

Supporting Information for

Kinetics and Regioselectivity in Diels-Alder Reaction of Fulleroids vs Methanofullerene and C₆₀

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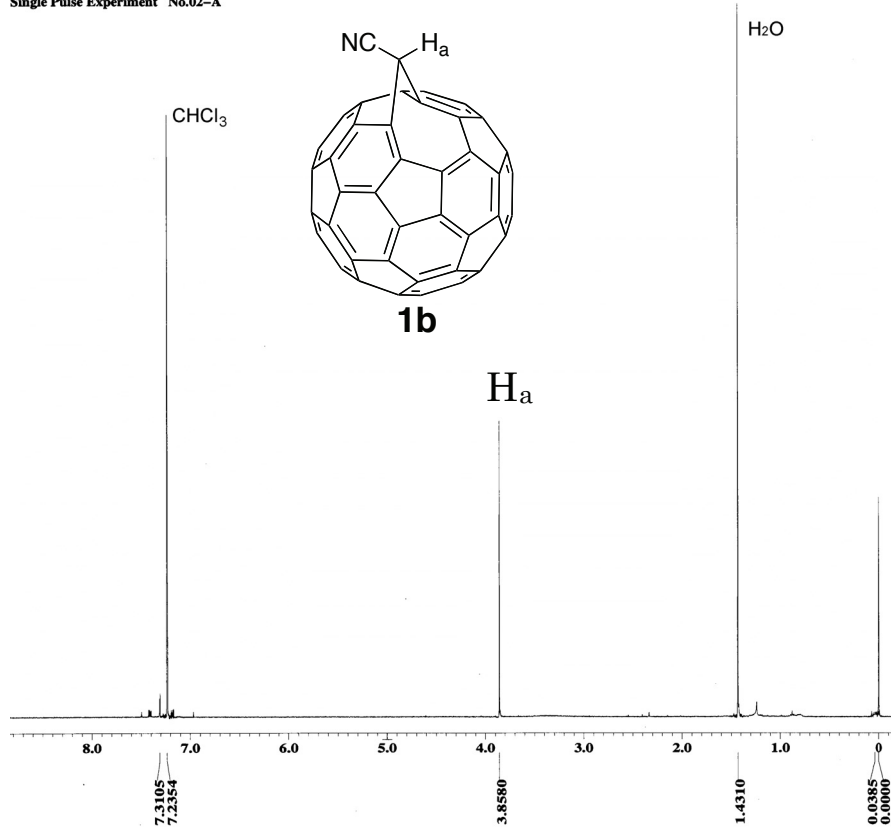
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(a)

Single Pulse Experiment No.02-A



(b)

