

**SUPPORTING
INFORMATION**

Supporting Information for

Fulleroid Addition Regiochemistry Is Driven By π -Orbital Misalignment

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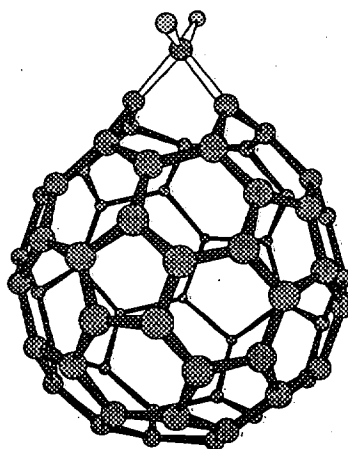
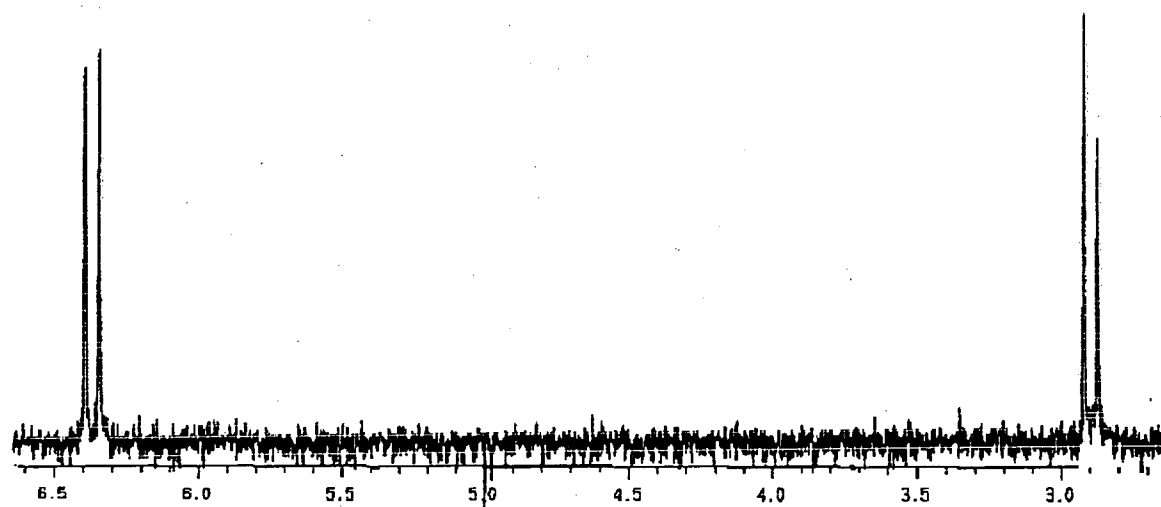
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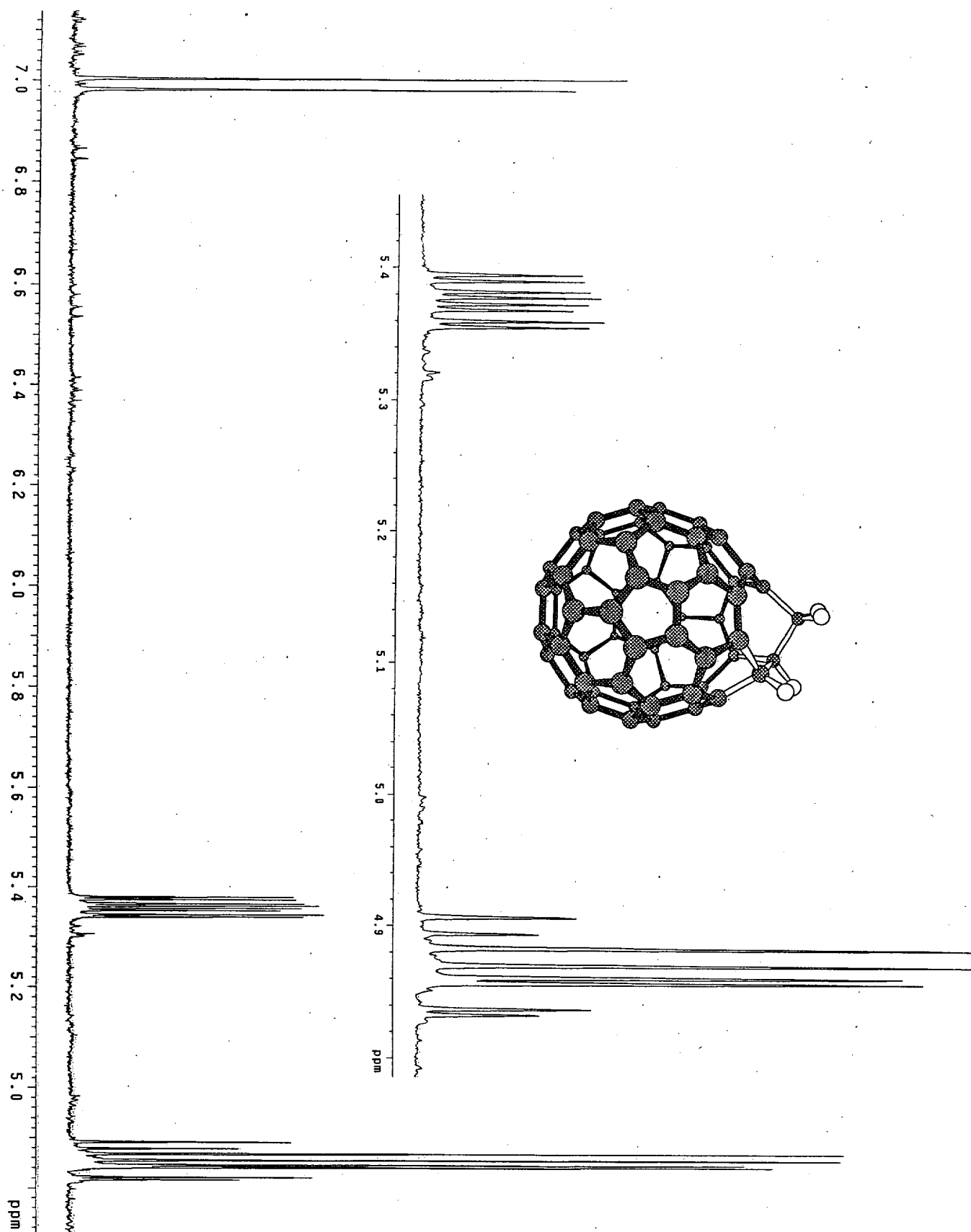
University of Kentucky, Lexington, KY 40506-0055

