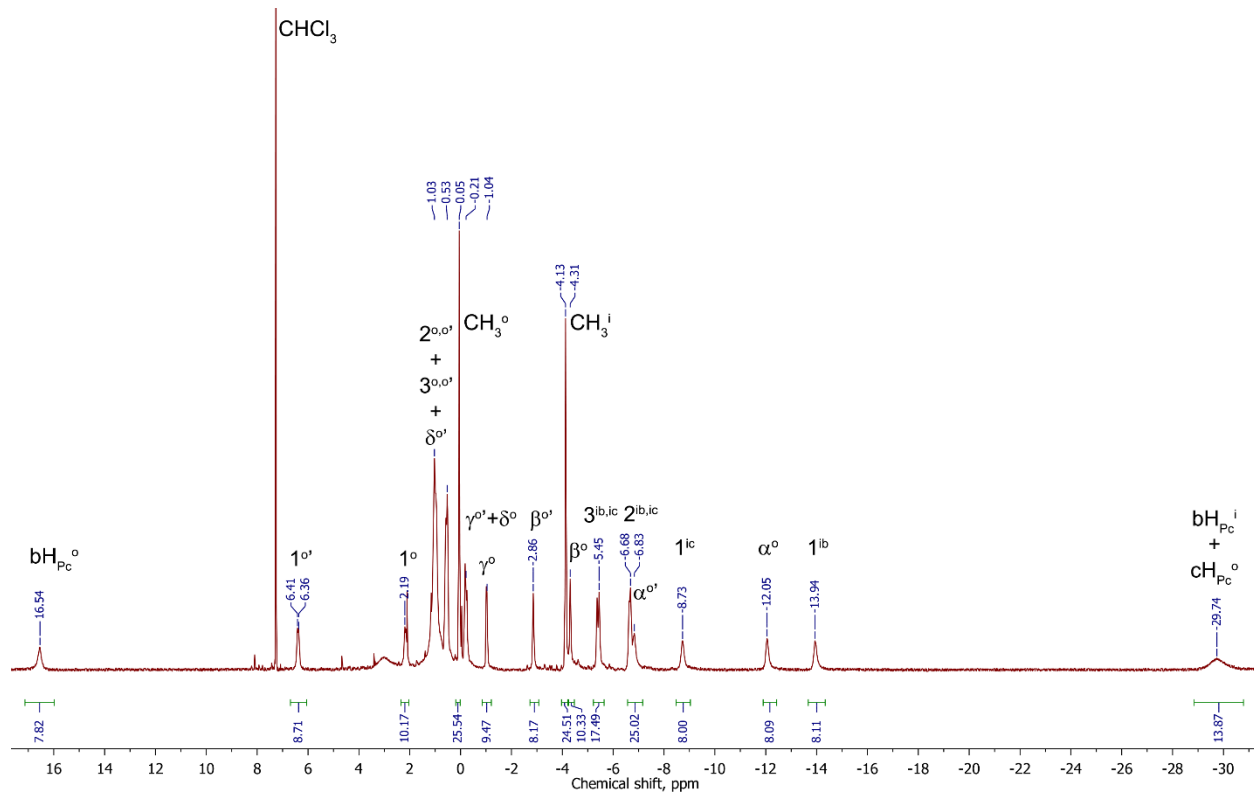


Figure S11. ^1H -NMR spectrum of $[\text{B}_4]\text{Y}[\text{B}_4]\text{Dy}[\text{C}_4]$ in CDCl_3 .

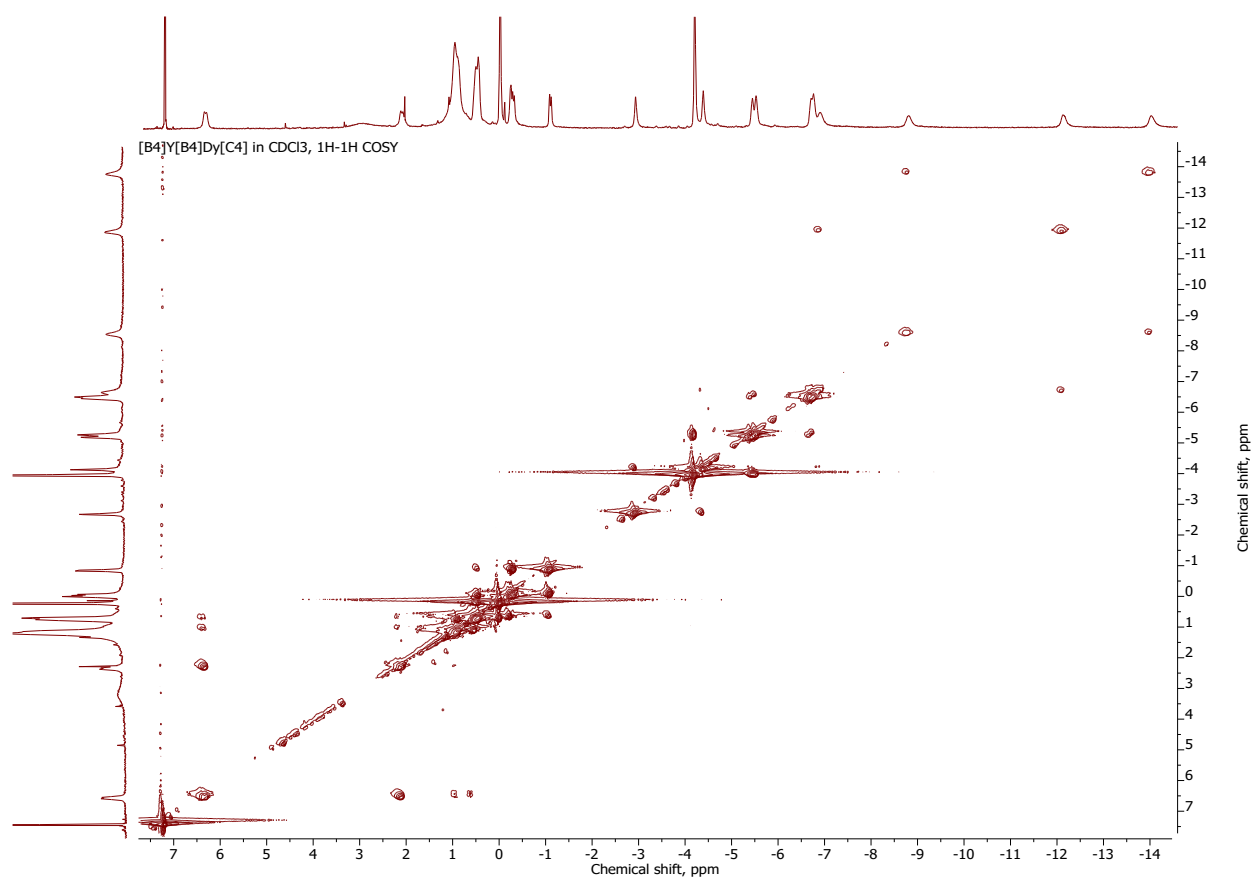


Figure S12. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Y}[\text{B}_4]\text{Dy}[\text{C}_4]$ in CDCl_3 .