Single Pulse with Broadband Decoupling No.02-A

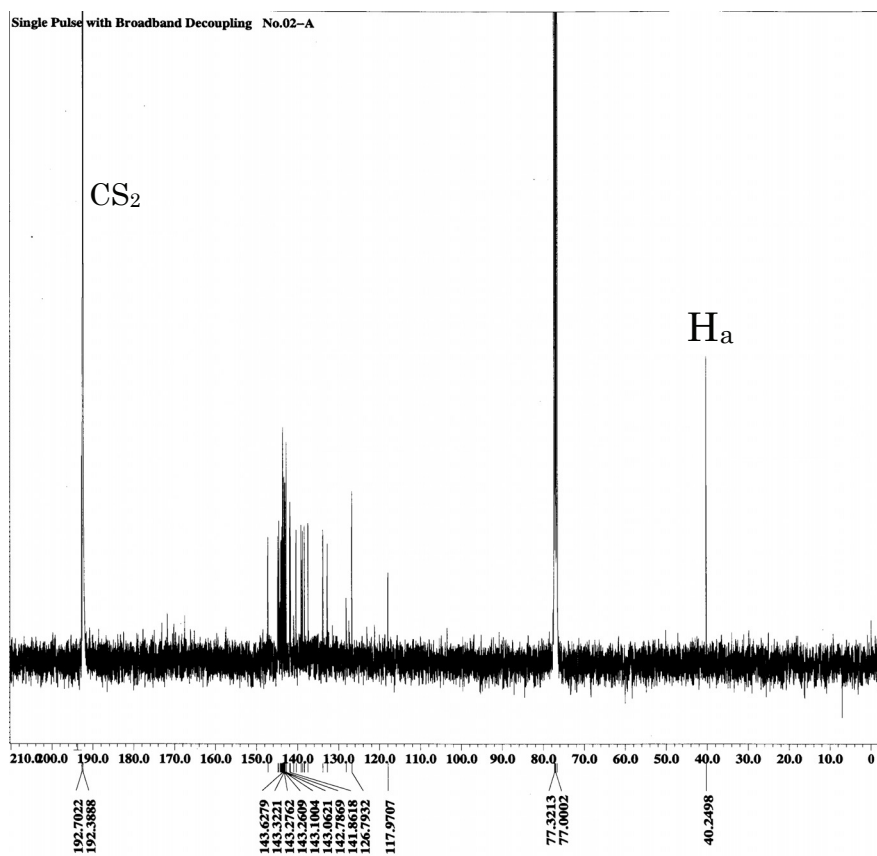
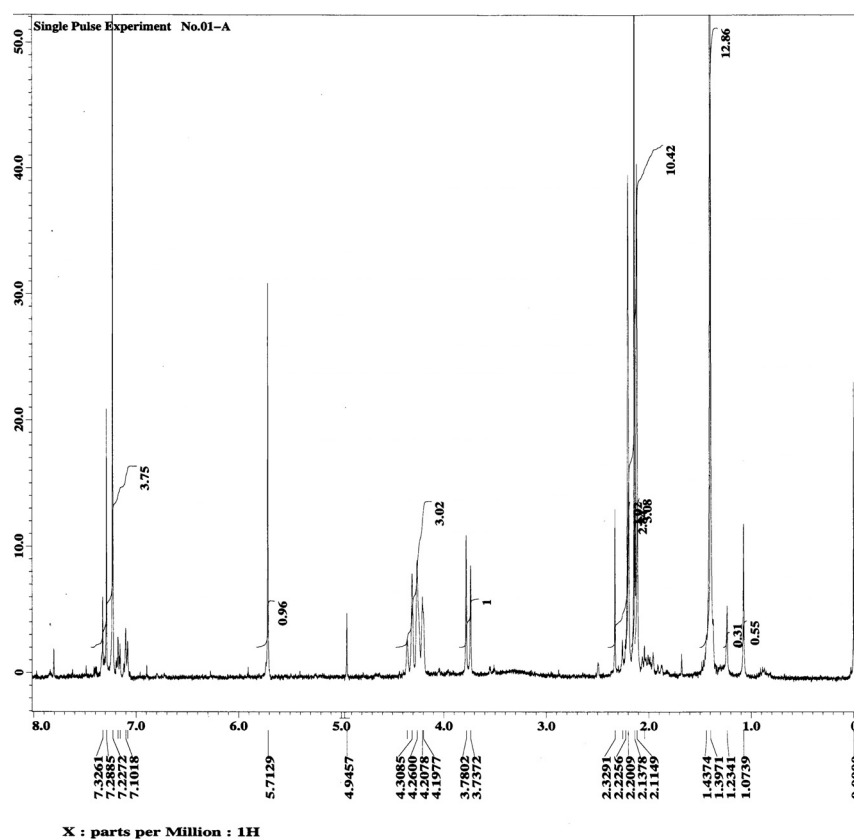


Fig. S1. (a) ¹H NMR and (b) ¹³C NMR spectrum of **1b** in CS₂/CDCl₃=1/1 (v/v).