- S-2. ¹H NMR spectrum of **1**.
- S-3. ¹H NMR spectrum of **2**.
- S-4. ¹H NMR spectrum of **3**.
- S-5. ¹³C NMR spectrum (sp² region only) of **1**.
- S-6. ¹³C NMR spectrum (sp² region only) of **2**.
- S-7. ¹³C NMR spectrum (sp² region only) of **3**.
- S-8. ¹H-¹³C coupled NMR spectrum (sp² region only) of **1**.
- S-9. ¹H-¹³C coupled NMR spectrum (sp² region only) of **2**.
- S-10. ¹H-¹³C coupled NMR spectrum (sp² region only) of **3**.
- S-11. Expansion of downfield resonance in ¹H-¹³C coupled NMR of **3**.
- S-12. ¹H NMR decoupling spectra of **2**.
- S-13. UV-vis absorption spectrum of **2**.
- S-14. UV-vis absorption spectrum of **3**.

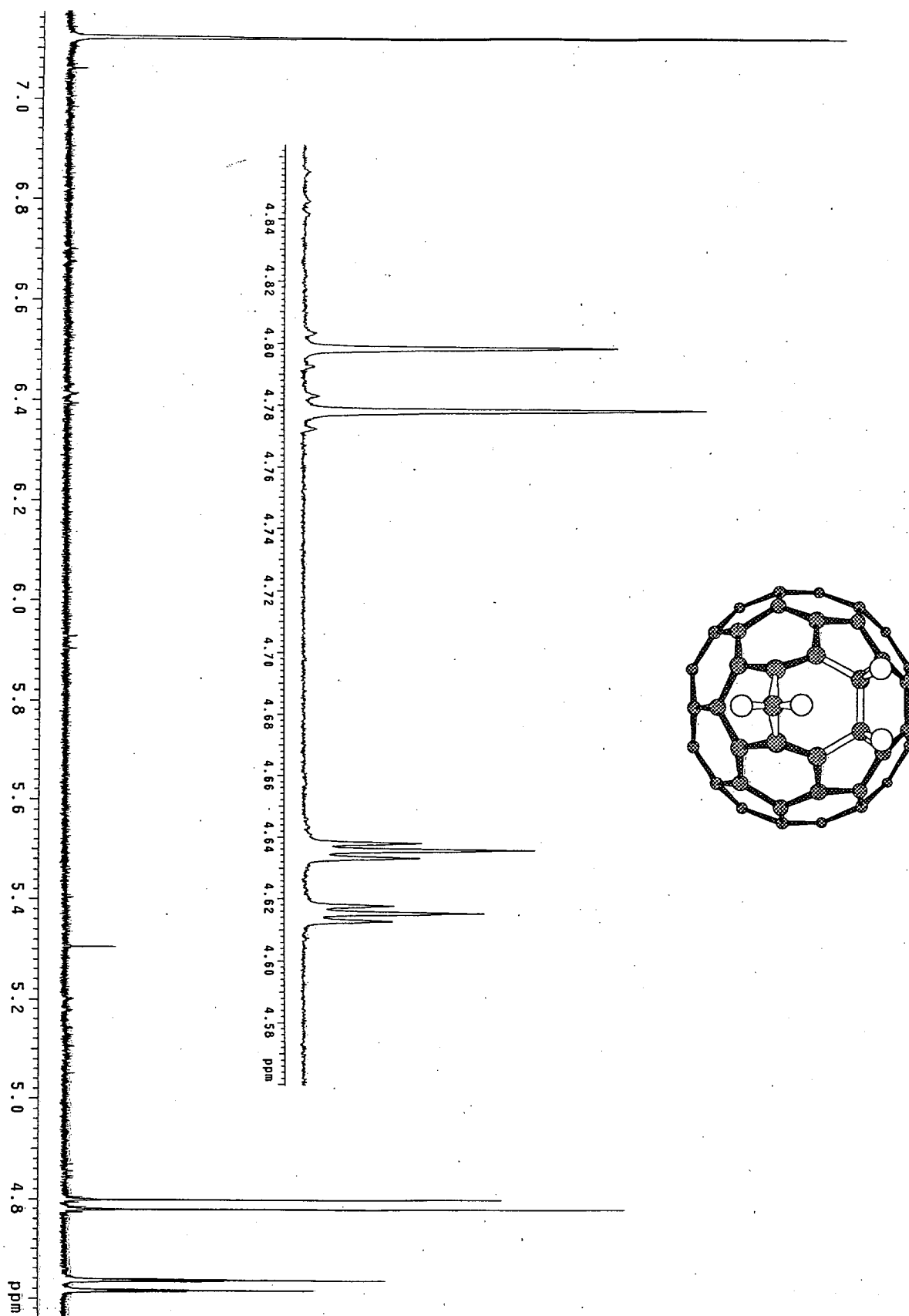
^1H NMR spectrum of C_{61}H_2 (1) at 200 MHz.



