

Supplementary Information

Influence of the Capping Agent PVP of the Outer Layer of Pd Nanocubes Surface on the Catalytic Hydrogenation of Unsaturated C–C Bonds

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Table S1. Experimental values obtained by FAAS to determine the amount of PVP

Washing times	Pd / (% m m ⁻¹)	Average Pd / %	PVP / (% m m ⁻¹)	Average PVP / %	Error
1 (Pd-NC85)	16.06	85.42	83.94	85.42	2.10
	13.09		86.91		
2 (Pd-NC70)	26.08	70.88	73.92	70.88	4.29
	32.15		67.85		
4 (Pd-NC55)	48.05	54.39	51.95	54.395	3.45
	43.16		56.84		
6 (Pd-NC39)	66.04	38.97	37.97	38.97	1.42
	64.8		39.98		
8 (Pd-NC20)	81.10	34.58	33.96	20.35	0.87
	80.20		35.2		

FAAS: flame atomic absorption spectrophotometry; PVP: polyvinylpyrrolidone; Pd-NC85, Pd-NC70, Pd-NC55, Pd-NC39, Pd-NC20: amount of PVP on the Pd-NCs from 85 to 20% (m m⁻¹) after the washing procedure.

Table S2. Calculated R_G and e_c from the R_S and σ values obtained from the SAXS fitted scattering curves

Sample	R _S / nm	R _G / nm	e _c / nm	σ
Pd-NC85	6.027	4.668	9.337	0.180
Pd-NC70	5.738	4.444	8.889	0.153
Pd-NC55	6.018	4.661	9.323	0.178
Pd-NC39	6.097	4.717	9.445	0.147

R_G: radius of gyration; R_S: sphere radius; e_c: cube edge length; σ: dispersity; Pd-NC85, Pd-NC70, Pd-NC55, Pd-NC39: amount of PVP on the Pd-NCs from 85 to 39% (m m⁻¹) after the washing procedure.

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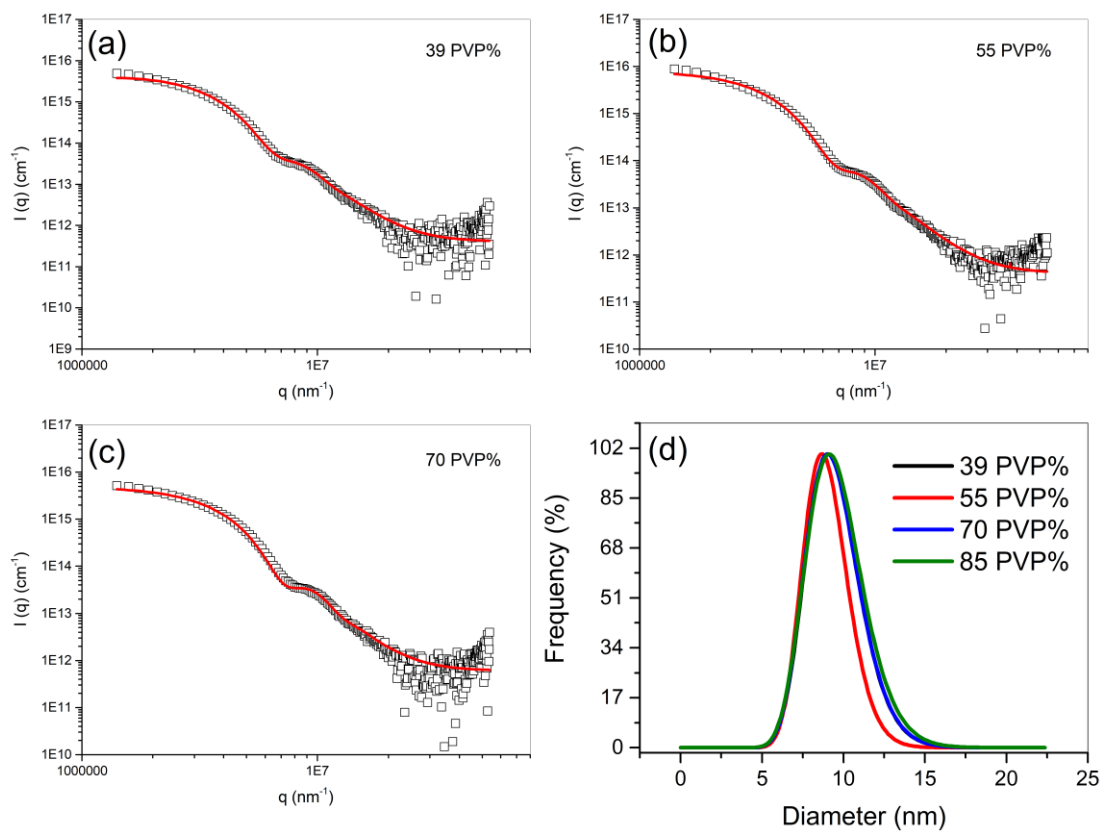


Figure S1. SAXS data and corresponding curve fitting for the Pd-NCs catalysts (a-c) and the size distribution plots (d).