(a)



(b)

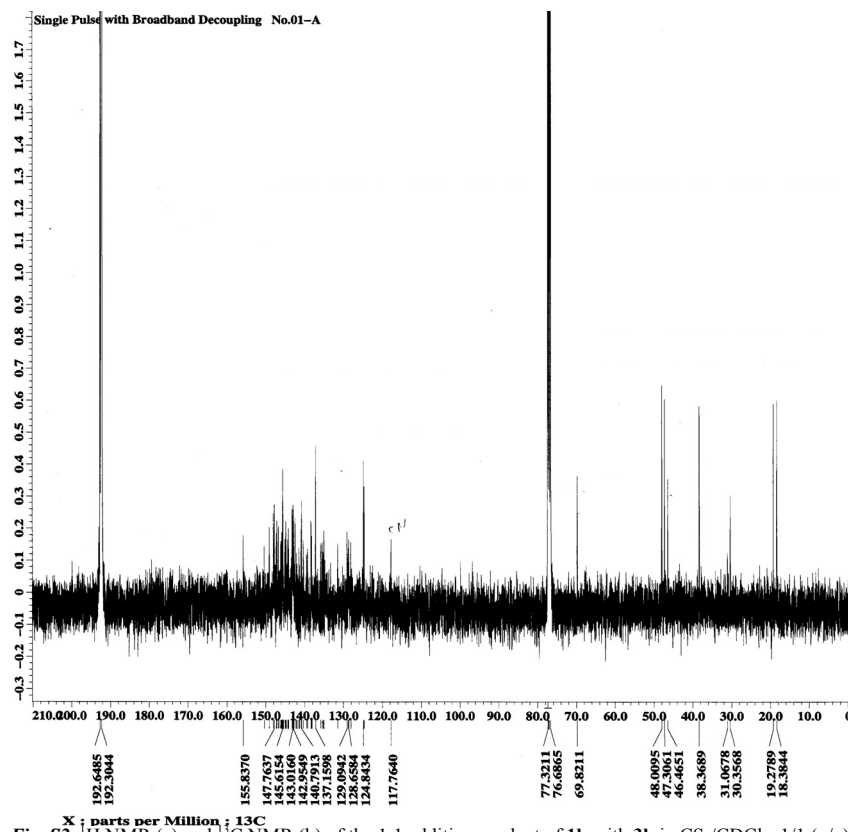


Fig. S2. ^1H NMR (a) and ^{13}C NMR (b) of the 1:1 addition product of **1b** with **3b** in $\text{CS}_2/\text{CDCl}_3=1/1$ (v/v).