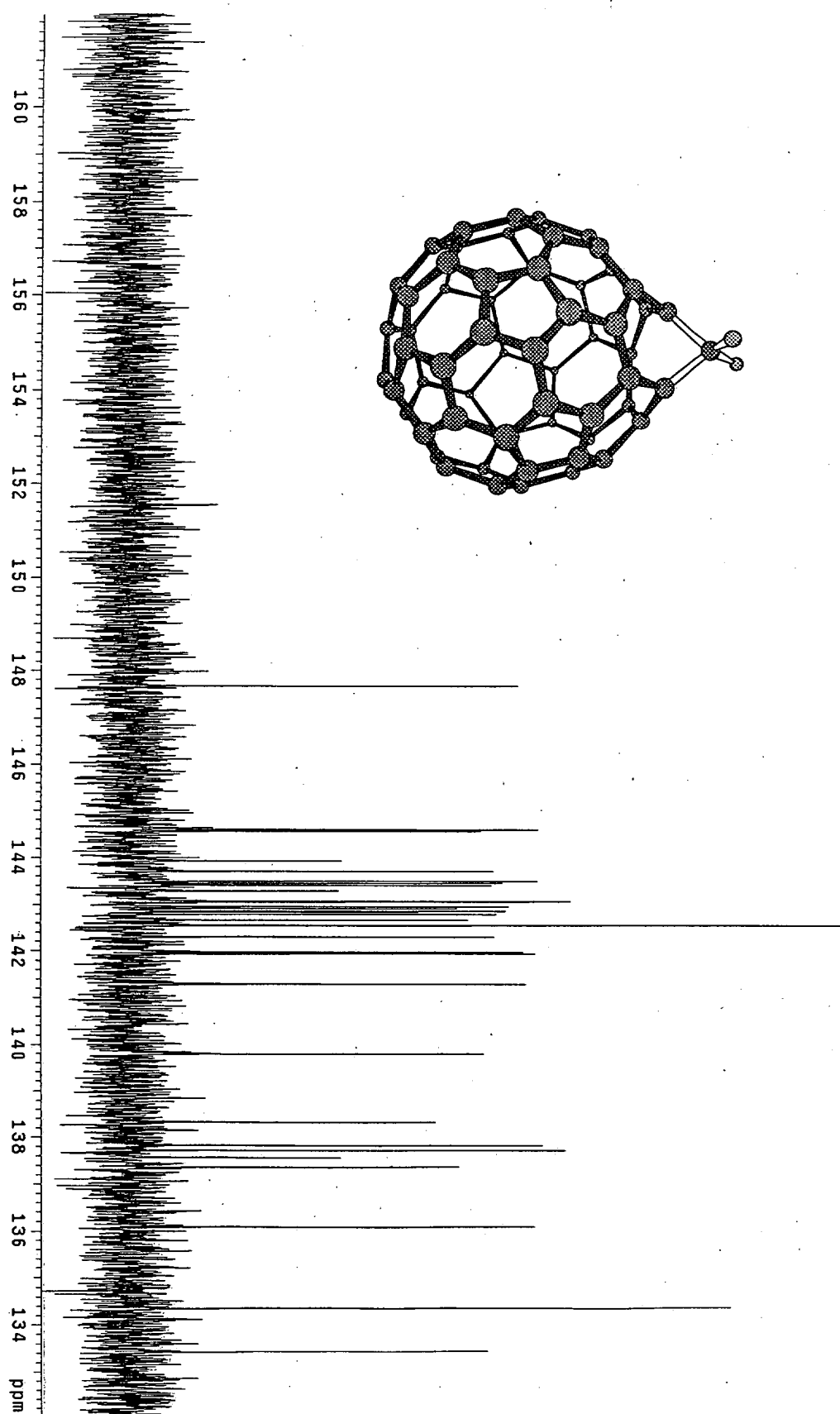
^1H NMR spectrum of C_{61}H_4 (2) at 500 MHz.



