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**SUPPORTING
INFORMATION**

Supporting Information for

Synthesis and Isolation of One Isomer of C₆₀H₆

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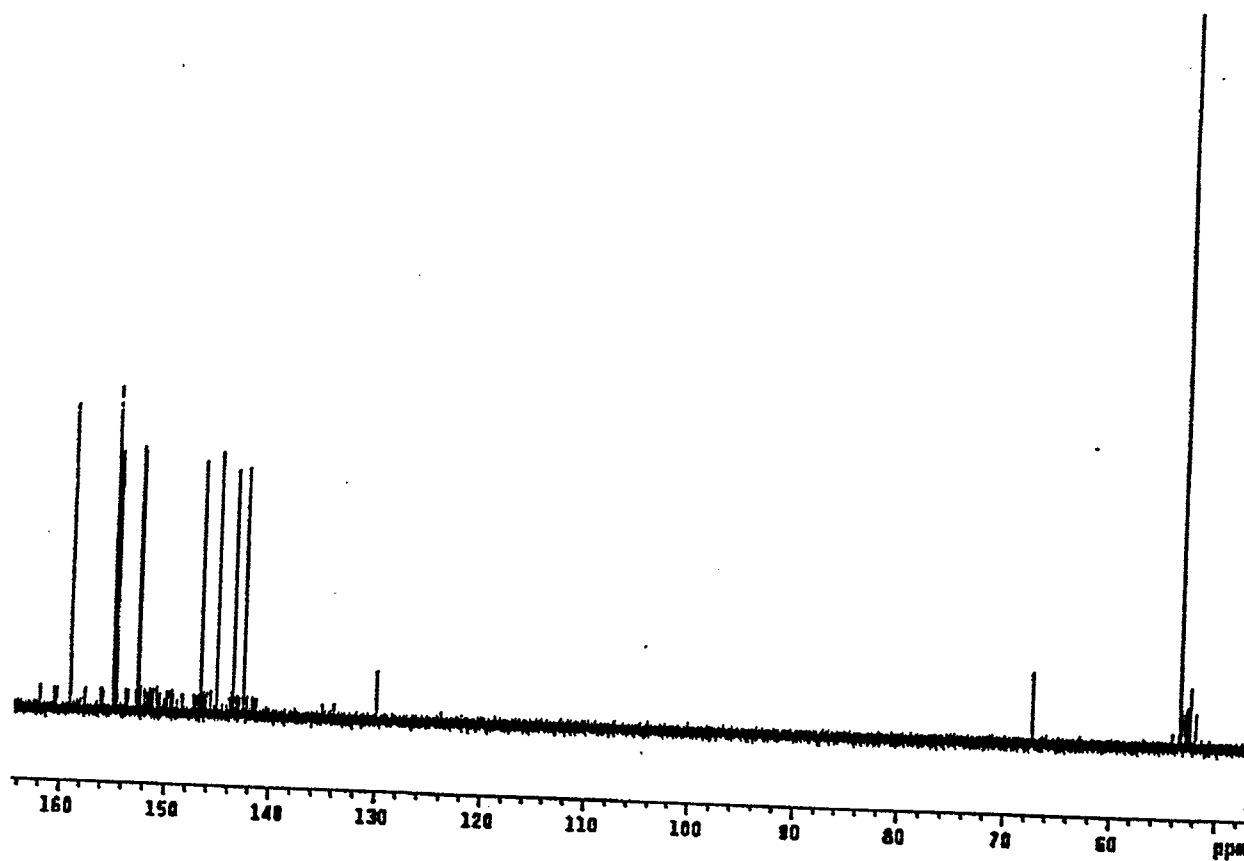
1. Experimental Procedure
2. ¹³C NMR Spectra of 1
 - a) ¹H-¹³C Decoupled spectrum
 - b) ¹H-¹³C Coupled spectra
 - c) Expansion of the downfield region
3. UV/visible Spectra of the major and minor isomers of C₆₀H₆
4. FABS Mass Spectrum