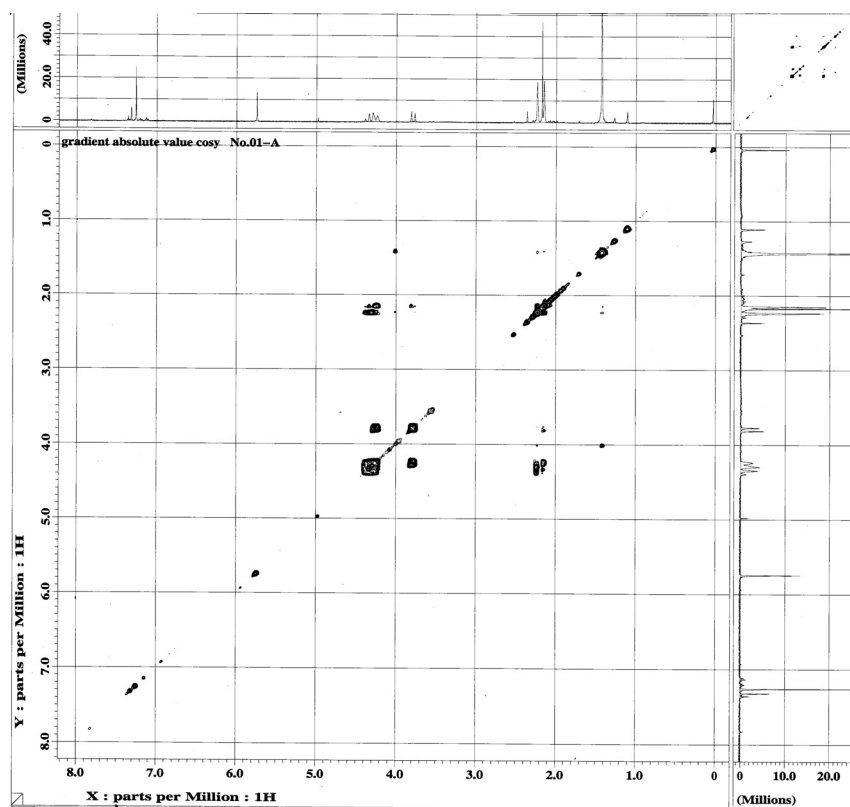


Fig. S3. ^1H - ^1H COSY of the 1:1 addition product of **1b** with **3b** in $\text{CS}_2/\text{CDCl}_3=1/1$ (v/v).

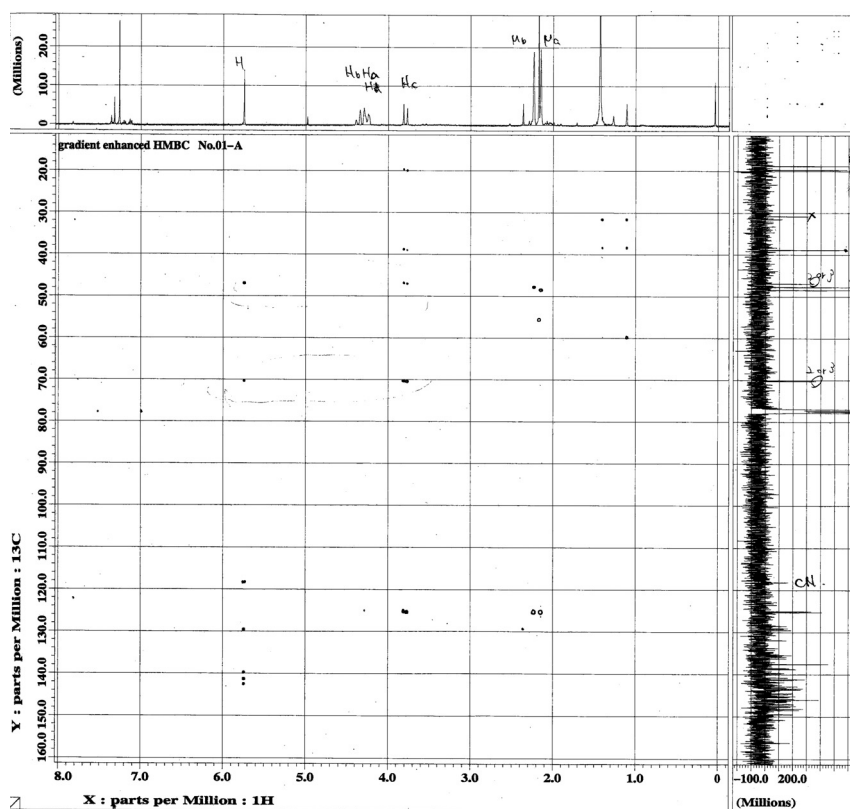


Fig. S4. HMBC of the 1:1 addition product of **1b** with **3b** in $\text{CS}_2/\text{CDCl}_3=1/1$ (v/v).