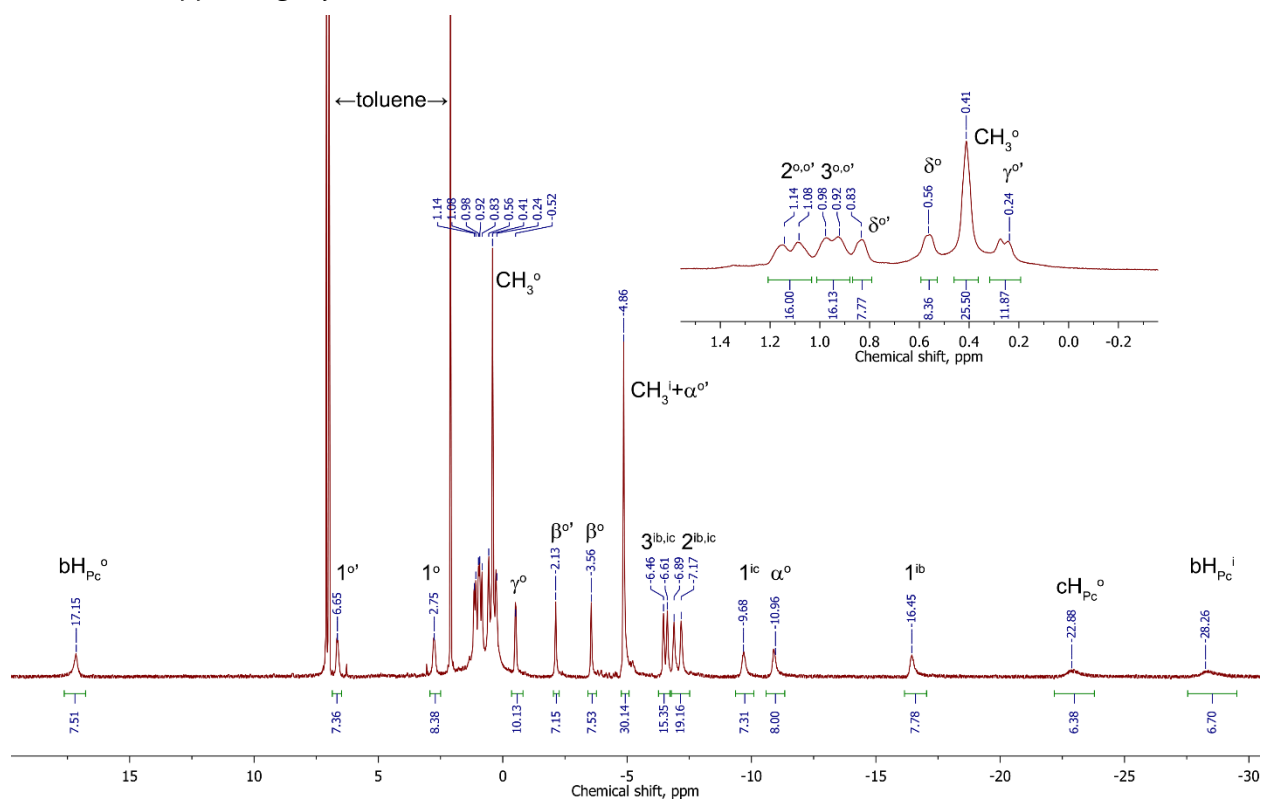


Figure S13. ^1H -NMR spectrum of $[\text{B}_4]\text{Y}[\text{B}_4]\text{Dy}[\text{C}_4]$ in toluene- d_8 .

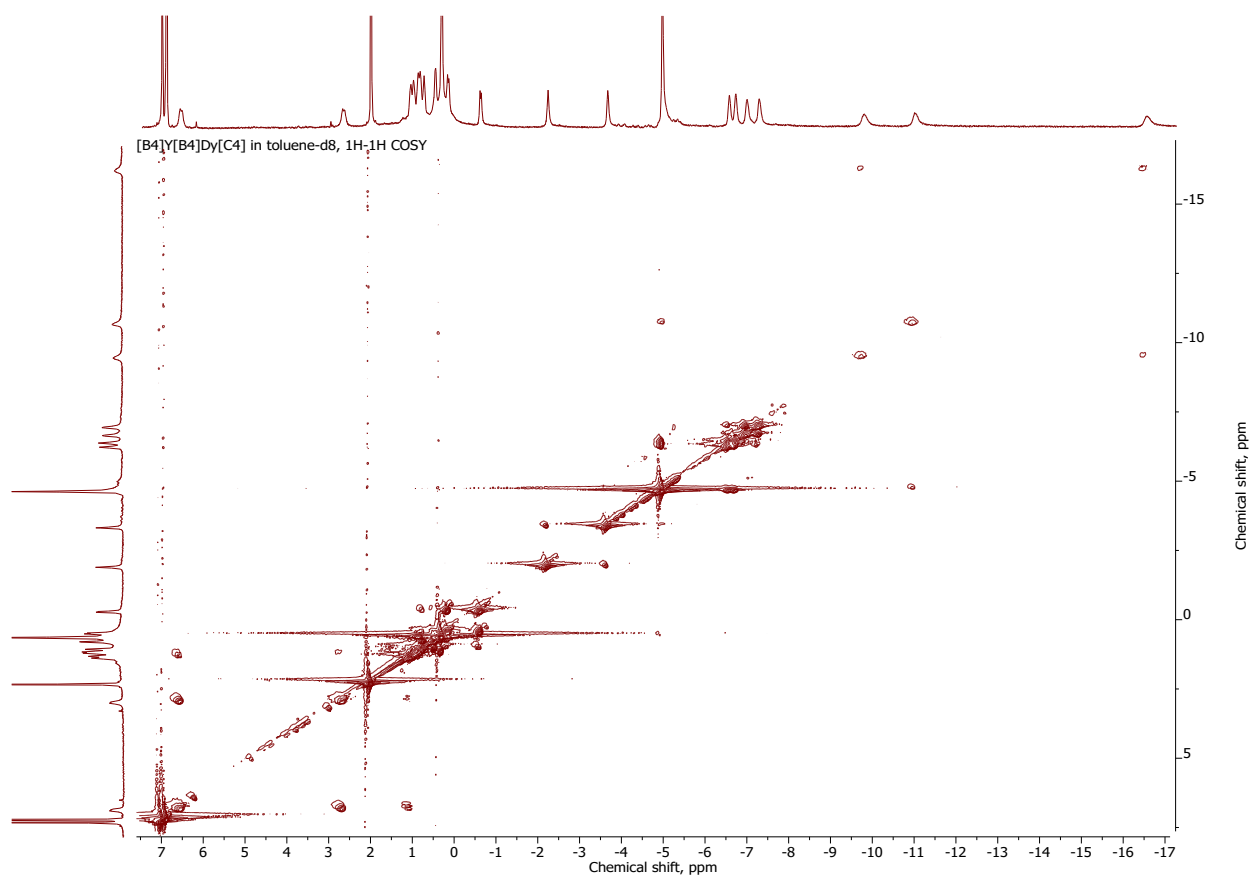


Figure S14. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Y}[\text{B}_4]\text{Dy}[\text{C}_4]$ in toluene- d_8 .

