

## **SUPPORTING INFORMATION**

### **Straight-Chain Alkanes Template the Assembly of Water-Soluble Nano-Capsules**

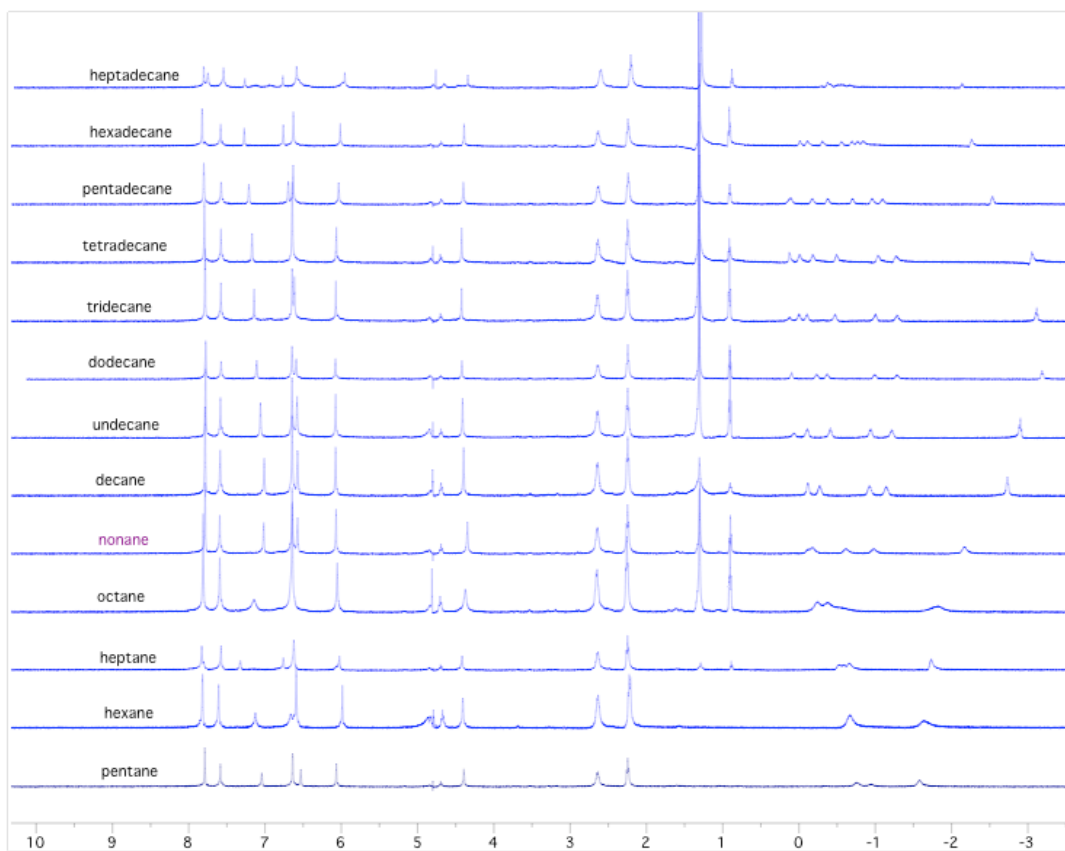
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## **<sup>1</sup>H-NMR spectra of the complexes of **1**<sub>2</sub> and hydrocarbons pentane through heptadecane**

In all cases an excess of guest was added to host **1**. To 0.6 mL of 1 mM host **1** and 10 mM sodium tetraborate, 10  $\mu$ L of the guest was added and the NMR spectra recorded (Figure S1). Integration of the host peaks versus the bound guest methyl peaks gave ratio of host to guest



**Figure S1:** <sup>1</sup>H-NMR spectra of the complexes of **1**<sub>2</sub> and hydrocarbons pentane through heptadecane.

## Pulse-Gradient Stimulated Spin-Echo NMR Studies

Diffusion measurements were performed on an INOVA 500 MHz (Varian Inc.) instrument equipped with a Performa II pulsed field gradient (PFG) module capable of producing pulses up to 52 gauss/cm. The experiments were carried out on a 5 mm PFG indirect detection probe. The STE (stimulated echo) diffusion experiment using the Varian pulse sequence “pge” (stimulated option on) were performed with pulse gradients of 2 ms in duration separated by 155 ms. Calibration utilized D<sub>2</sub>O samples with a diffusion constant of  $1.88 \times 10^{-5} \text{ cm}^2/\text{s}$ . The data was analyzed using the optional Varian diffusion software. The experiments were run at 25 °C, at a host concentration of 1mM (in 10 mM sodium tetraborate). The given diffusion constants were an average of three measurements. This signal attenuation (Figure S2) follows the equation:

$$\ln(I_g/I_o) = -\gamma^2 D G^2 \delta^2 (\Delta - \delta/3)$$

Where:  $I_g$  is the observed intensity

$I_o$  is the reference intensity

D is the diffusion constant

$\gamma$  is the gyromagnetic ratio of the observed nucleus

G is the gradient strength (arrayed in the experiment)

