

Diffusion of Linear Polymers within Microcapsules

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NMR Diffusion Experiment Conditions:

Sample	Concentration	Temp	Sweep Width	Pulse Width	Acq Time
Triphenylphosphine	27 mg/mL	20 °C	10000 Hz	10.7	0.7 s
TPP-PS	25.6 mg/mL	20°C	10000 Hz	10.7	0.3 s
TPP-PS	88 mg/mL	20°C	10000 Hz	10.7	0.3 s
TPP-PS Cap	Packed tube	20°C	10000 Hz	10.7	0.3 s
Tris-(o-tolyl)phosphine	29 mg/mL	20°C	10000 Hz	10.75	0.7 s
OTP-PS	26.4 mg/mL	20°C	10000 Hz	9.75	0.3 s
OTP-PS	39.6 mg/mL	21°C	10000 Hz	9.75	0.3 s
OTP-PS	77.6 mg/mL	20°C	10000 Hz	9.75	0.3 s
OTP-PS Cap	Packed Tube	20°C	10000 Hz	9.75	0.3 s

Sample	Recycle						Minimum g	Maximum g
	Delay	Δ	δ	τ	Steps	nt		
Triphenylphosphine	40 s	0.5 s	2 ms	0.8 ms	10	1	0.0099 T/m	0.3358 T/m
TPP-PS	14 s	1 s	5 ms	0.8 ms	10	64	0.002 T/m	0.553 T/m
TPP-PS	14 s	4 s	5 ms	0.8 ms	10	64	0.002 T/m	0.553 T/m
TPP-PS Cap	14 s	5 s	5 ms	0.8 ms	8	180	0.002 T/m	0.553 T/m
Tris-(o-Tolyl)phosphine	20 s	0.5 s	2 ms	0.8 ms	10	6	0.0099 T/m	0.3358 T/m
OTP-PS	14 s	1 s	5 ms	0.8 ms	10	64	0.002 T/m	0.553 T/m
OTP-PS	14 s	2 s	5 ms	0.8 ms	10	64	0.002 T/m	0.553 T/m
OTP-PS	14 s	4 s	5 ms	0.8 ms	10	64	0.002 T/m	0.553 T/m
OTP-PS Cap	14 s	5 s	5 ms	0.8 ms	8	180	0.002 T/m	0.553 T/m

Determination of Diffusion Constants:

$$\ln\left(\frac{I}{I_o}\right) = -D * g^2 * \gamma^2 * \delta^2 * \left(\Delta + \frac{4}{3}\delta + \frac{3}{2}\tau\right) \Rightarrow \ln\left(\frac{I}{I_o}\right) = -D * g^2 * k \Rightarrow \ln\left(\frac{I}{I_o}\right) = -D * Q$$

Definition of Variables:

g = gradient strength in Tesla/m

γ = magnetogyric ratio

δ = gradient length (total duration of bipolar gradient pulse)

Δ = diffusion delay

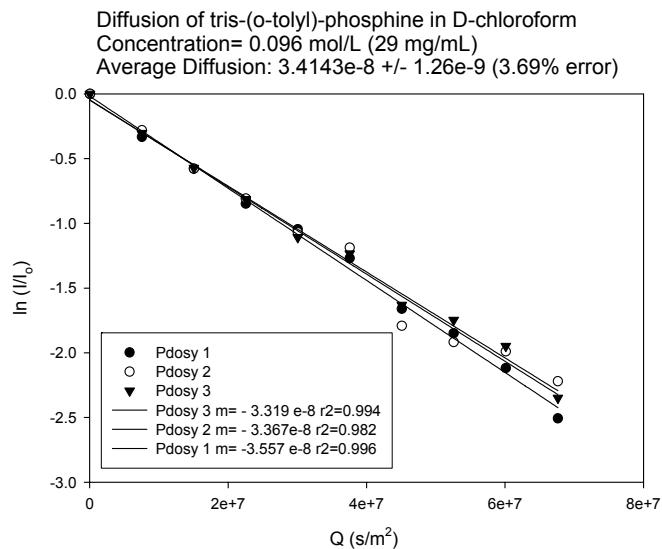
τ = gradient recovery delay

Relaxation Times for the Molecules under Investigation:

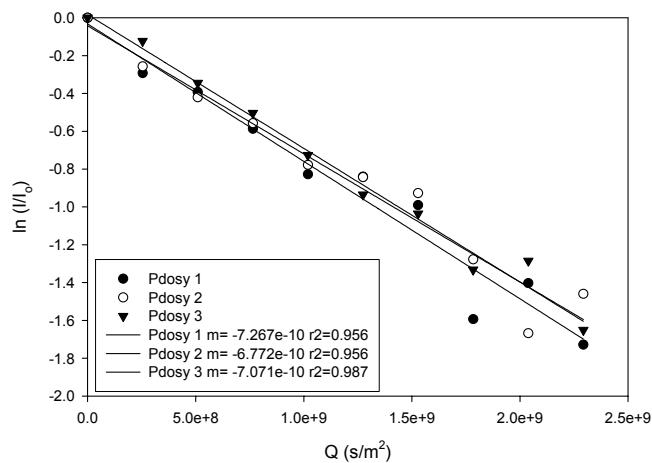
Sample	Concentration*	T ₁ (s)	T ₂ (s)
Triphenylphosphine	25.9 mg/mL	17.4	6.0
TPP-PS	88 mg/mL	3.96	0.56
TPP-PS Cap	Packed tube	4.06	0.18
Tris-(o-tolyl)phosphine	31.5 mg/mL	9.07	4.9
OTP-PS	40 mg/mL	5.42	0.70
OTP-PS Cap	Packed tube	6.32	0.65
TPP-PS Bead	Packed tube	5.33	< 0.02

*The concentrations are exact for the T₂ measurements. The polymer T₁ values were collected at lower concentrations.

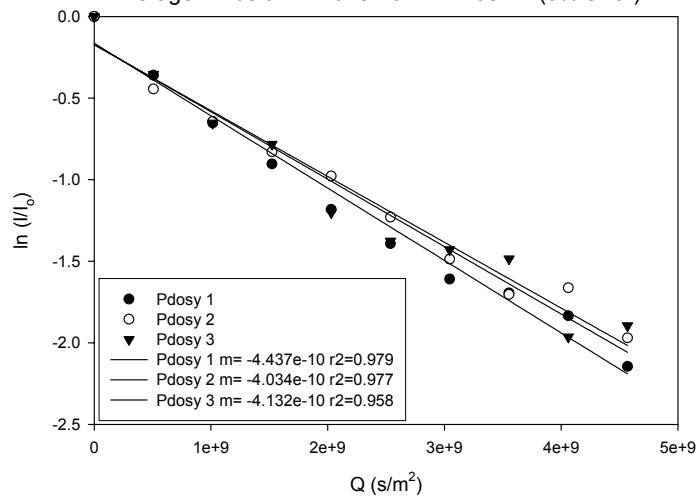
NMR Diffusion Data: Error reflects deviation in diffusion rates, does not take r^2 into account.



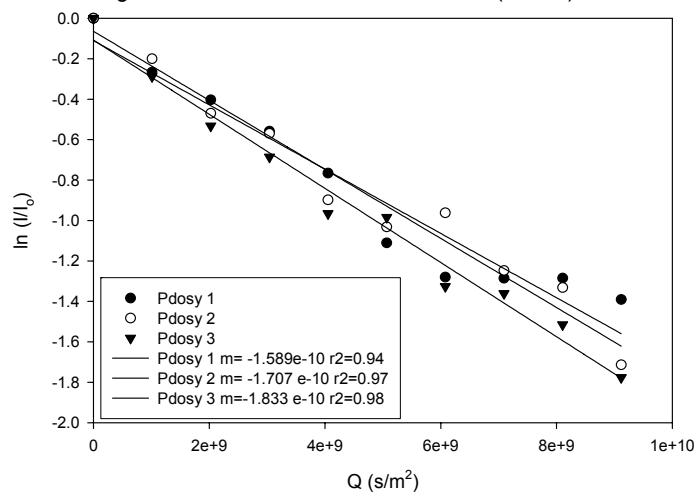
Diffusion of o-tolyl-phosphine Modified Polystyrene in Chloroform
Concentration= 26.4 mg/mL
Average Diffusion: 7.0367e-10 +/- 2.49e-11 (3.54% error)