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

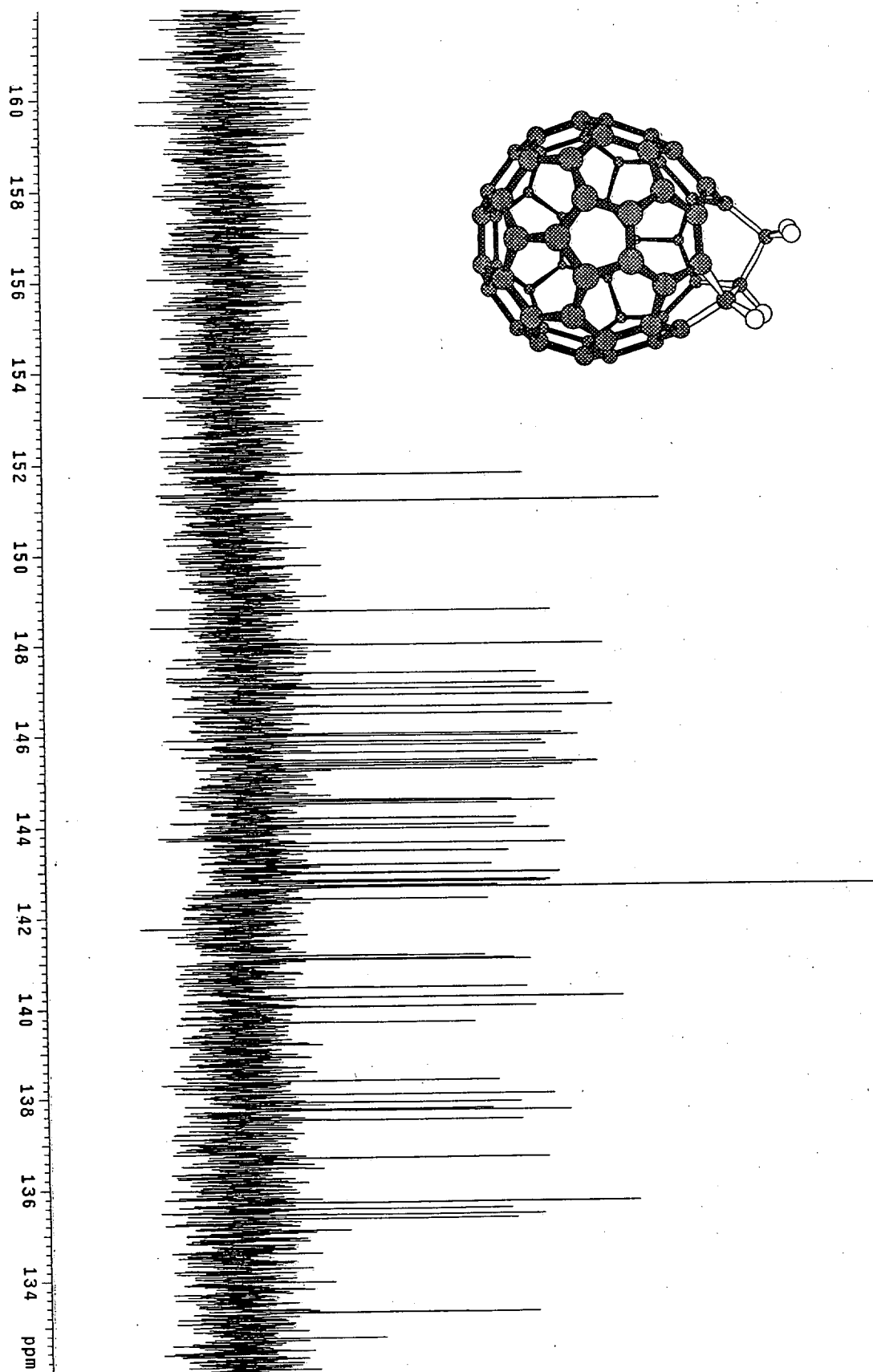


^{13}C NMR spectrum of C_{61}H_2 (1) at 125 MHz (sp^2 region only).



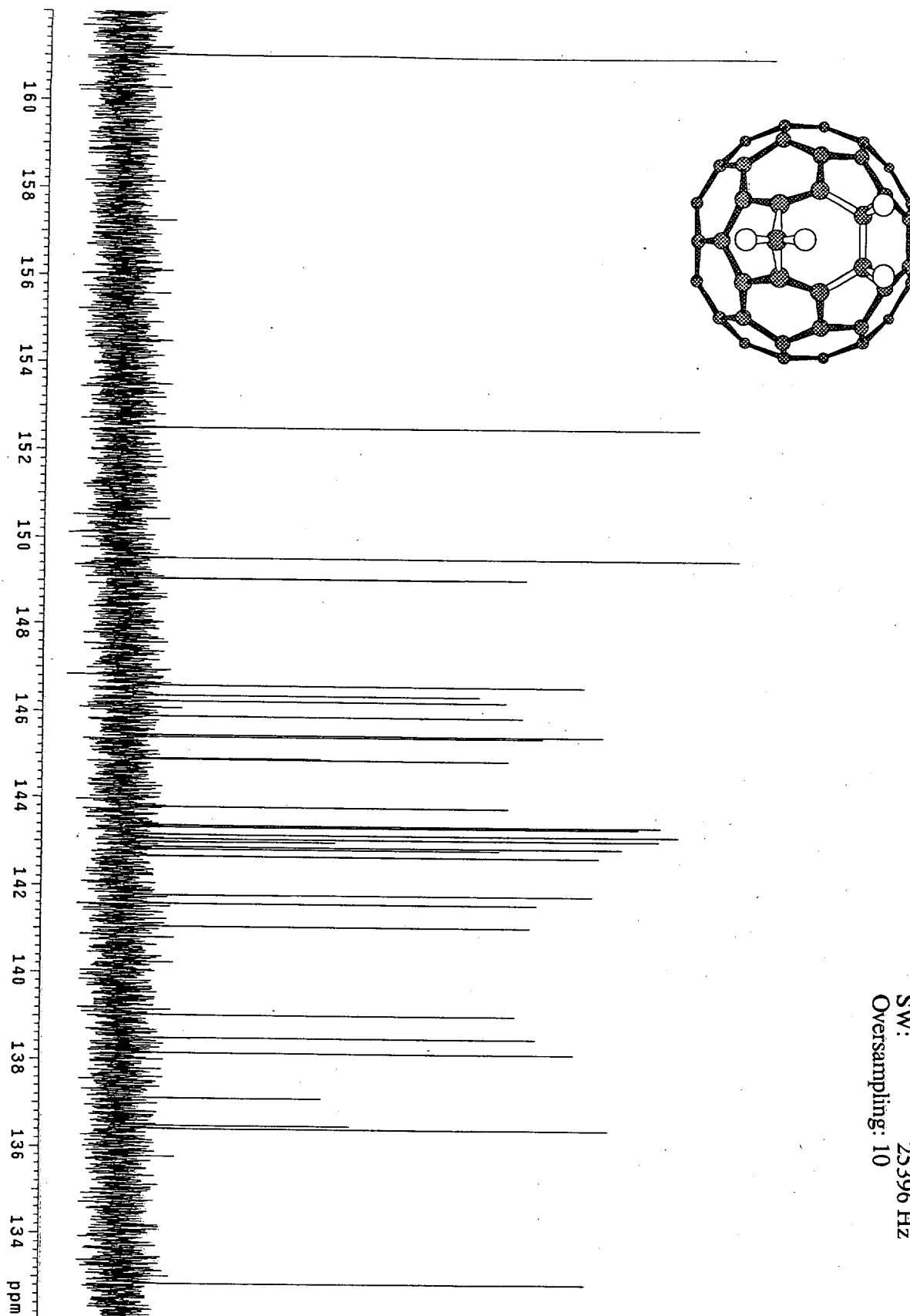
Experimental Conditions:
 Transients: 1728
 Acq. Time: 5.161 sec
 Flip angle: 25°
 SW: 25396 Hz
 Oversampling: 10

