Supporting Information for

Fulleroid Addition Regiochemistry Is Driven By π-Orbital Misalignment

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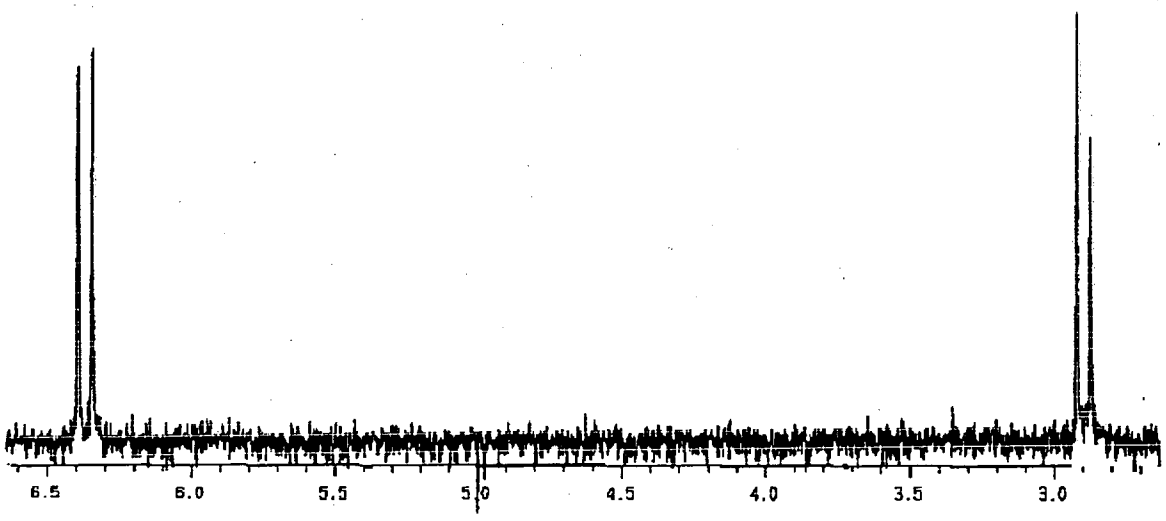
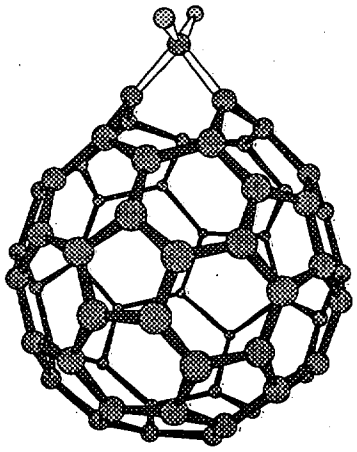
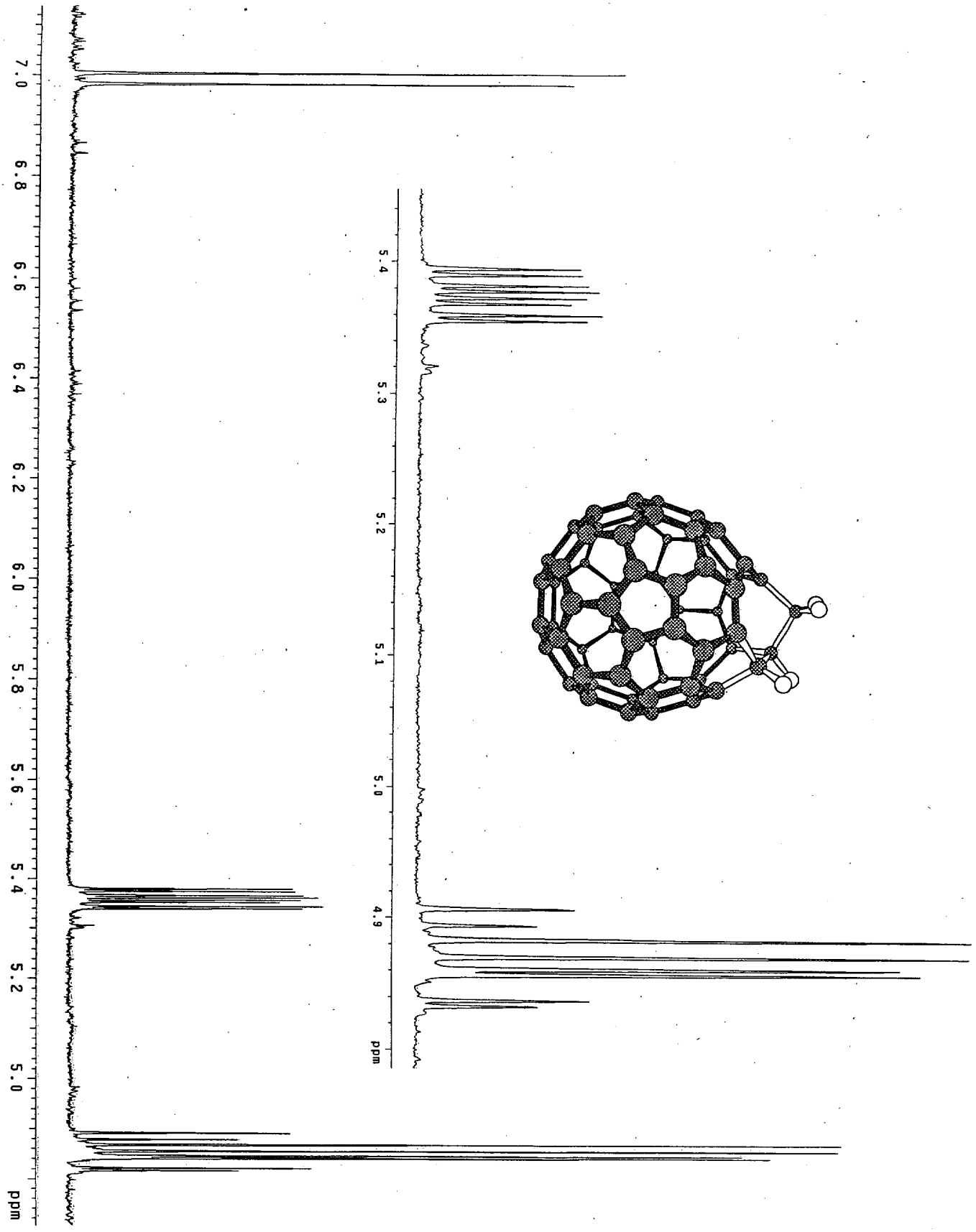
^{1}H NMR spectrum of $C_{61}H_2$ (**1**) at 200 MHz.