1. Experimental Procedures - Preparation of C₆₀H₆

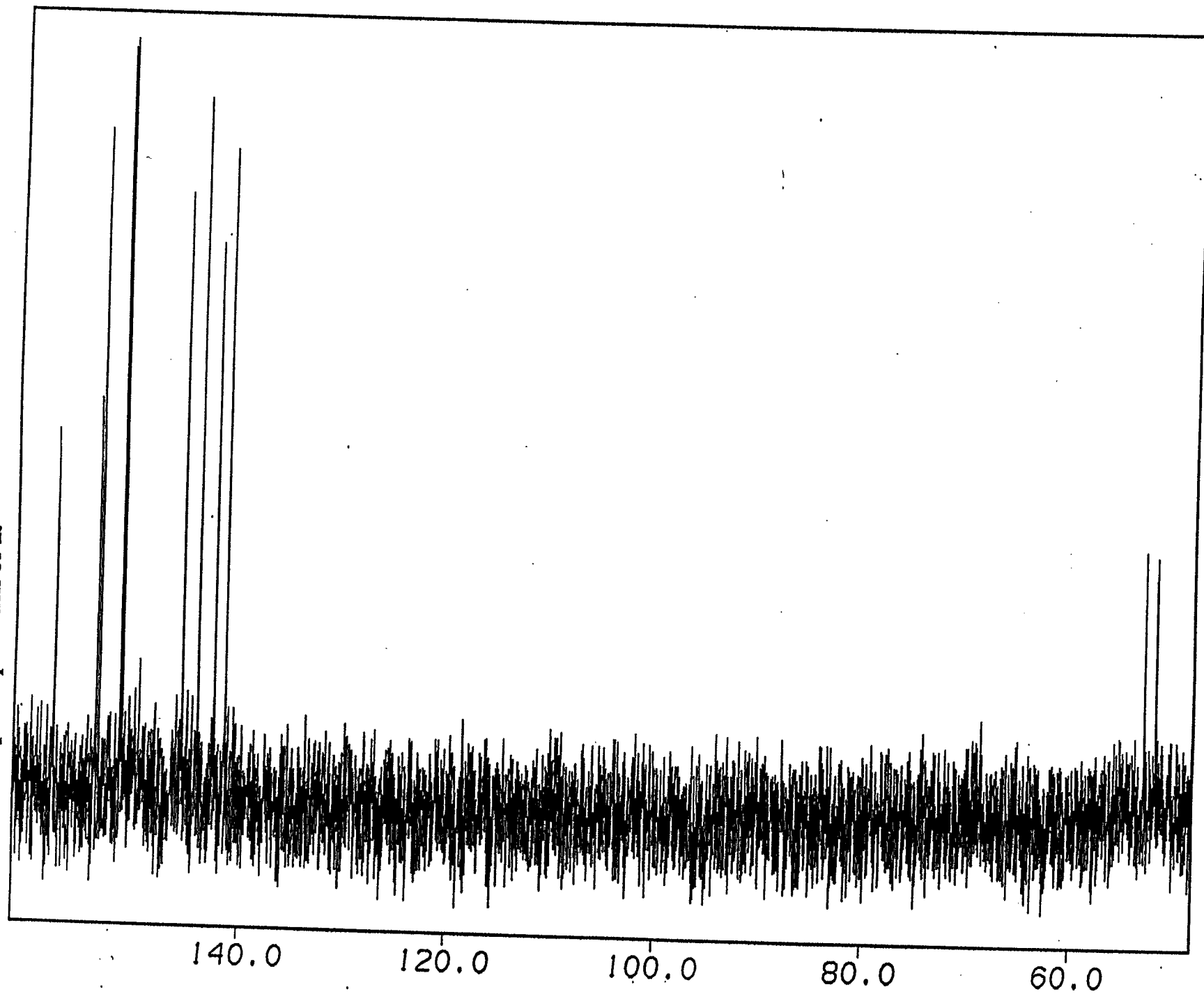
Zn-Cu couple was prepared from Zn dust and aqueous Cu(SO₄)₂ as described by Ekong.¹ C₆₀ (60.1 mg, 0.0835 mmol) and 60 mL toluene were combined in a 100 mL 3-neck flask and deoxygenated with argon. Zn-Cu couple (1.2003 g, 18.36 mmol Zn) and water (0.75 mL) were added. The resulting mixture was heated in a 50 °C oil bath and stirred vigorously with a 3/4" x 3/8" egg-shaped magnetic stir bar. After 3 hours the mixture was cooled to room temperature, the supernatant was decanted and the residual solid was washed twice with 1.5 mL portions of toluene. The combined supernatant and washings were concentrated, filtered through a 0.2 μm nylon filter, and purified by HPLC as described in the text. The C₆₀H₆ band (21.2 mg) was isolated as a 5:1 mixture of two peaks in 35% yield.