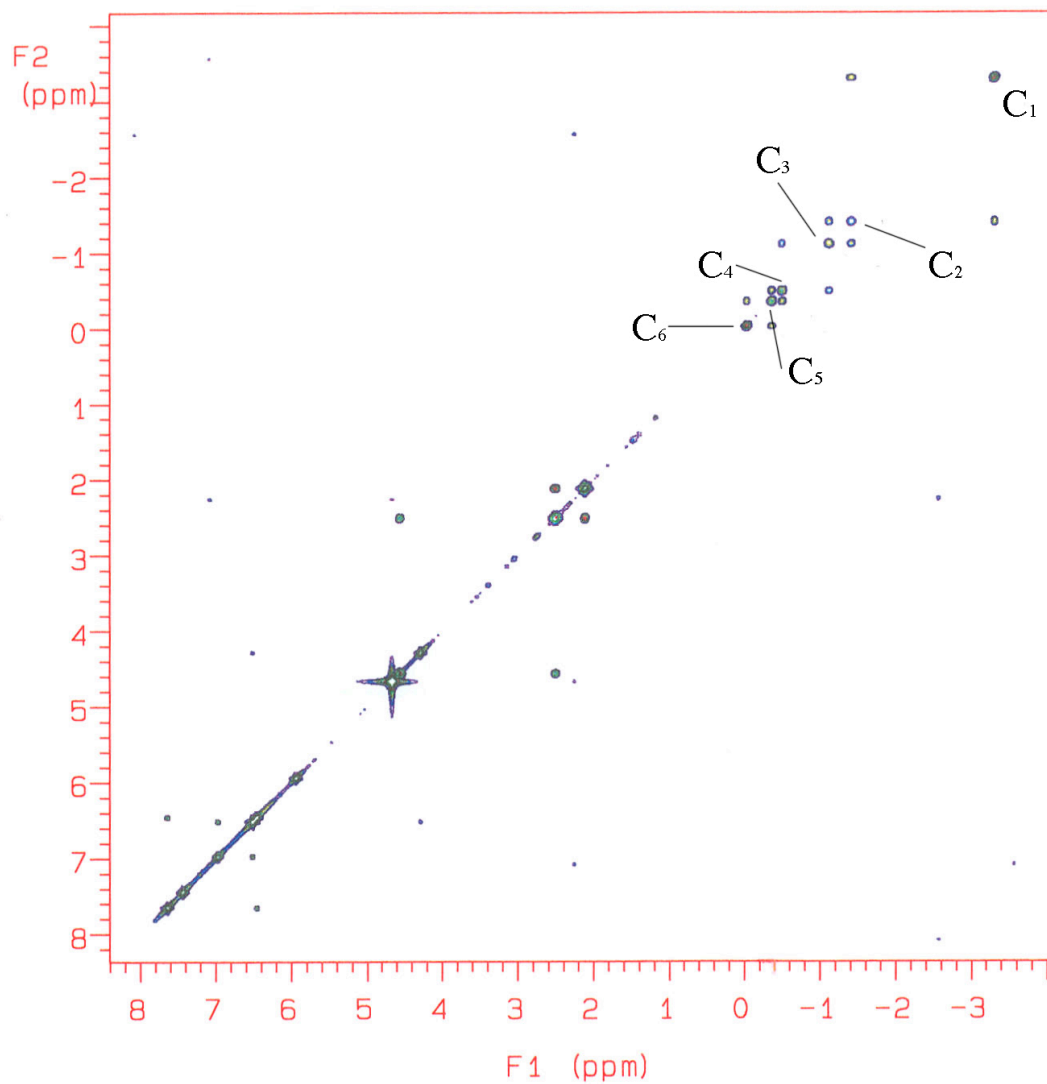
$\delta$  is the length of the gradient

$\Delta$  is the diffusion time

The slope of the plot  $\ln(I/I_o)$  versus the square of the gradient strength yielded the diffusion constant. This calculation is performed automatically by the diffusion macro from Varian, and gave for example a value of  $D = 1.82 \times 10^{-6} \text{ cm}^2\text{s}^{-1}$  for free host **1**.