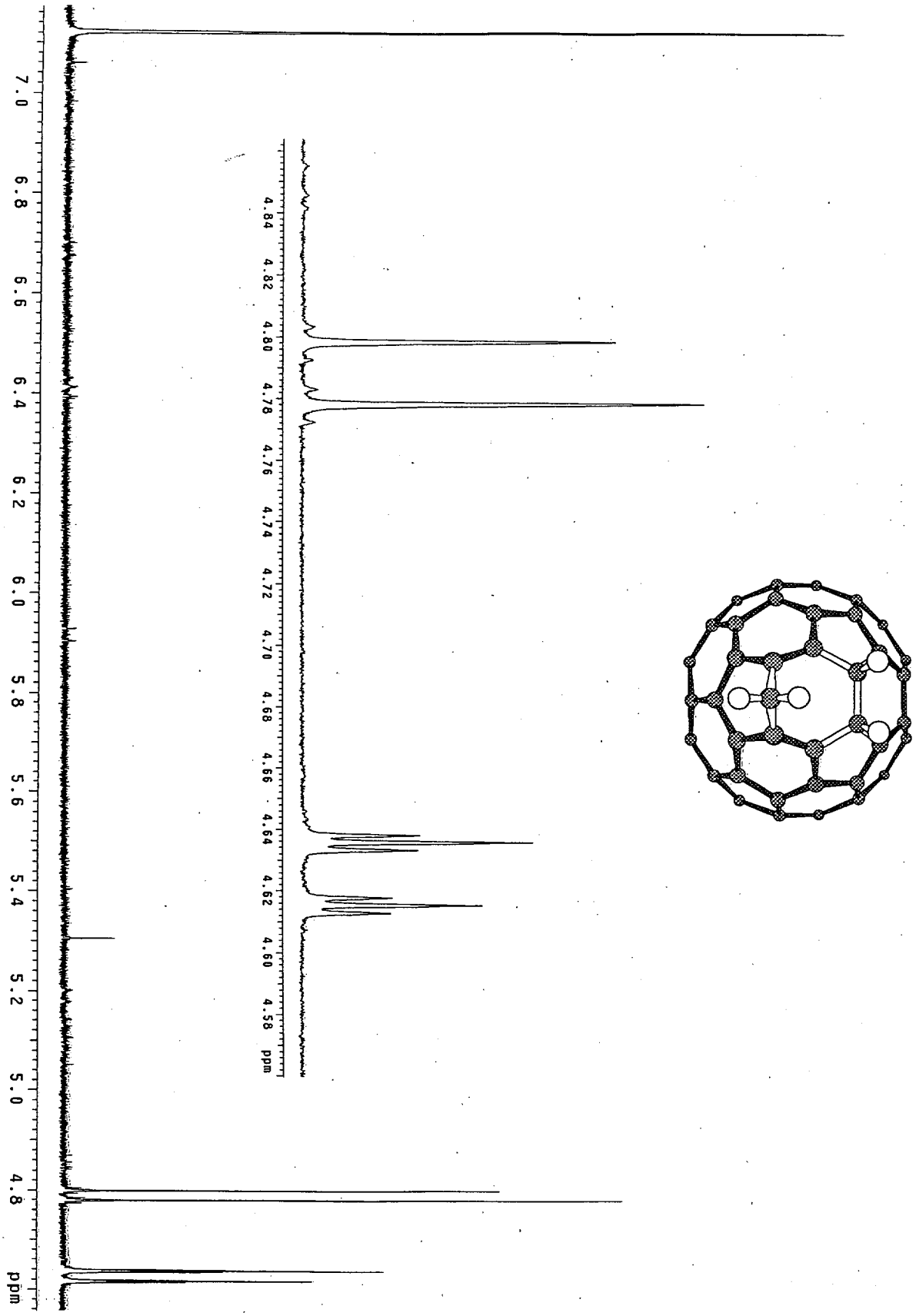




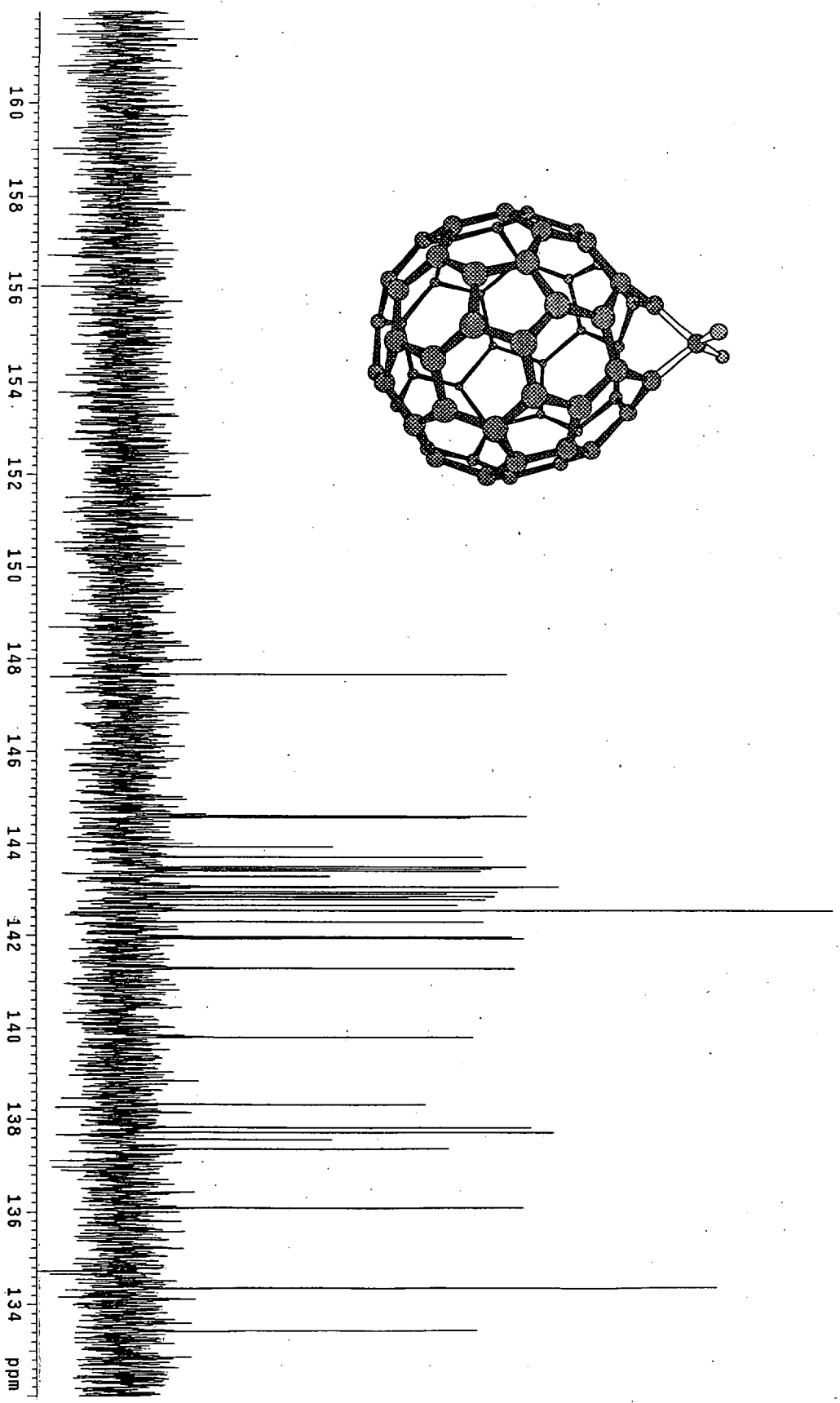
^{1}H NMR spectrum of $C_{61}H_4$ (**2**) at 500 MHz.