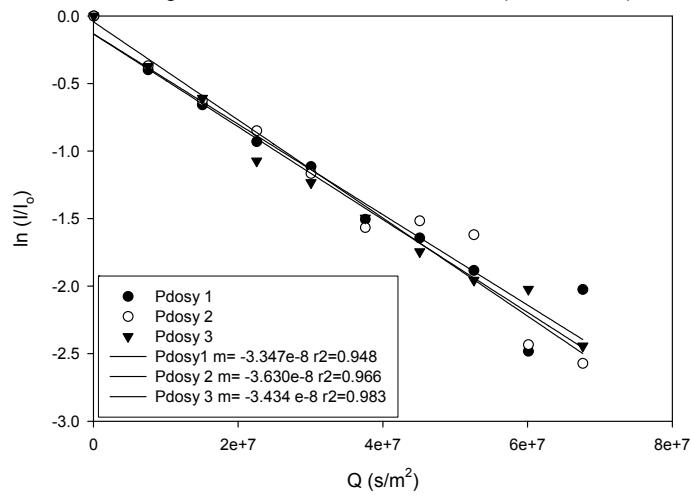
Diffusion of o-tolyl-phosphine Modified Polystyrene
 Concentration= 39.6 mg/mL
 Average Diffusion: 4.201e-10 +/- 2.10e-11 (5% error)



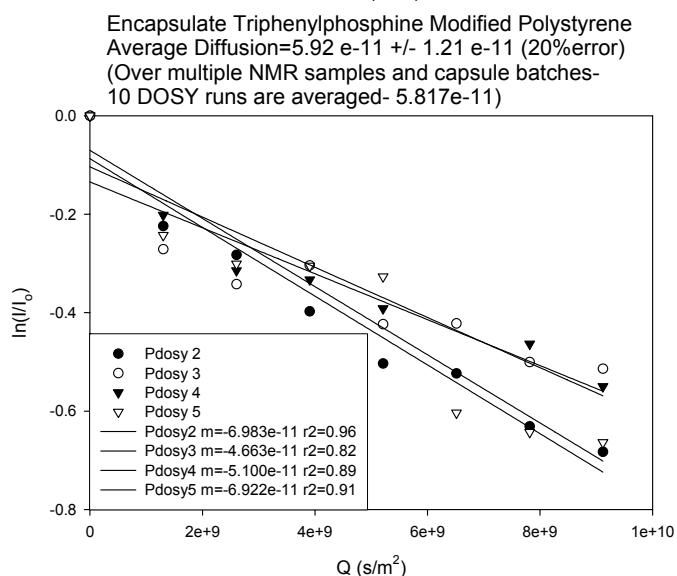
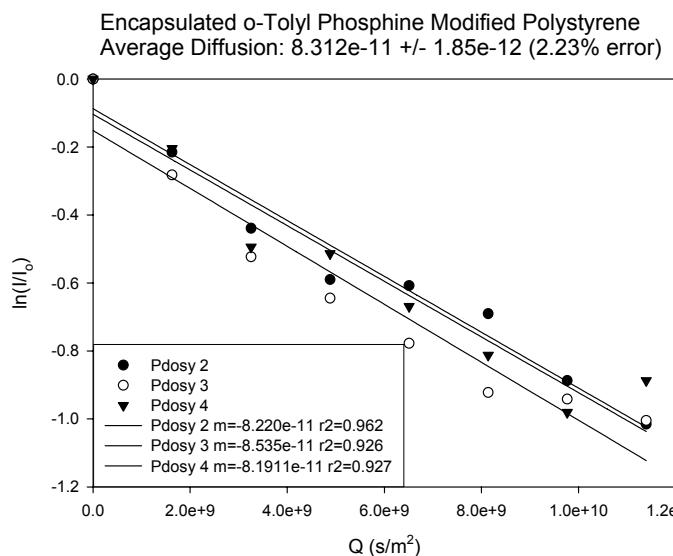
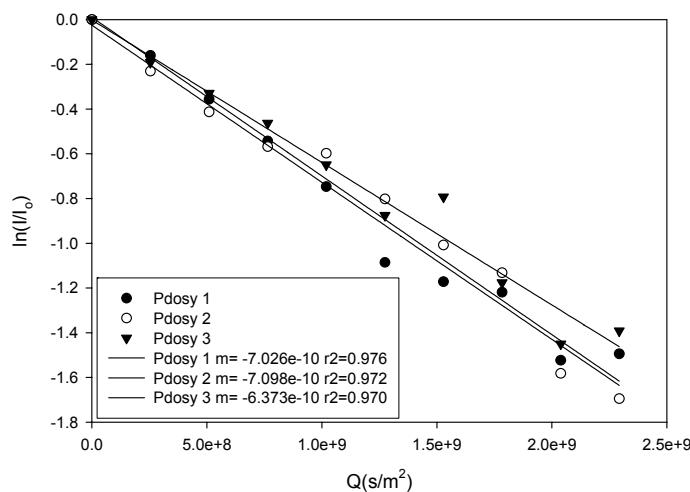
Diffusion of o-tolyl-phosphine Modified Polystyrene in Chloroform
 Concentration=77.6 mg/mL
 Average Diffusion: 1.7097e-10 +/- 1.22e-11 (7.14%)