^{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

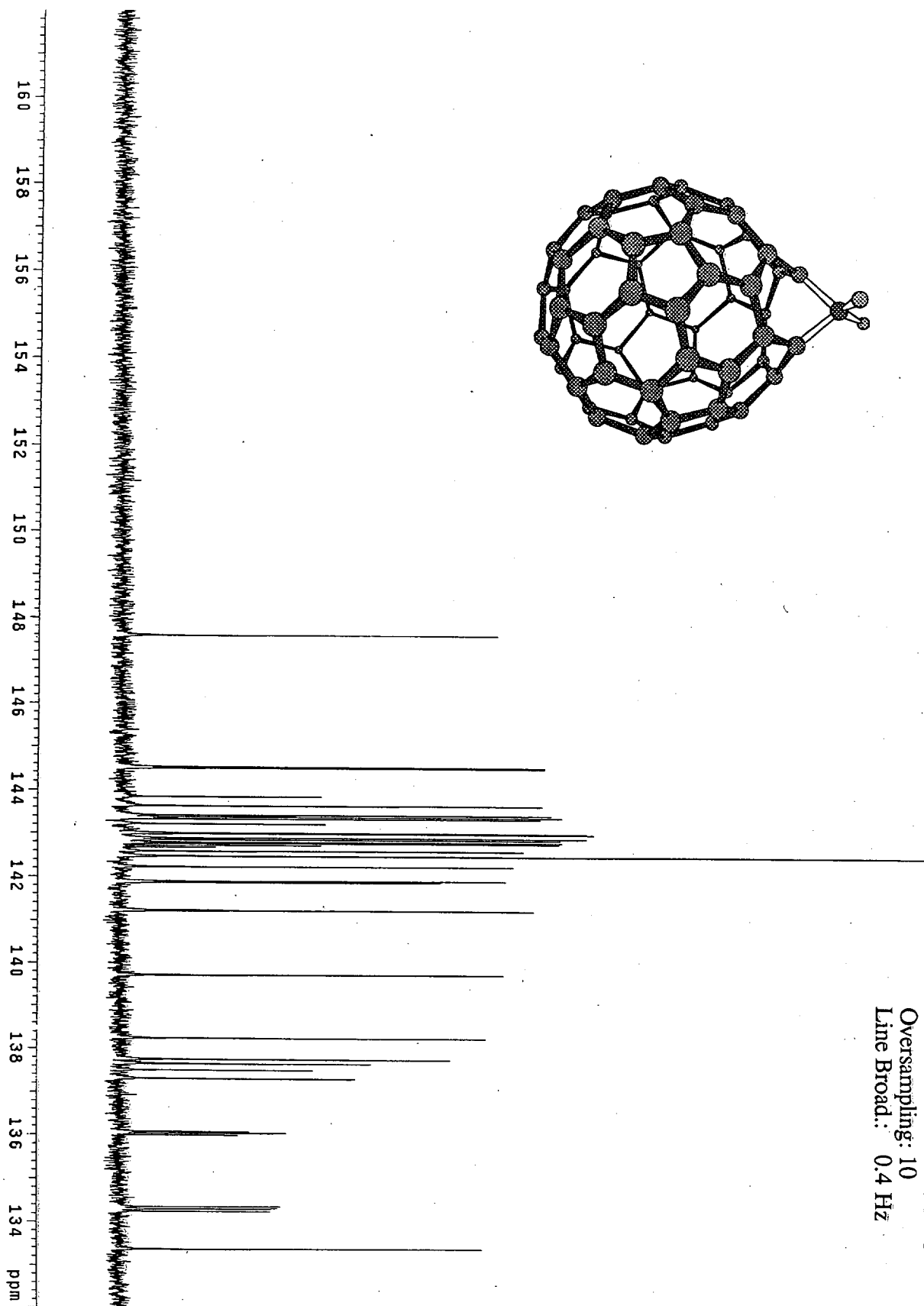
^{13}C NMR spectrum of C_{61}H_4 (3) at 125 MHz (sp^2 region only).



Experimental Conditions:

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

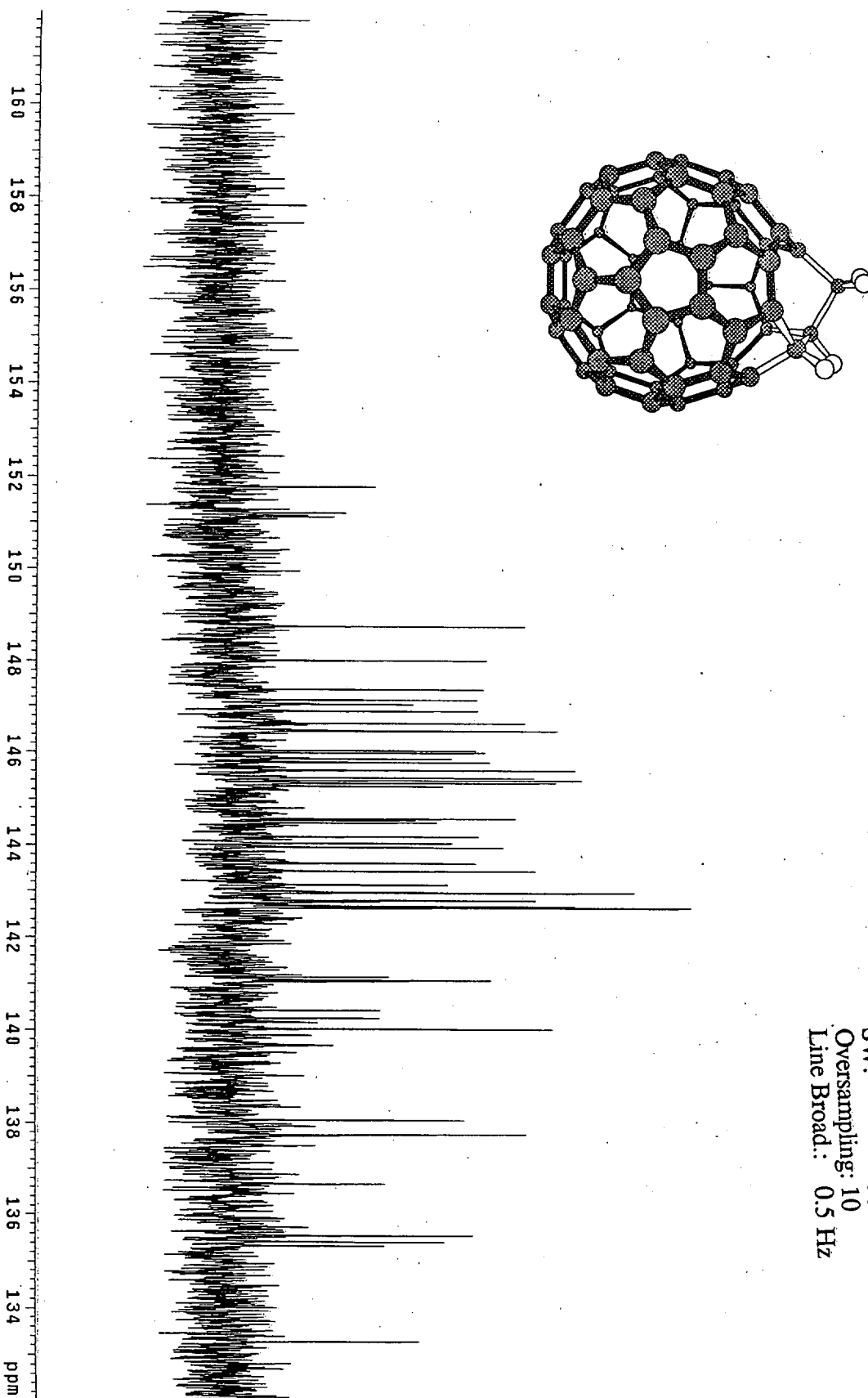
^1H - ^{13}C coupled NMR spectrum of **1** at 125 MHz (sp^2 region only).