^{1}H NMR spectrum of $C_{61}H_4$ (**3**) at 500 MHz.

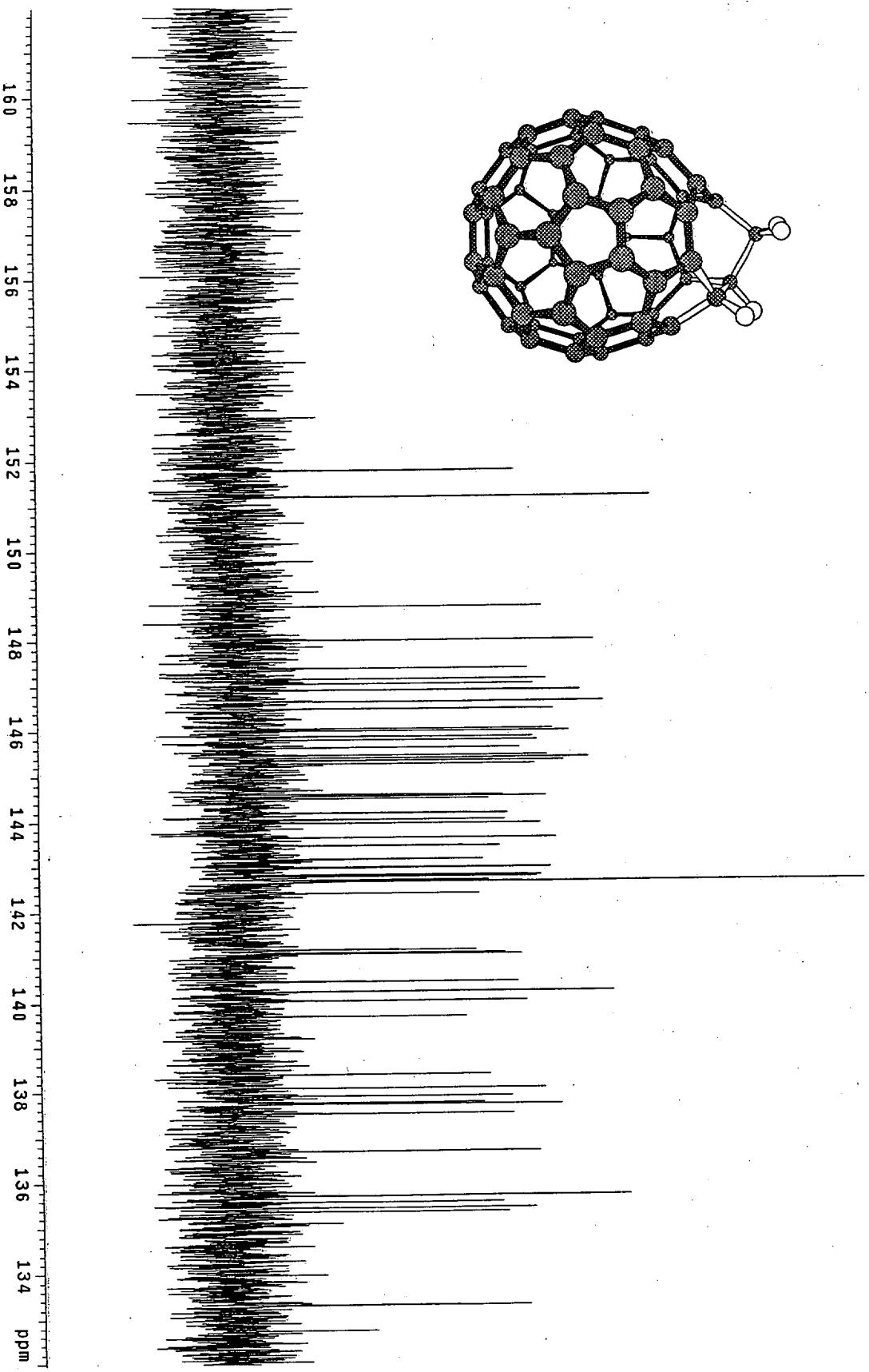


^{13}C NMR spectrum of $C_{61}H_2$ (**1**) at 125 MHz (sp^2 region only).