## COSY $^1\text{H-NMR}$ of the complex of $\mathbf{1}_2$ with dodecane

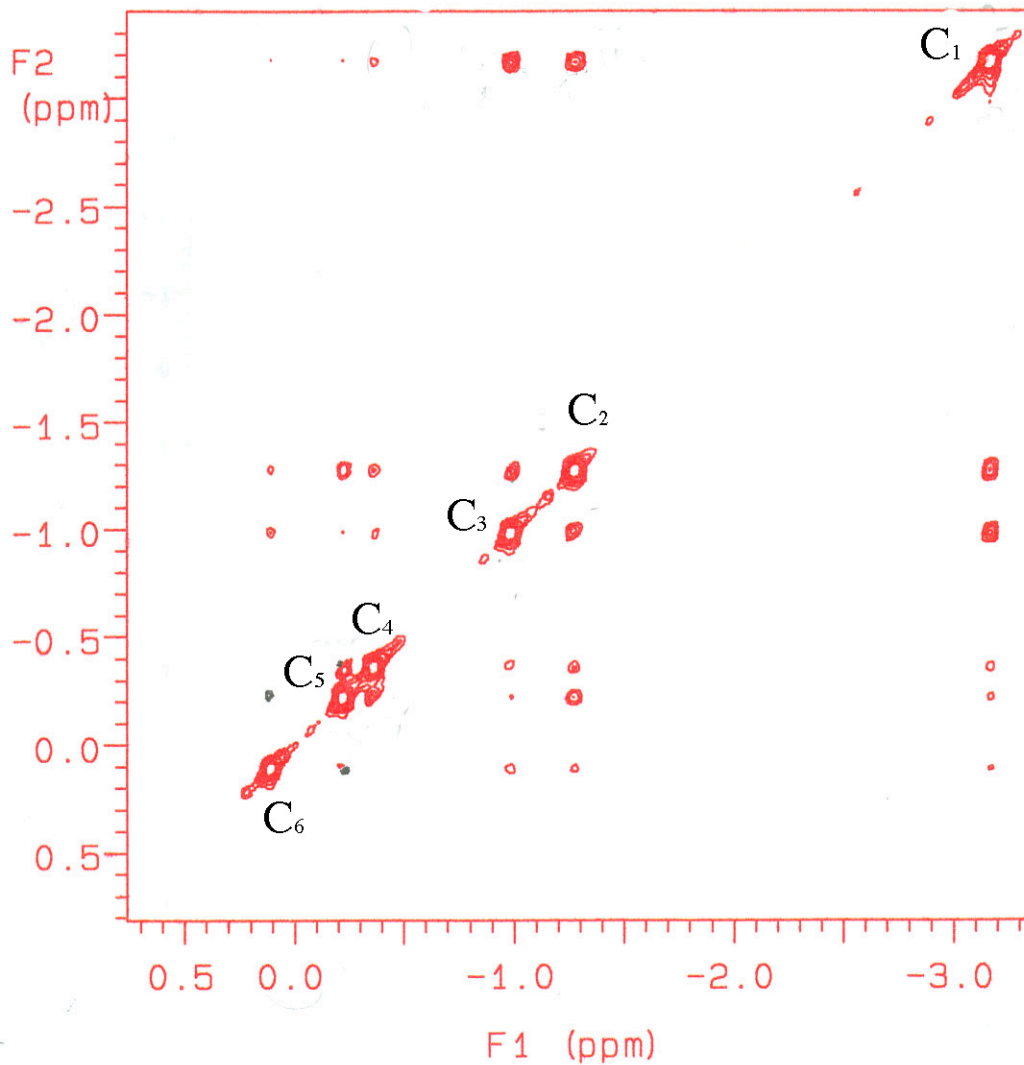
The proton COSY for the complex between  $\mathbf{1}_2$  and dodecane is shown in Figure S2. This COSY is representative of the spectra recorded for the other complexes.



**Figure S2:** COSY  $^1\text{H-NMR}$  of the complex of  $\mathbf{1}_2$  with dodecane. C-atoms of the terminal methyl group or methylene groups are indicated.

### NOESY $^1\text{H-NMR}$ of the complex of $\mathbf{1}_2$ with dodecane (bound guest peak region)

The proton NOESY for the complex between  $\mathbf{1}_2$  and dodecane is shown in Figure S3. This NOESY is representative of the spectra recorded for the other complexes.



**Figure S3:** NOESY  $^1\text{H-NMR}$  of the complex of  $\mathbf{1}_2$  with dodecane (bound guest peak region). C-atoms of the terminal methyl group or methylene groups are indicated.