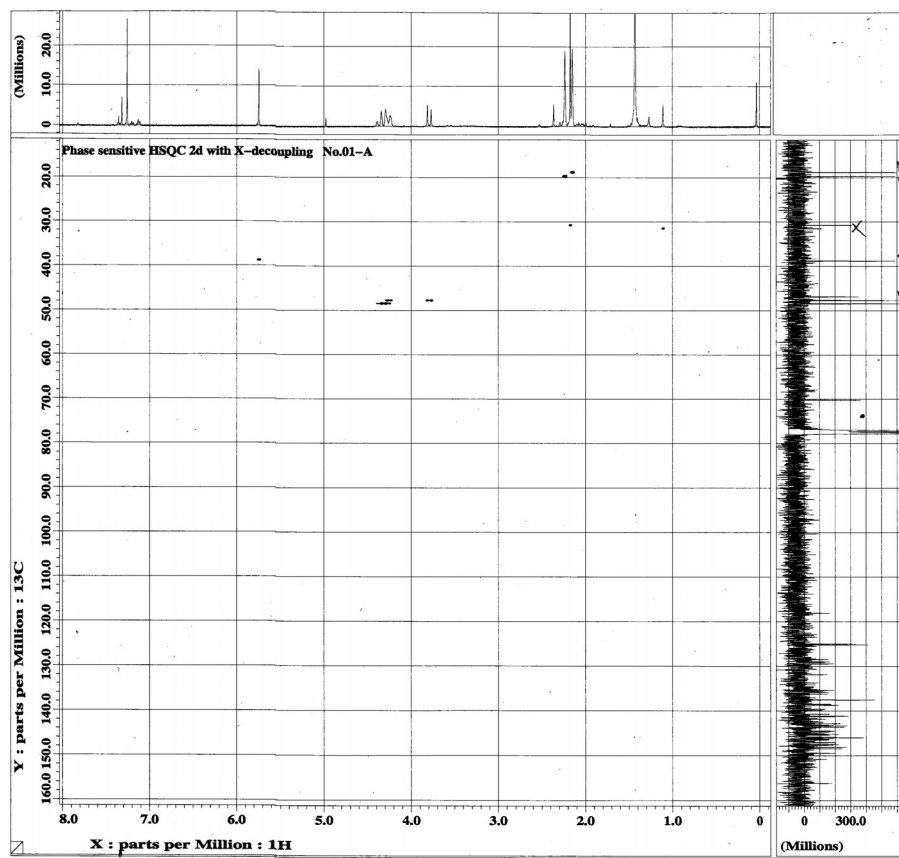
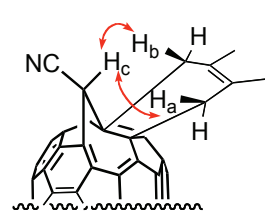


Fig. S5. HMQC of the 1:1 addition product of **1b** with **3b** and in $\text{CS}_2/\text{CDCl}_3=1/1$ (v/v).