Experimental Conditions:

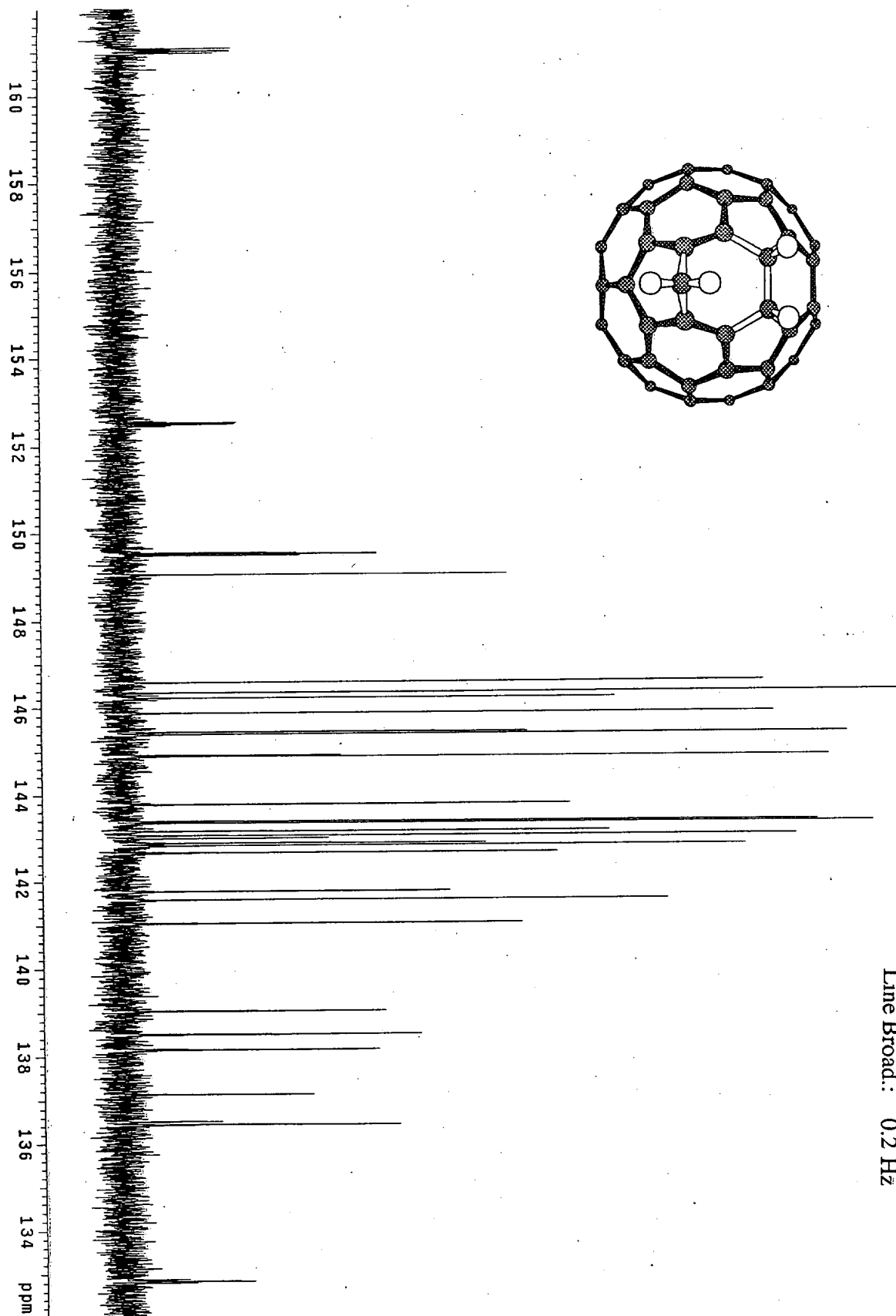
Transients: 44928
 Acq. Time: 5.161 sec
 Flip angle: 25°
 SW: 25396 Hz
 Oversampling: 10
 Line Broad.: 0.4 Hz