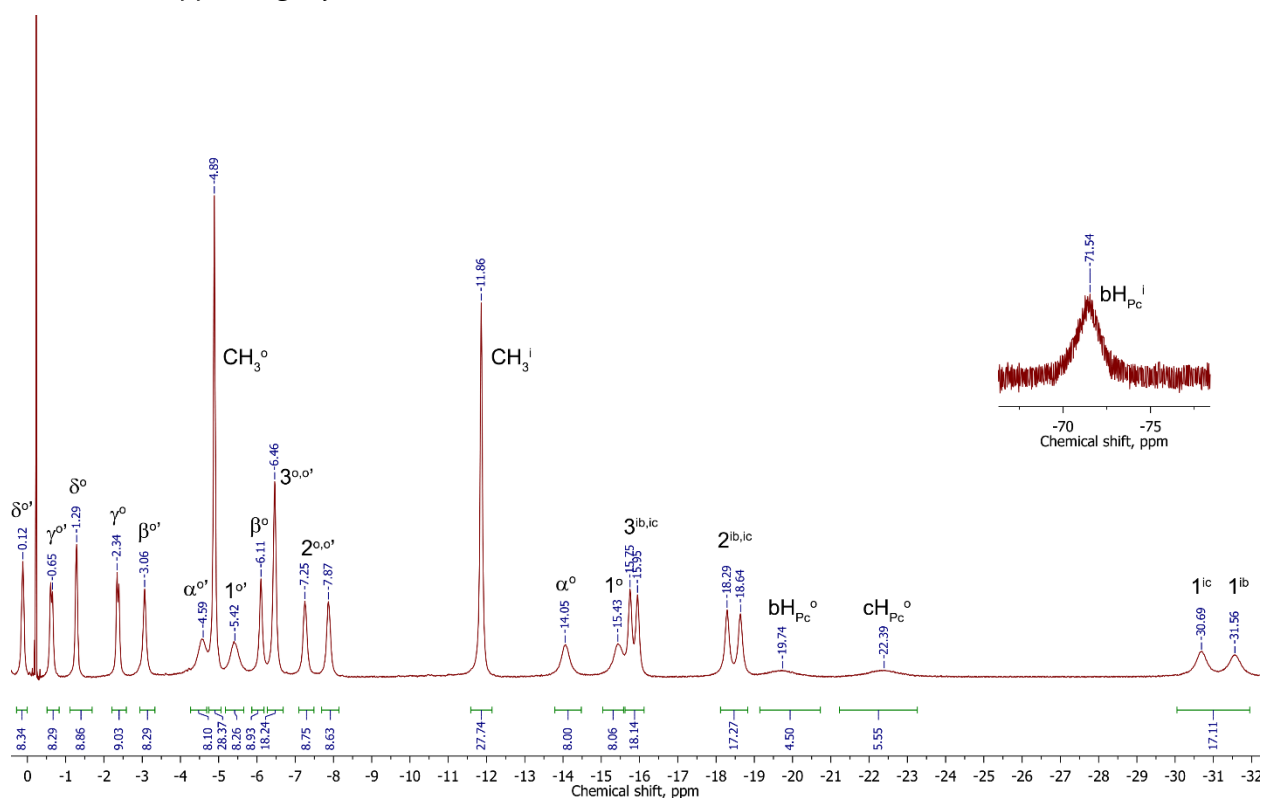


Figure S15. ^1H -NMR spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Dy}[\text{C}_4]$ in CDCl_3 .

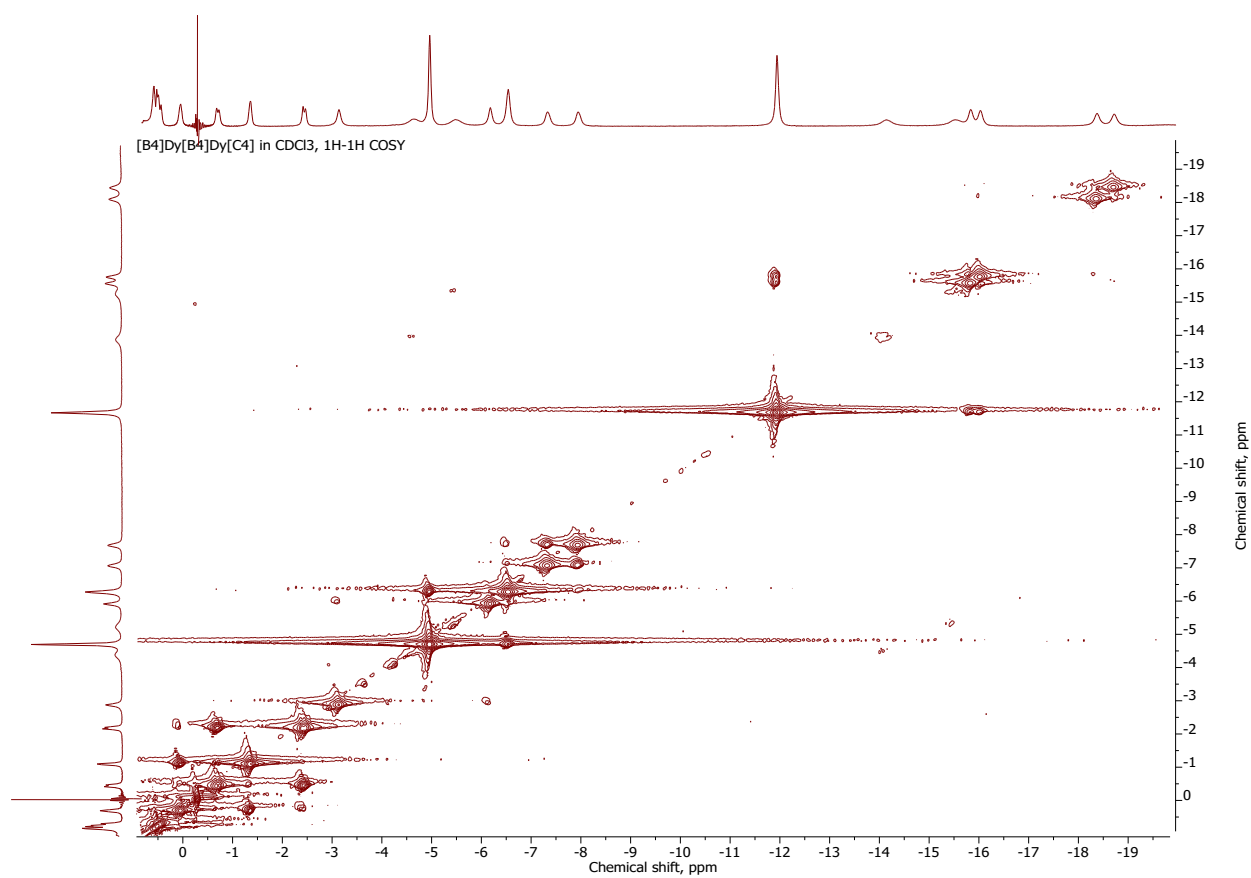


Figure S16. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Dy}[\text{C}_4]$ in CDCl_3 .