Attacked from **1b** and **3b**

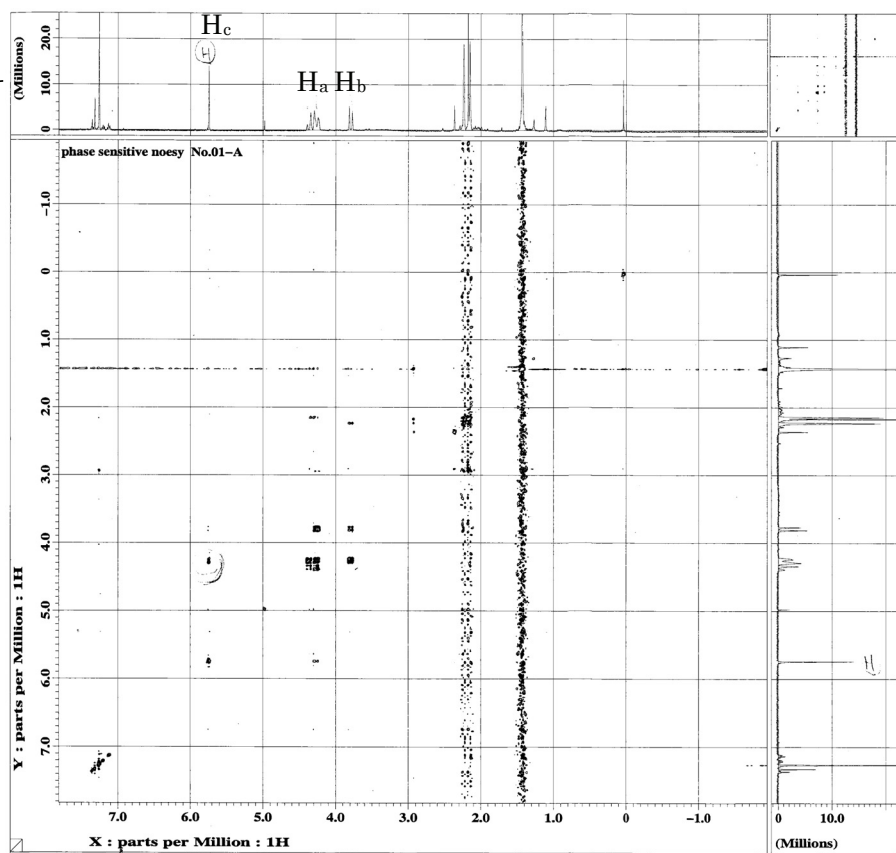
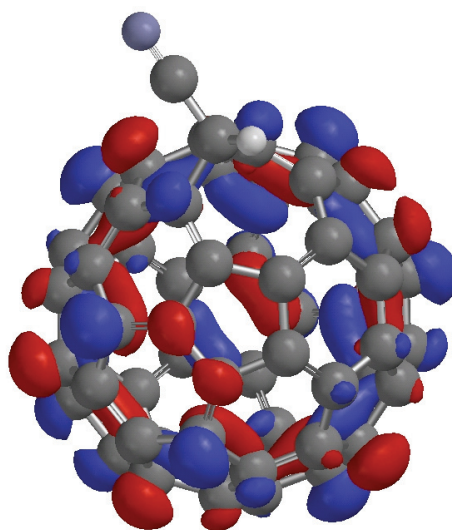
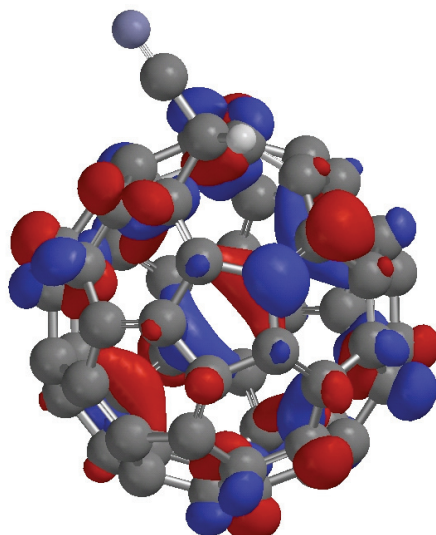


Fig. S6. NOESY of the 1:1 addition product of **1b** with **3b** in $\text{CS}_2/\text{CDCl}_3=1/1$ (v/v).

(a)



(b)



(c)

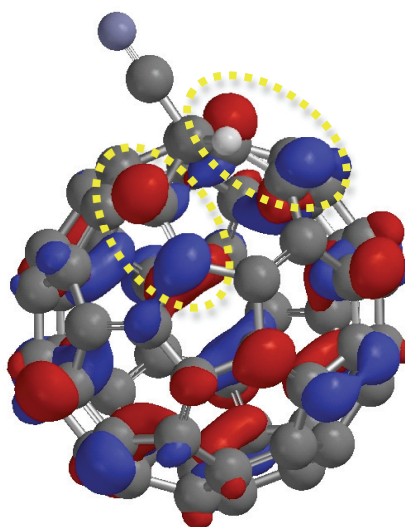


Fig. S7. (a) LUMO, (b) LUMO+1 and (c) LUMO+2 orbital of cyano-substituted fulleroid **1b** by B3LYP/6-31G* calculation. Two yellow ellipsoids in (c) mean the bridgehead double bonds.