2. a) ^1H - ^{13}C Decoupled NMR Spectrum of **1**.

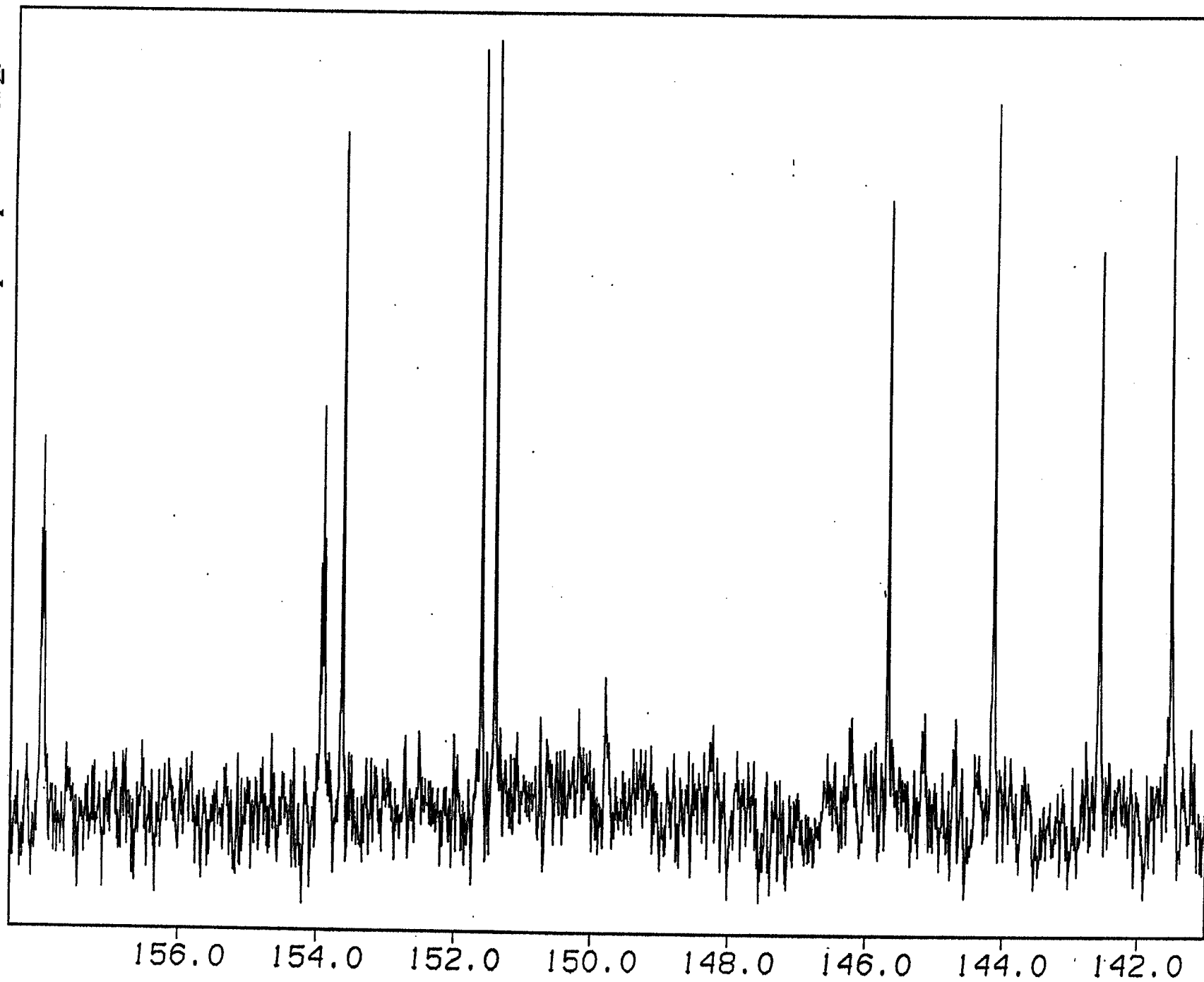
Peak List (9:1 CS_2 /acetone- d_6 , 125 MHz) δ 158.05, 153.97, 153.66, 151.65, 151.45, 145.71, 144.18, 142.60, 141.55, 52.28.