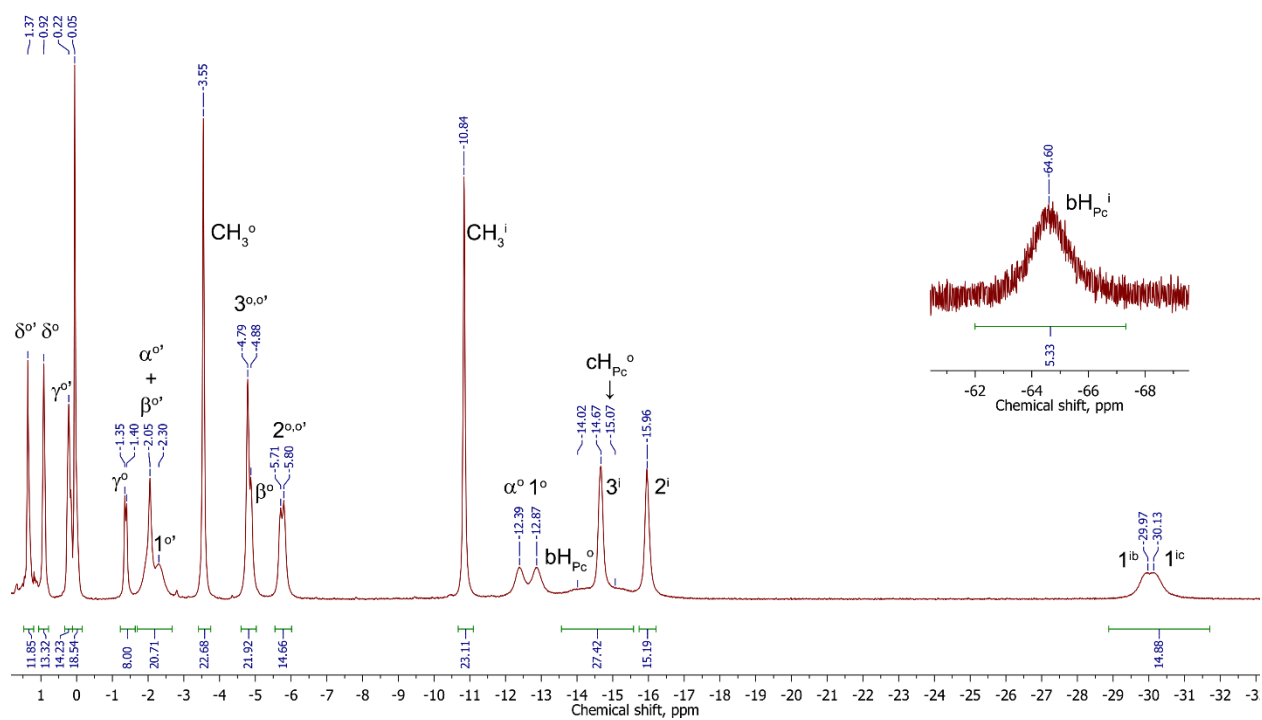


Figure S17. ¹H-NMR spectrum of [B₄]Dy[B₄]Dy[C₄] in toluene-d₈.