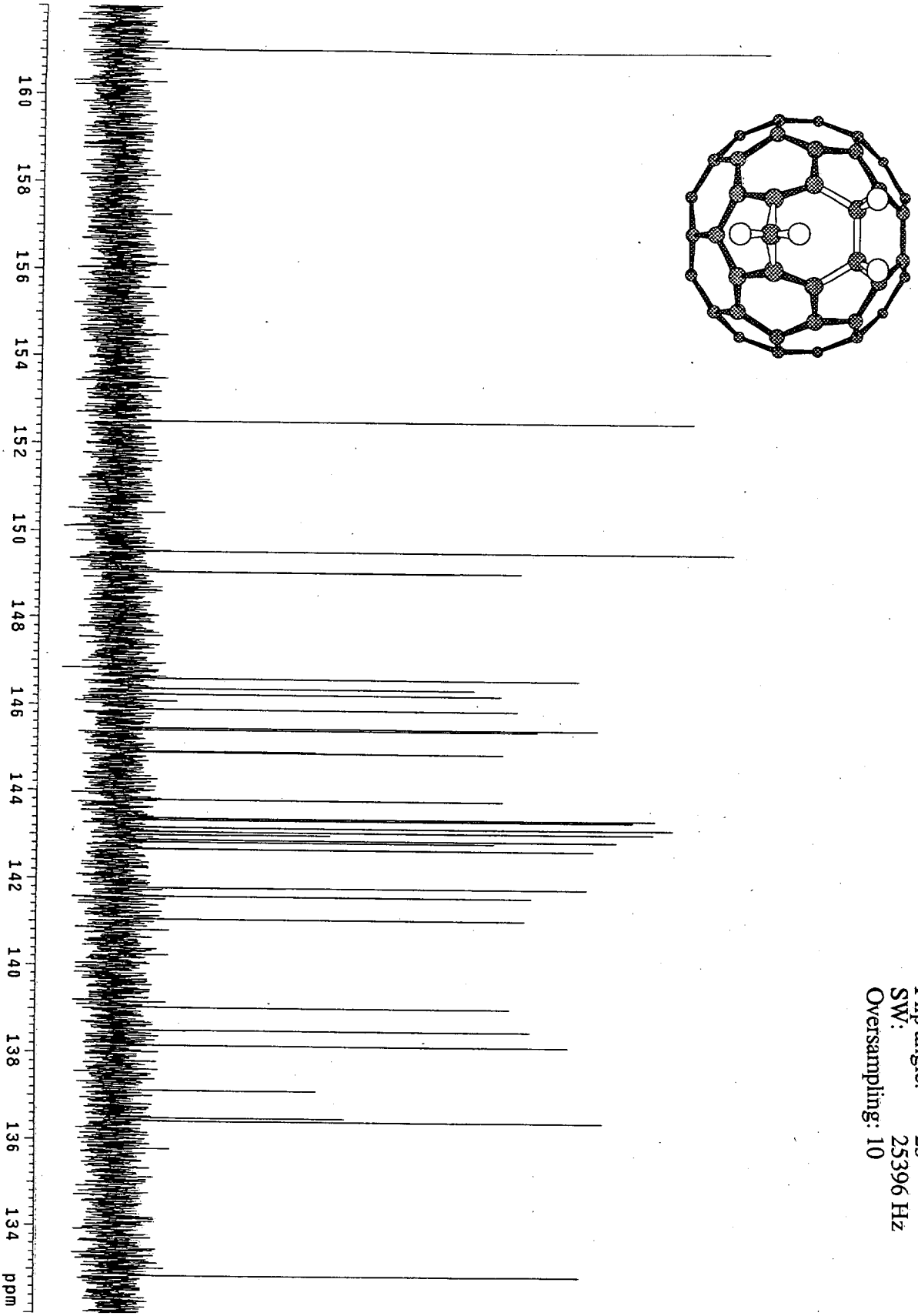
Experimental Conditions:
Transients: 1728
Acq. Time: 5.161 sec
Flip angle: 25 °
SW: 25396 Hz
Oversampling: 10

^{13}C NMR spectrum of $C_{61}H_4$ (**2**) at 125 MHz (sp^2 region only).