^1H - ^{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

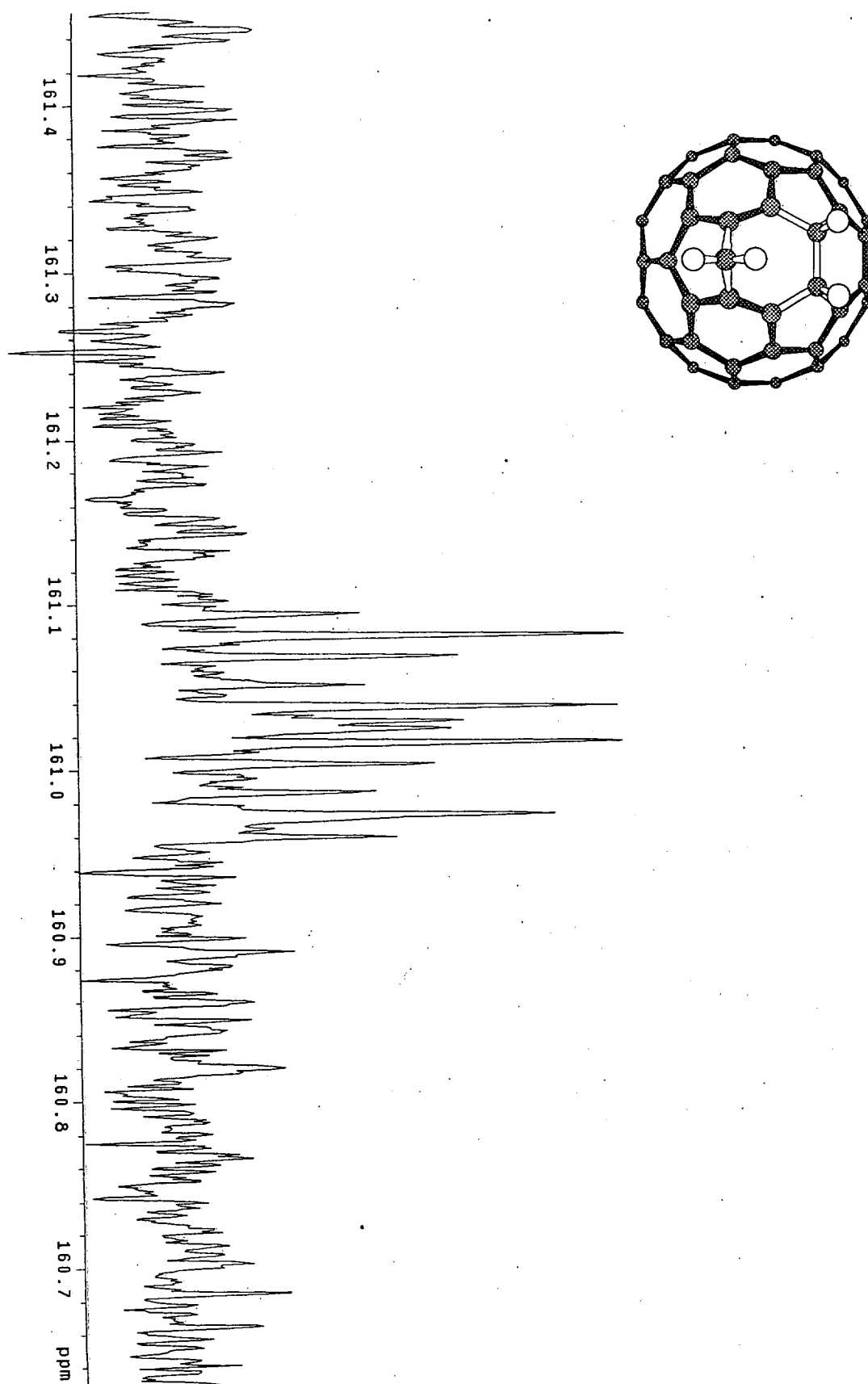
^1H - ^{13}C coupled NMR spectrum of **3** at 125 MHz (sp^2 region only).



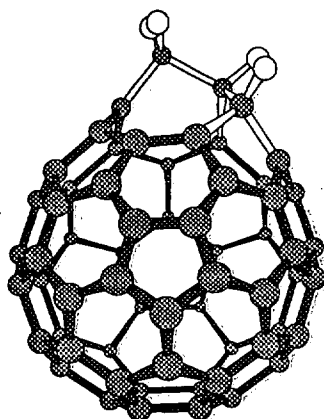
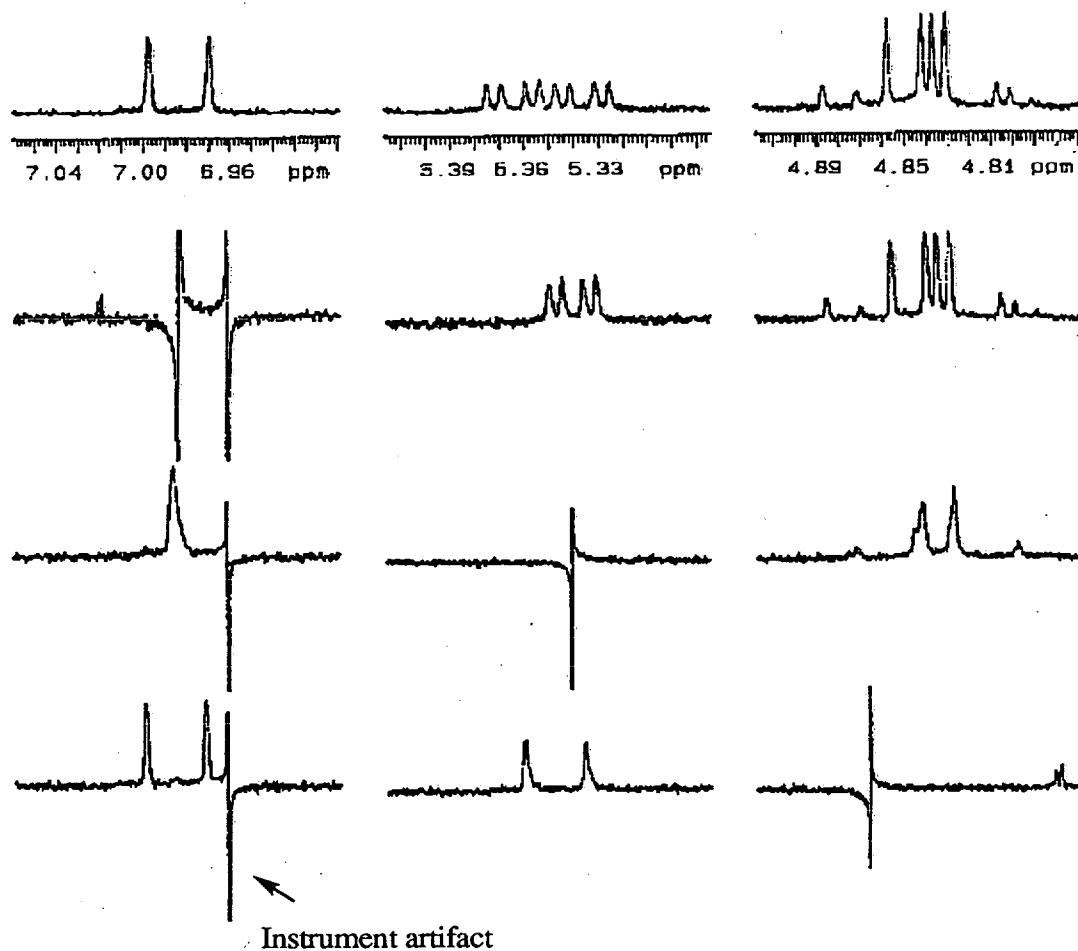
Experimental Conditions:

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

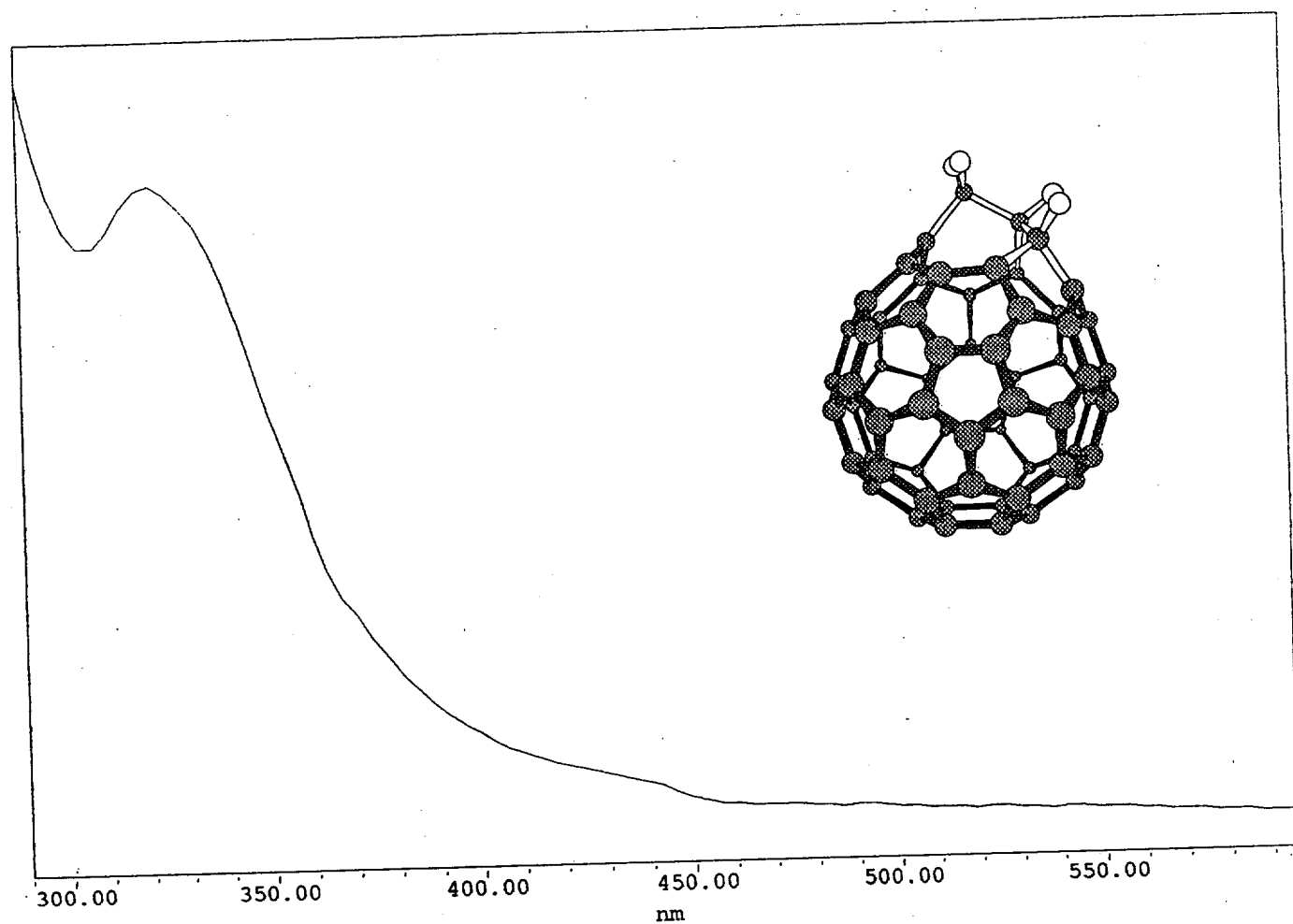
Expansion of downfield resonance in ^1H - ^{13}C coupled NMR of 3.



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



UV-Vis spectrum of **2**.



UV-Vis spectrum of 3.