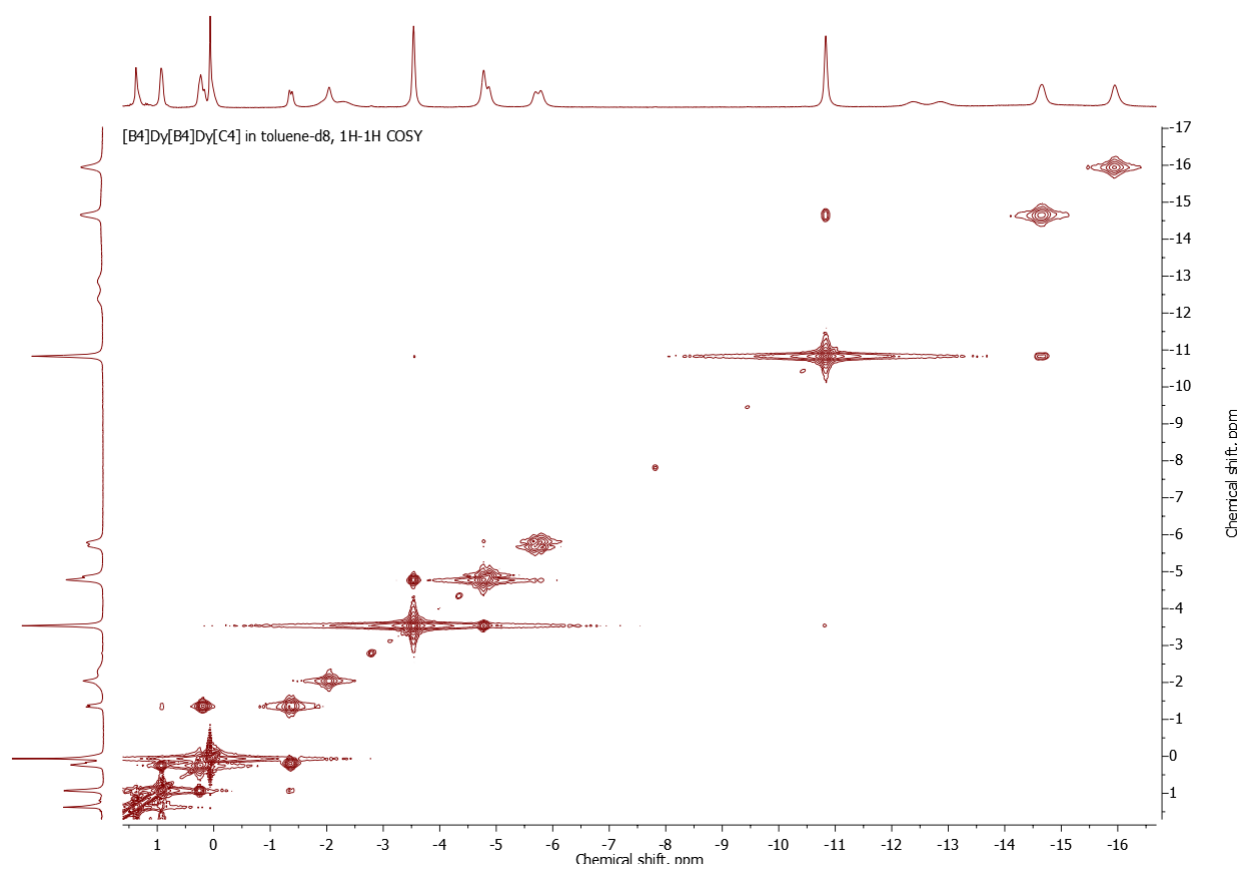
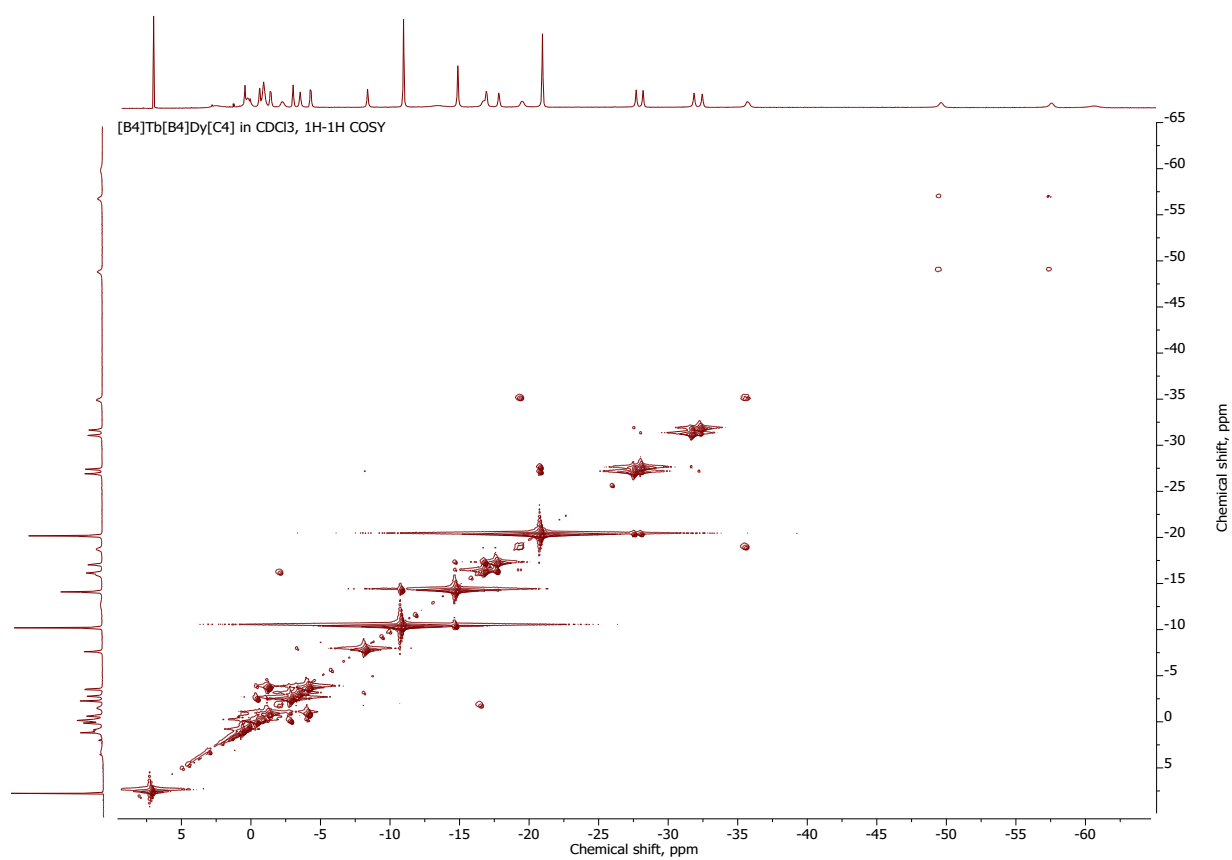
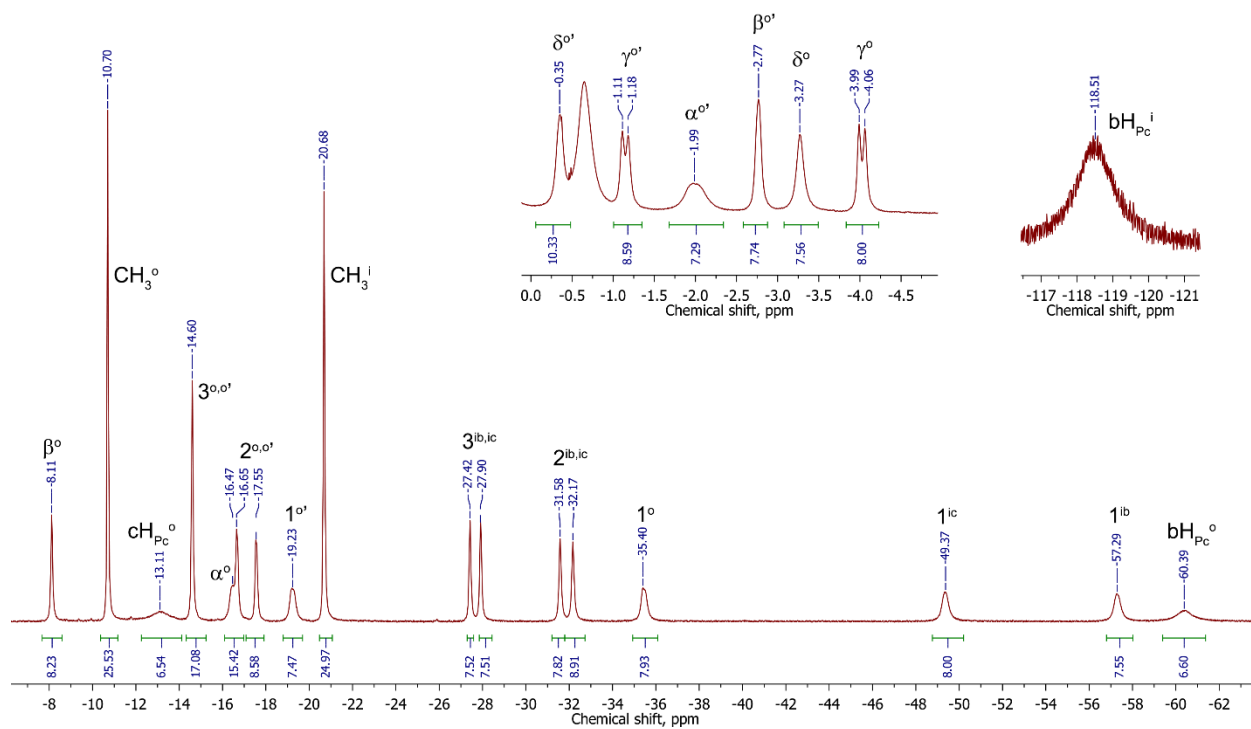


Figure S18. ¹H-¹H COSY spectrum of [B₄]Dy[B₄]Dy[C₄] in toluene-d₈.