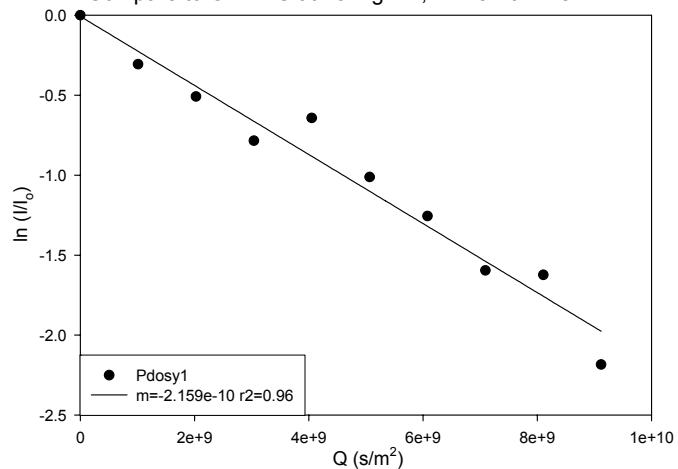
Diffusion of Triphenylphosphine in D-Chloroform
 Concentration= 0.102 mol/L (27 mg/mL)
 Average Diffusion: 3.470e-8 +/- 1.45e-9 (4.18% error)



Diffusion of Triphenylphosphine Modified Polystyrene in Chloroform
 Concentration= 25.6 mg/mL
 Average Diffusion: $6.832 \times 10^{-10} \pm 3.99 \times 10^{-11}$ (5.85% error)



Triphenylphosphine Modified Polystyrene in Chloroform
 Concentration: 88 mg/mL
 Only one test run, diffusion rate=2.159e-10 m²/s²
 Compare to OTP-PS at 78 mg/mL, 1.71e-10 m²/s



Diffusion of Methylene Chloride in
 1. Chloroform
 2. TPP-PS Chloroform Solution (66 mg/mL)
 3. TPP-PS Caps