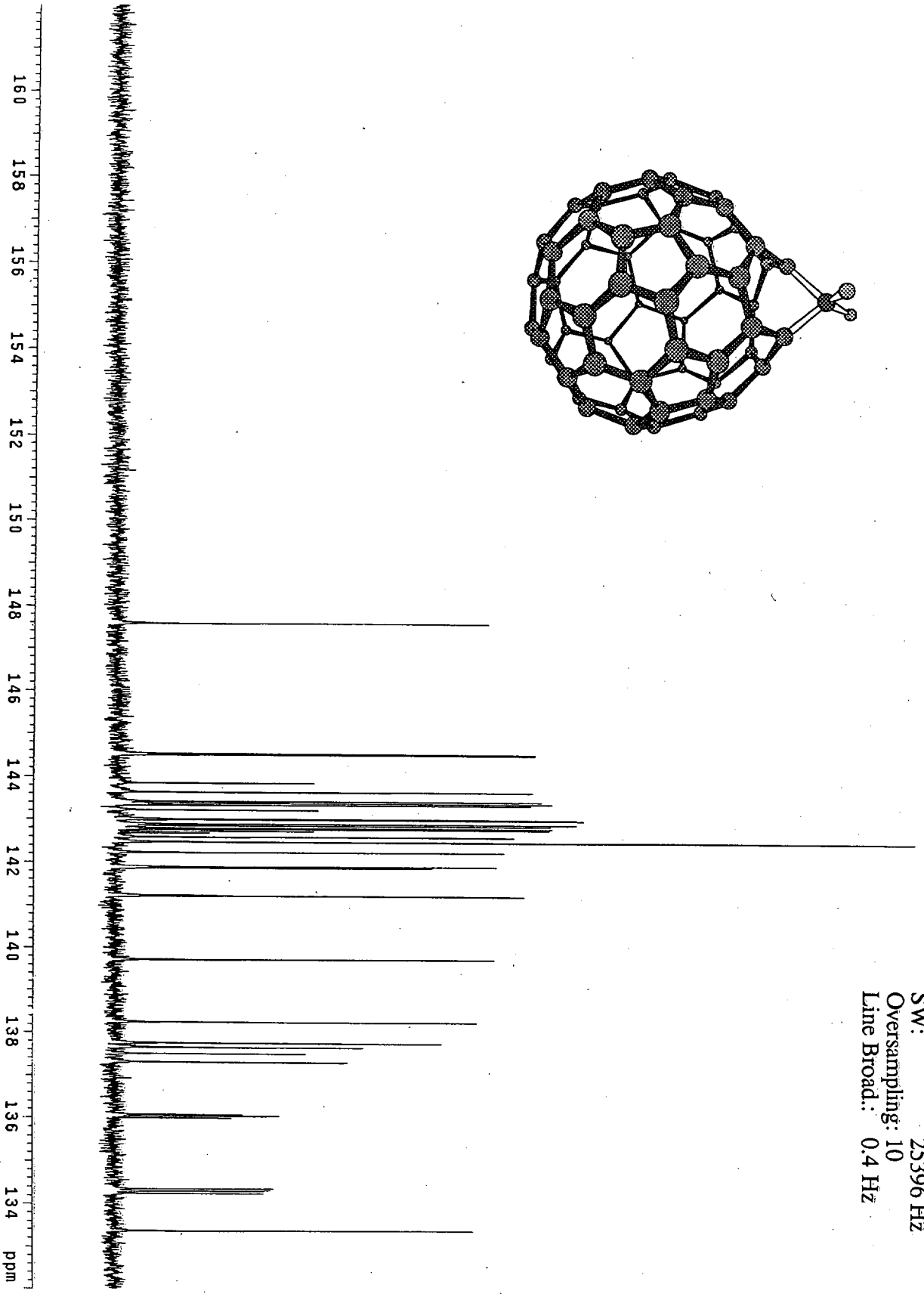
Experimental Conditions:
Transients: 30848
Acq. Time: 5.161 sec
Flip angle: 25 °
SW: 25396 Hz
Oversampling: 10

^{13}C NMR spectrum of $C_{61}H_4$ (**3**) at 125 MHz (sp^2 region only).



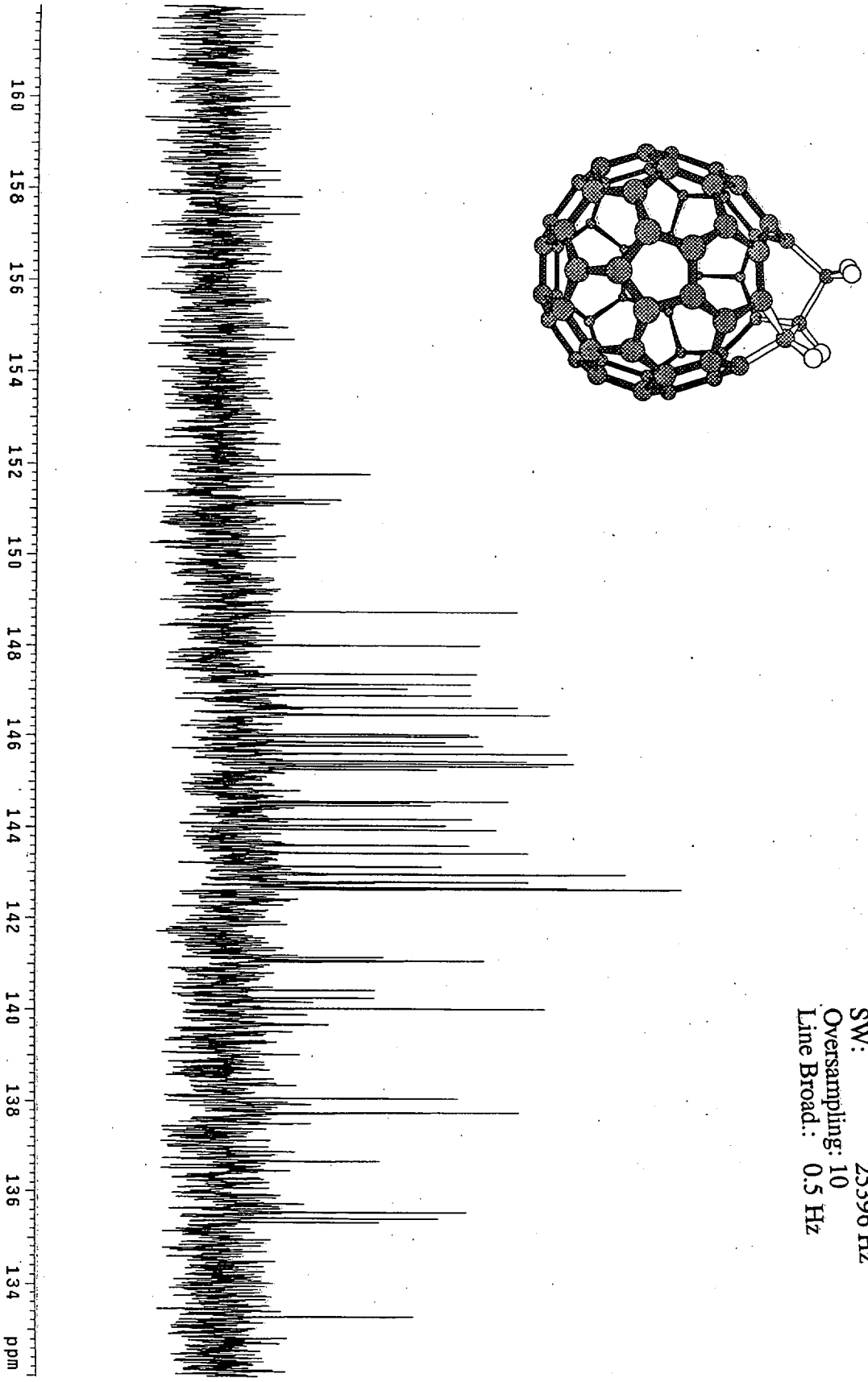
Experimental Conditions:
Transients: 9504
Acq. Time: 5.161 sec
Flip angle: 25°
SW: 25396 Hz
Oversampling: 10