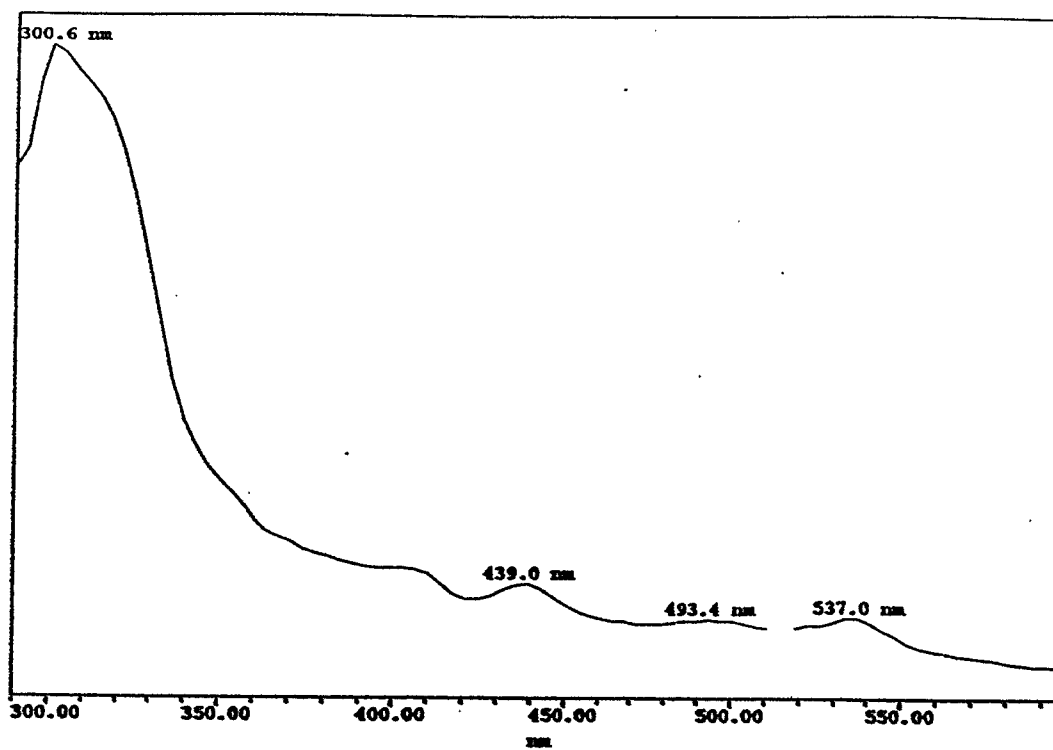
2 b) ^1H - ^{13}C Coupled Spectrum of 1.