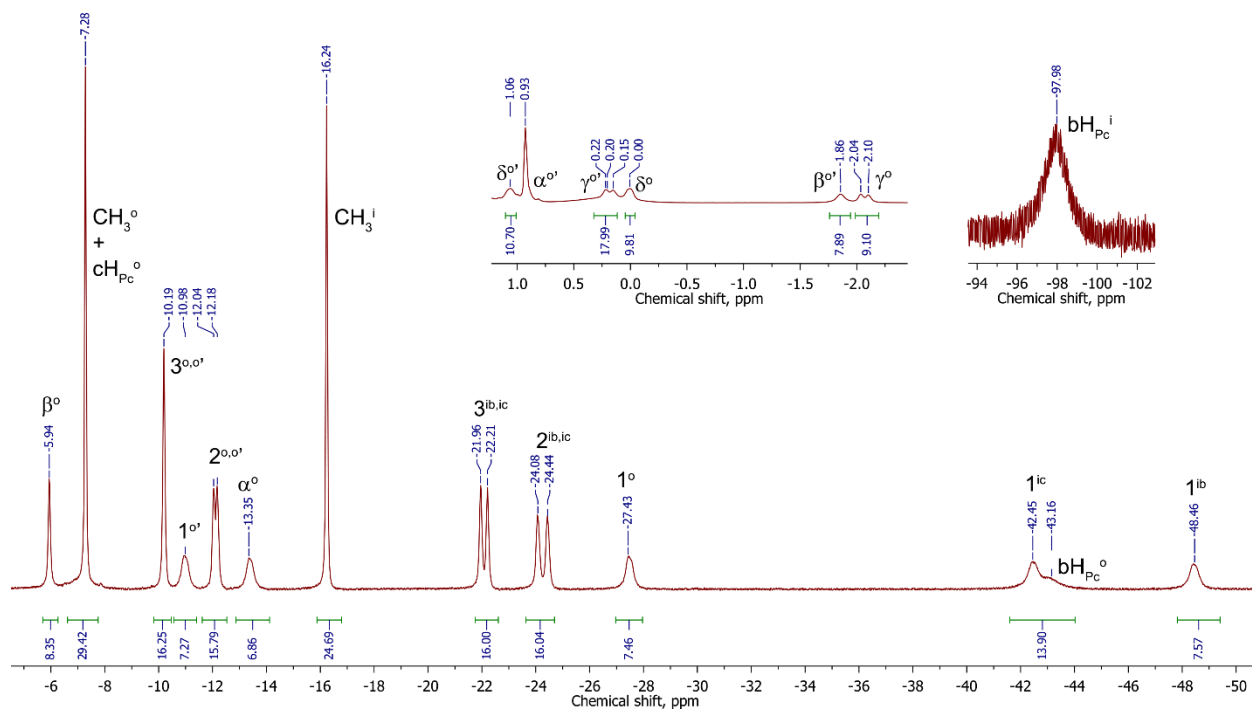


Figure S21. ^1H -NMR spectrum of $[\text{B}_4]\text{Tb}[\text{B}_4]\text{Dy}[\text{C}_4]$ in toluene- d_8 .

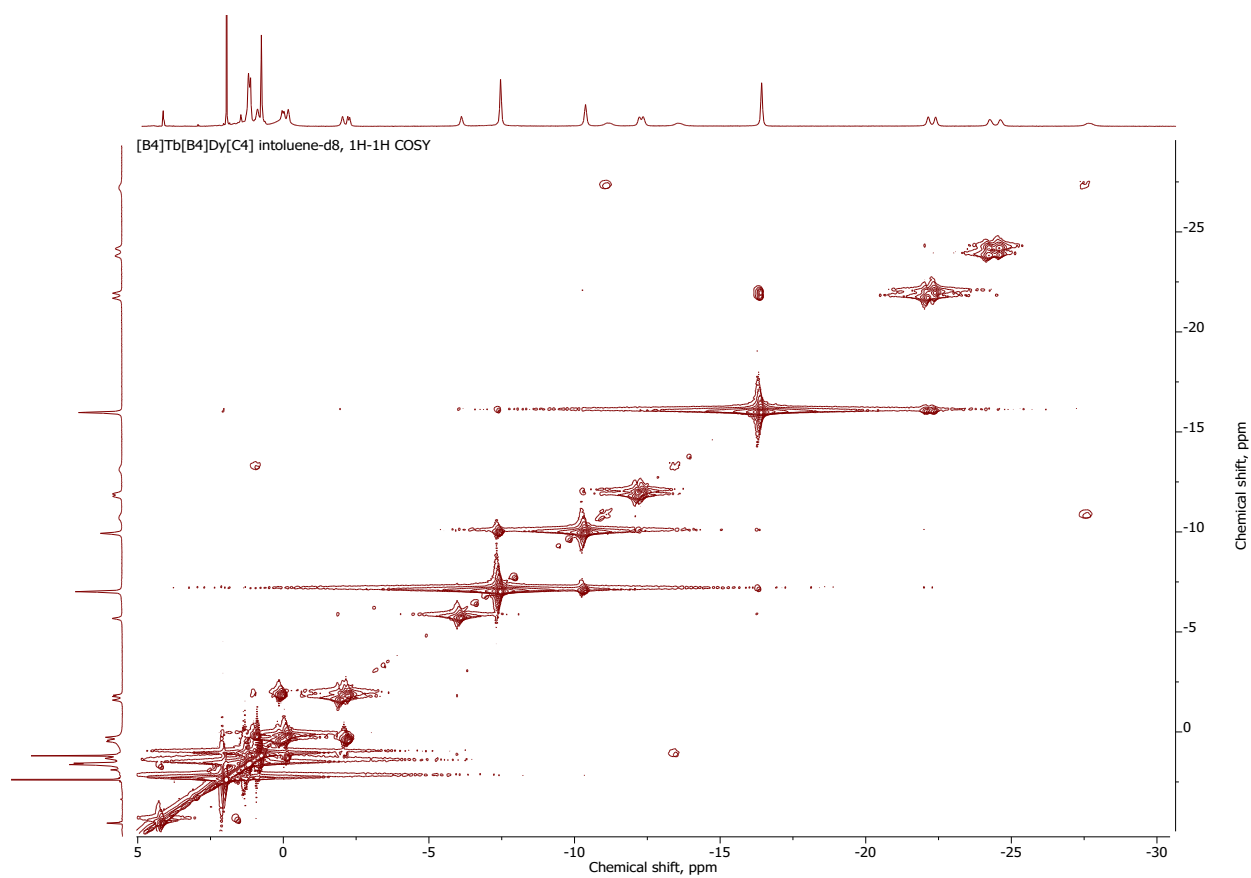


Figure S22. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Tb}[\text{B}_4]\text{Dy}[\text{C}_4]$ in toluene- d_8 .