^{1}H-^{13}C coupled NMR spectrum of **1** at 125 MHz (sp^2 region only).



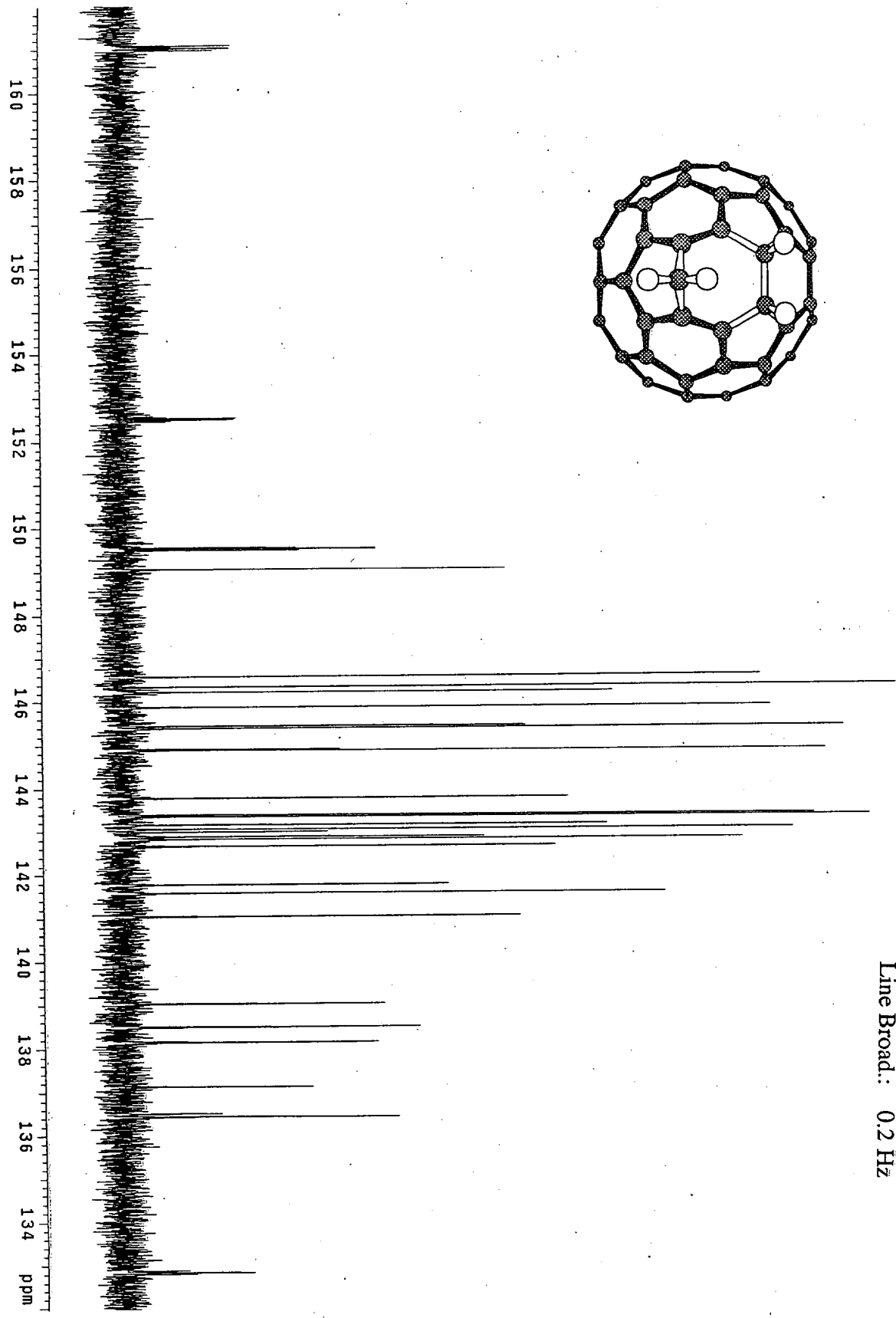
Experimental Conditions:
Transients: 44928
Acq. Time: 5.161 sec
Flip angle: 25 °
SW: 25396 Hz
Oversampling: 10
Line Broad.: 0.4 Hz

^{1}H-^{13}C coupled NMR spectrum of **2** at 125 MHz (sp^2 region only).