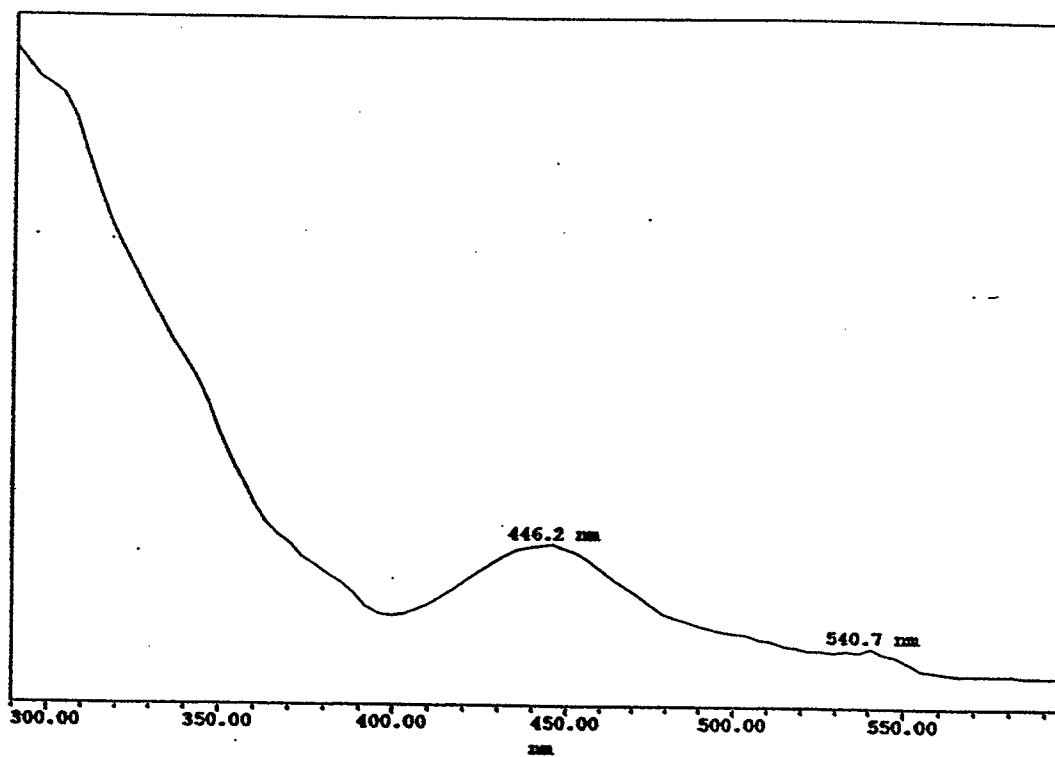
2 c) Expansion of the downfield region of the ^1H - ^{13}C Coupled Spectrum of **1**.



3. UV/Visible spectra of the major and minor isomers of $C_{60}H_6$

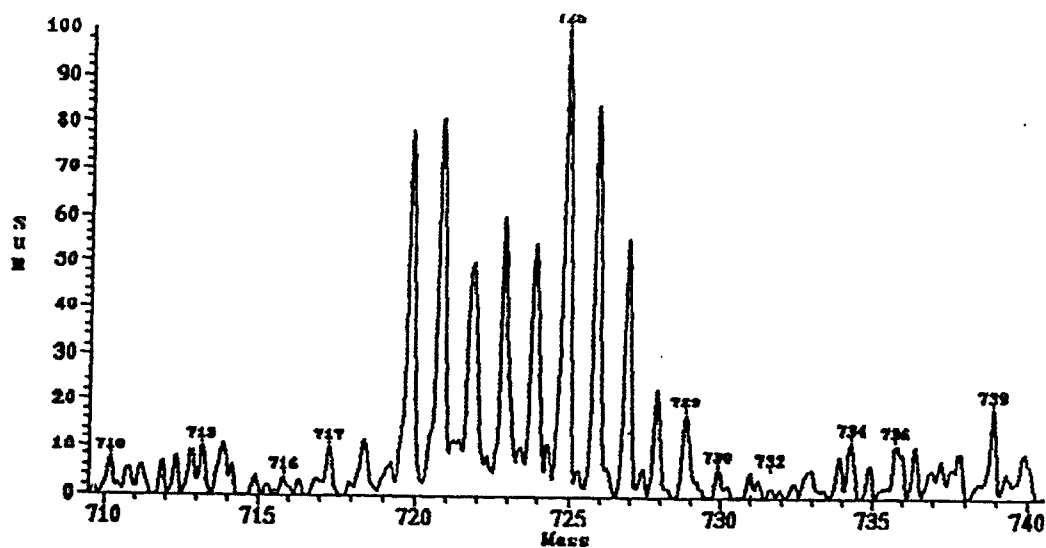


Major isomer (1)



Minor isomer

4. FABS Mass Spectrum of C₆₀H₆ Major Isomer



Negative-Ion FABS Mass Spectrum (*m*-nitrobenzyl alcohol matrix).