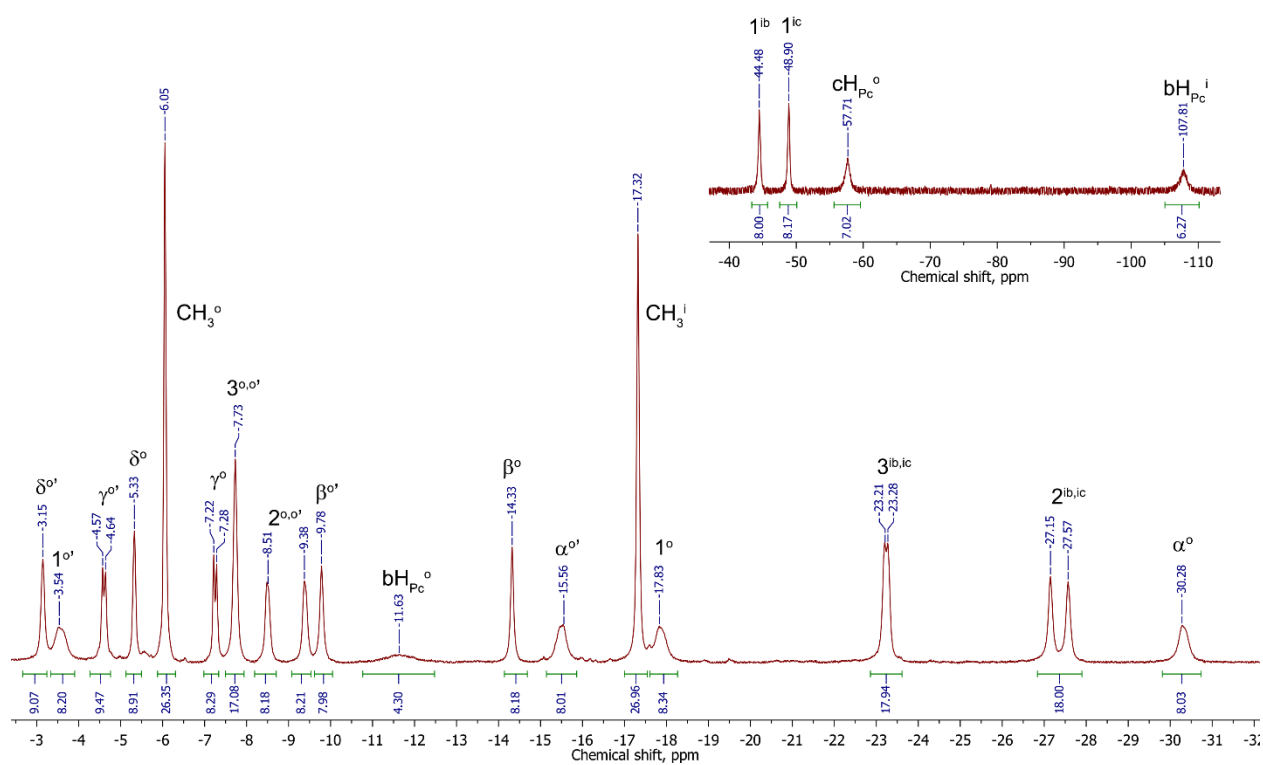


Figure S23. ^1H -NMR spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Tb}[\text{C}_4]$ in CDCl_3 .

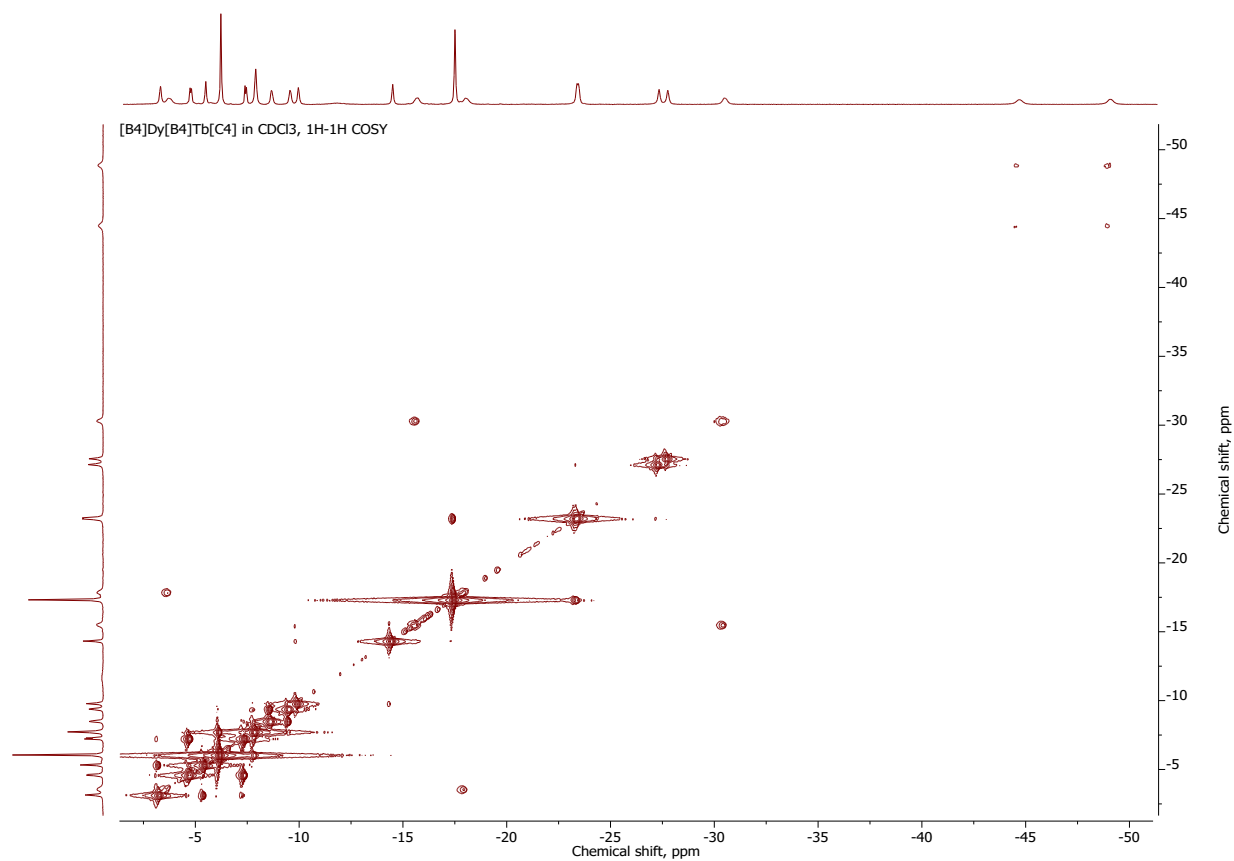


Figure S24. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Tb}[\text{C}_4]$ in CDCl_3 .