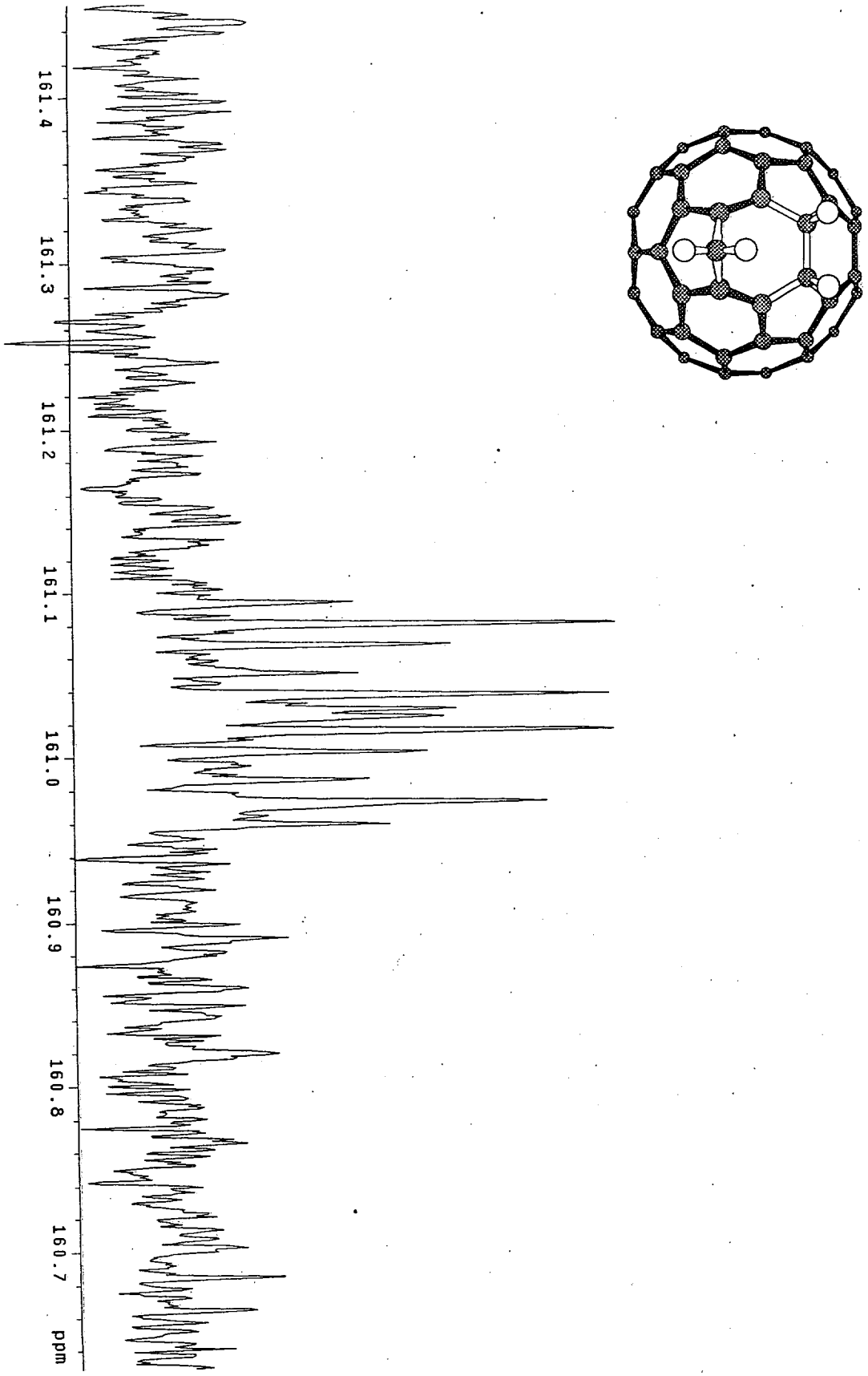
Experimental Conditions:
Transients: 58368
Acq. Time: 5.161 sec
Flip angle: 25 °
SW: 25396 Hz
Oversampling: 10
Line Broad.: 0.5 Hz

^{1}H-^{13}C coupled NMR spectrum of **3** at 125 MHz (sp^2 region only).