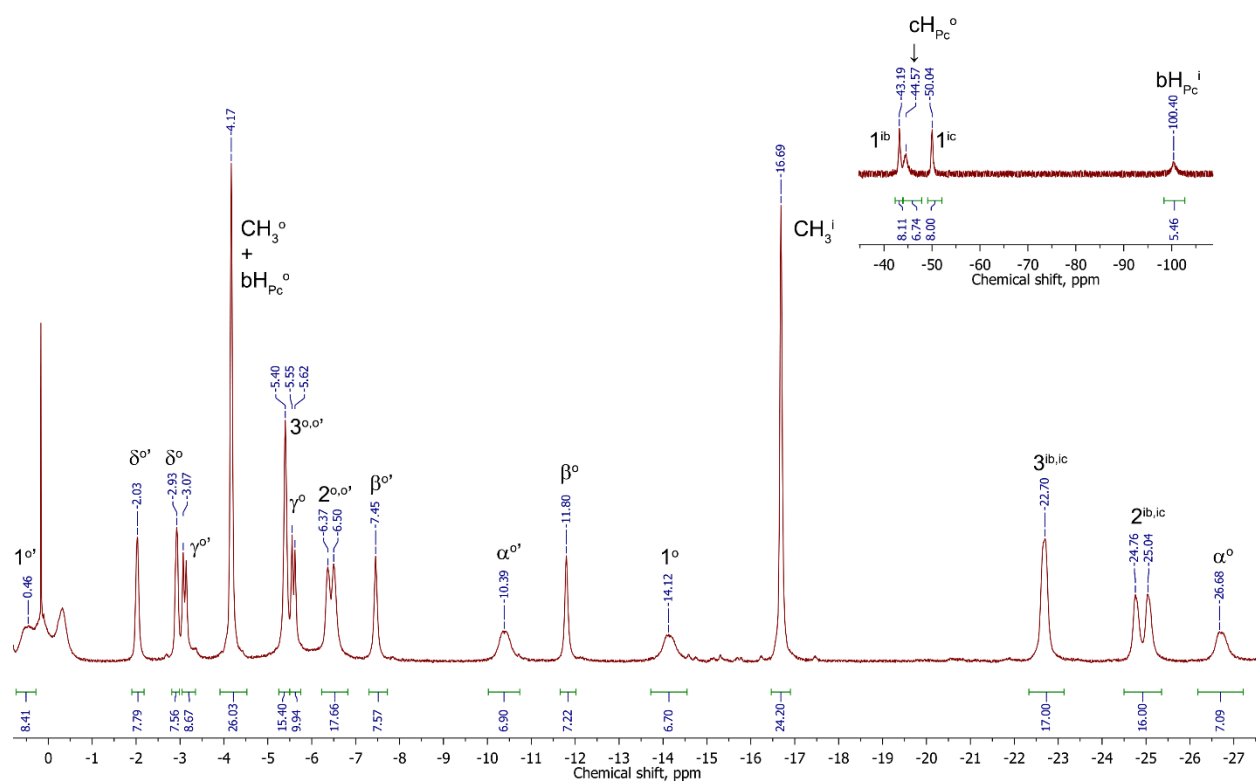


Figure S25. ^1H -NMR spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Tb}[\text{C}_4]$ in toluene- d_8 .

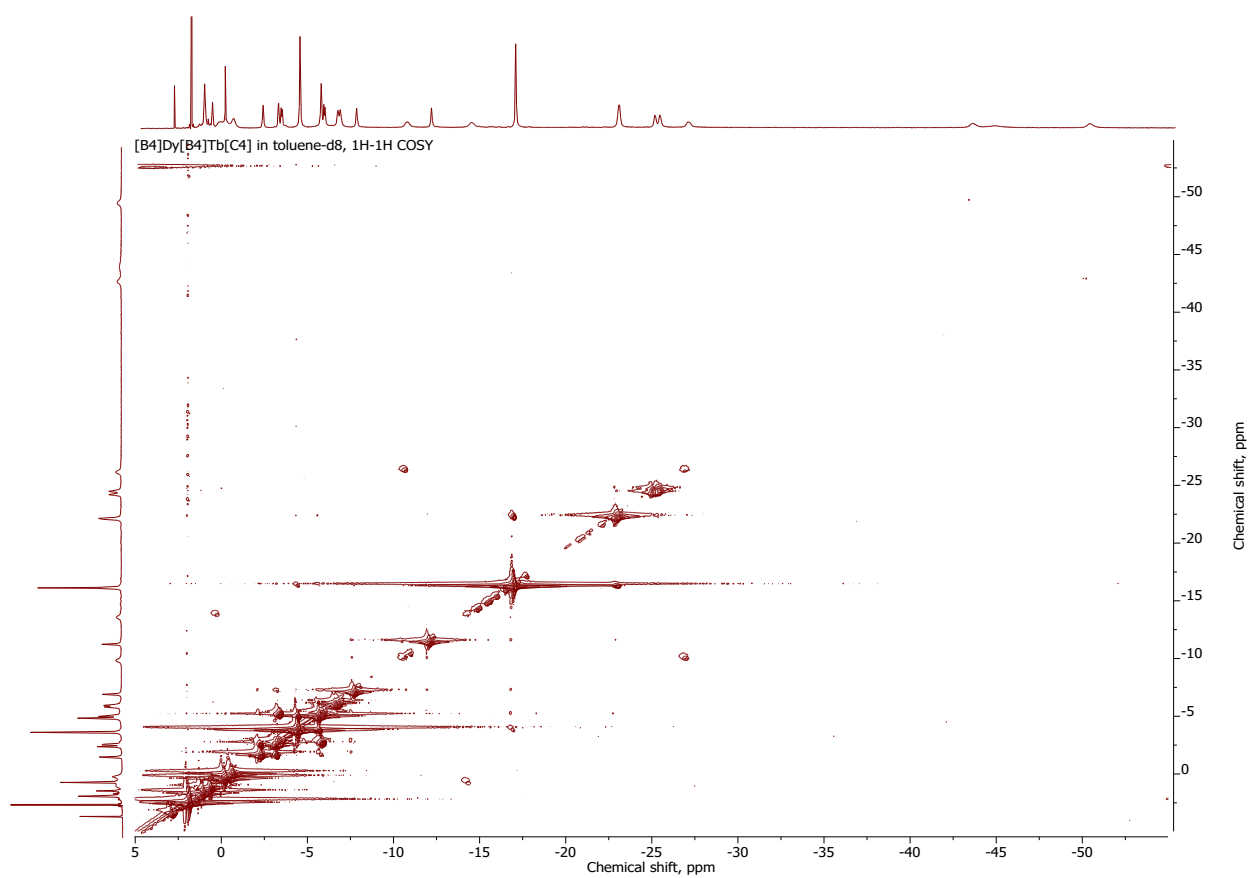


Figure S26. ^1H - ^1H COSY spectrum of $[\text{B}_4]\text{Dy}[\text{B}_4]\text{Tb}[\text{C}_4]$ in toluene- d_8 .