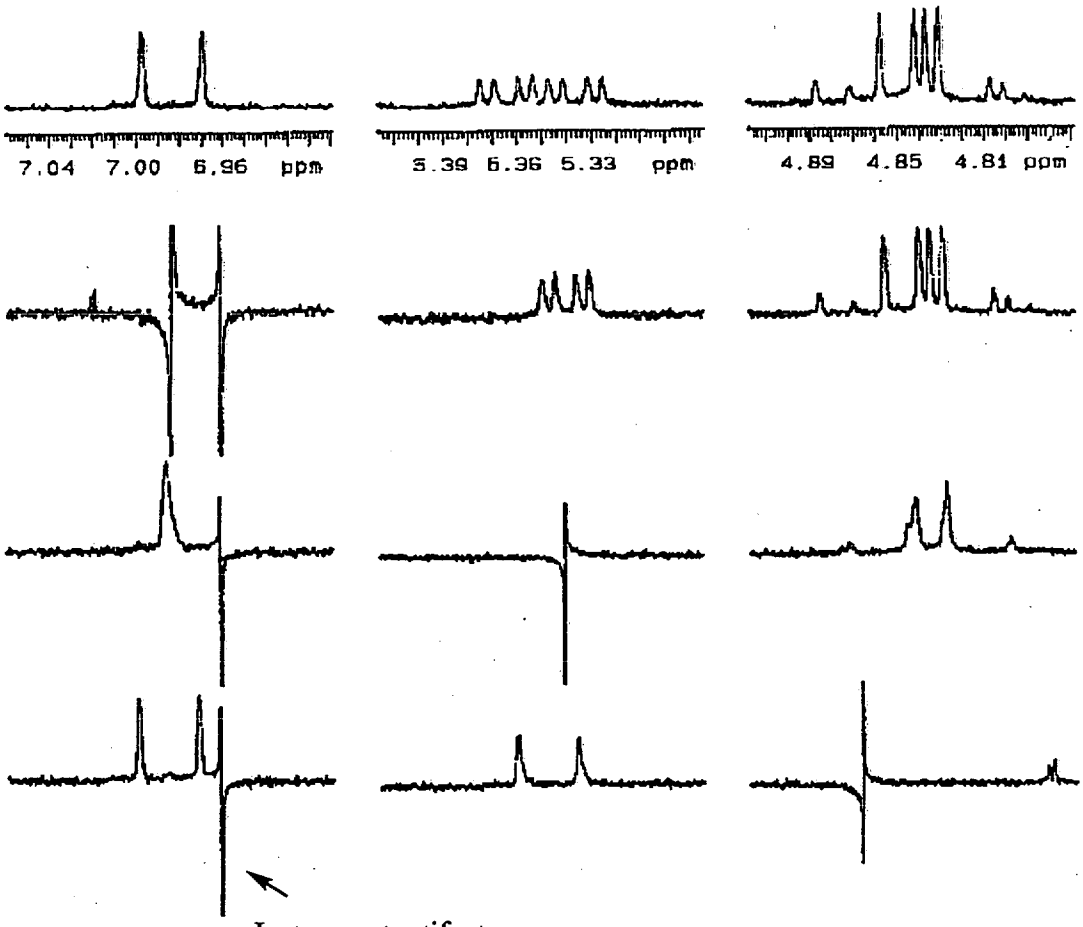


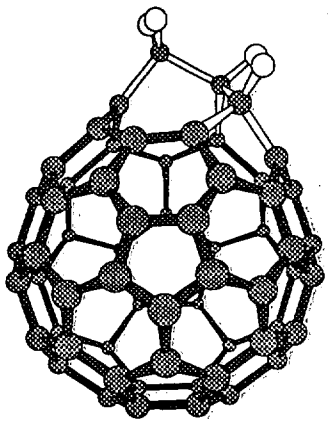
Experimental Conditions:
Transients: 67352
Acq. Time: 5.161 sec
Flip angle: 25 °
SW: 25396 Hz
Oversampling: 10
Line Broad.: 0.2 Hz

Expansion of downfield resonance in ^{1}H-^{13}C coupled NMR of **3**.

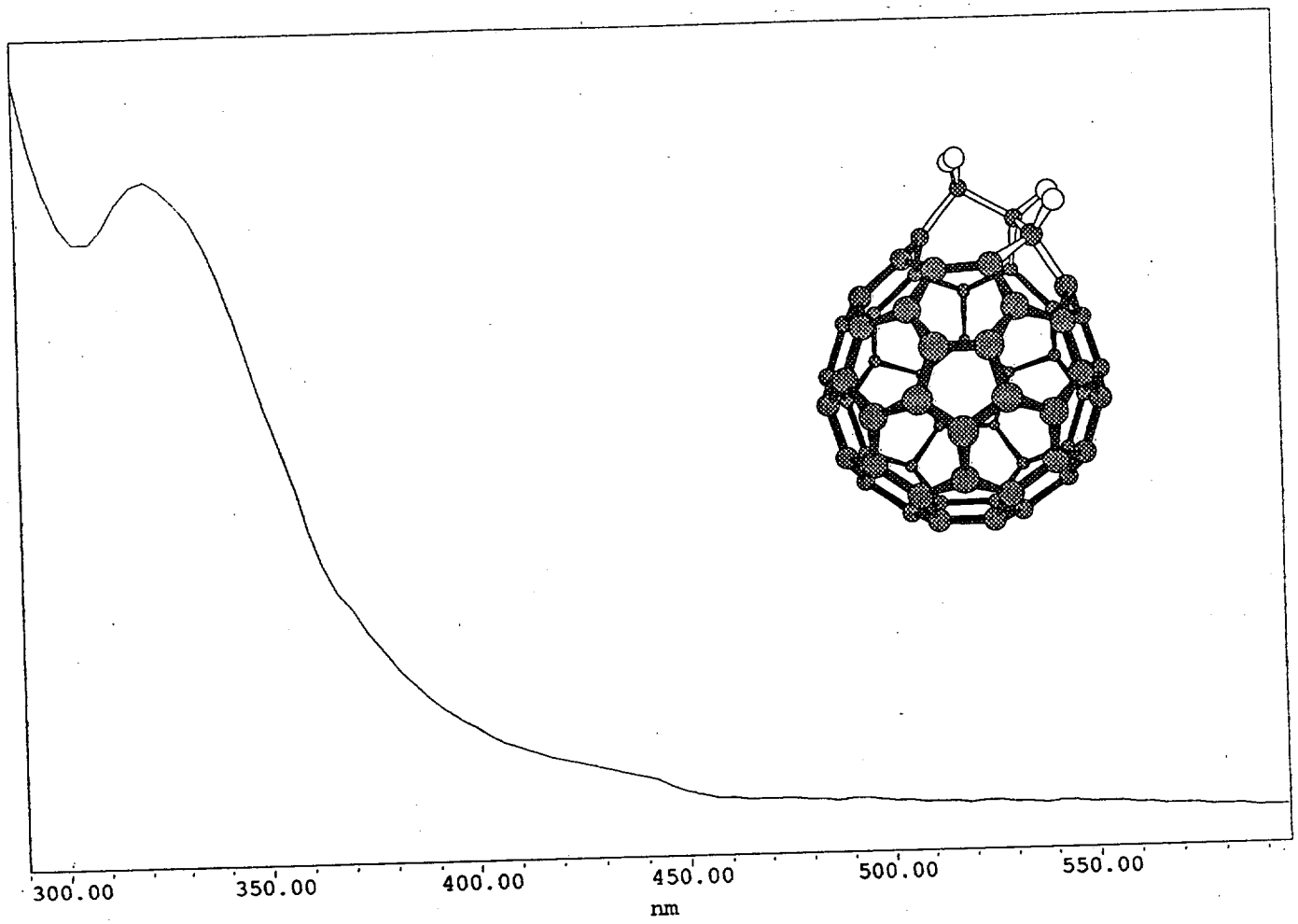


^{1}H NMR decoupling spectra of $C_{61}H_4$ (**2**) at 400 Mhz.





UV-Vis spectrum of **2**.



UV-Vis spectrum of **3**.