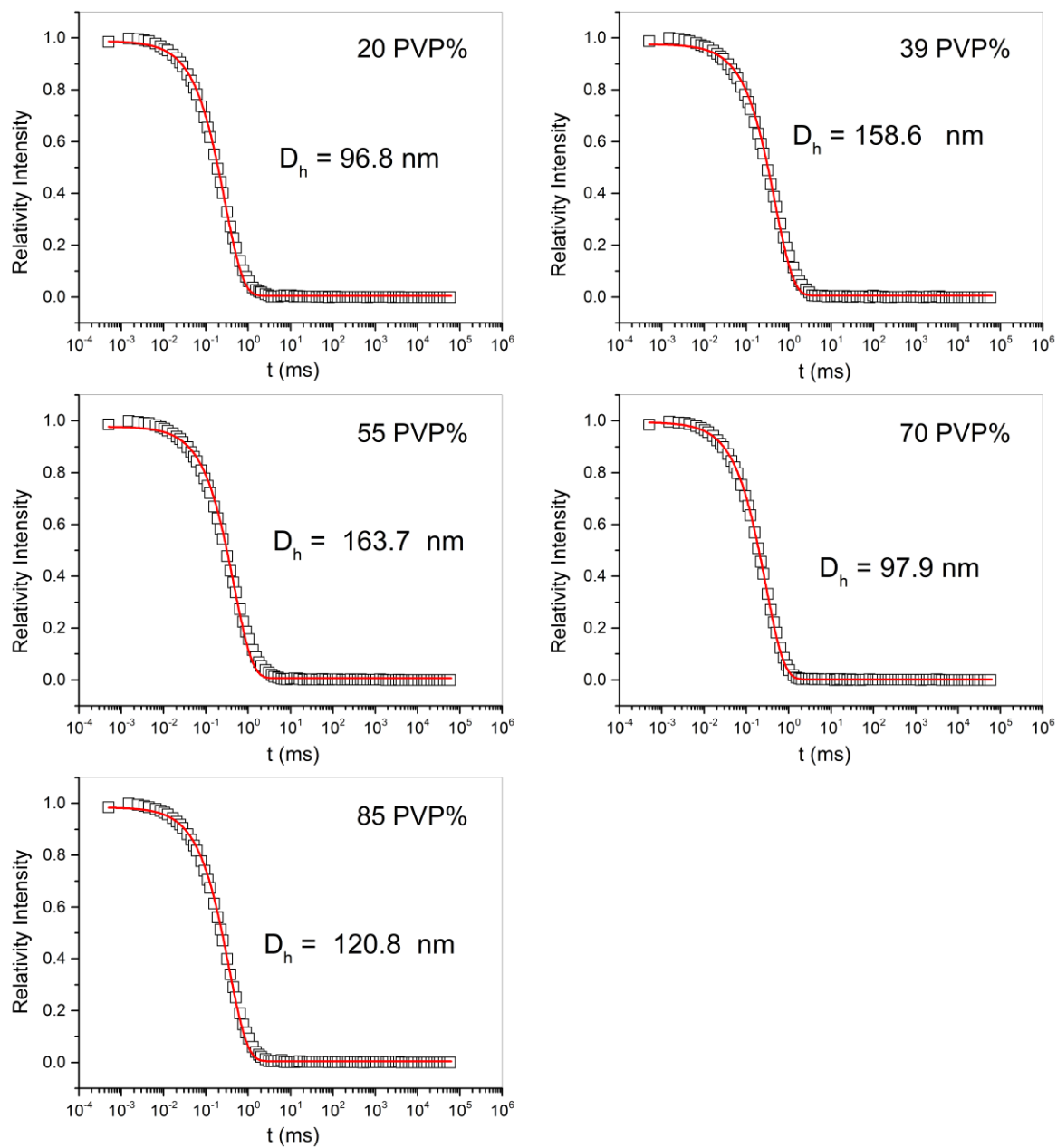


Figure S2. Volume-weighted DLS analysis for all Pd-NCs catalysts.

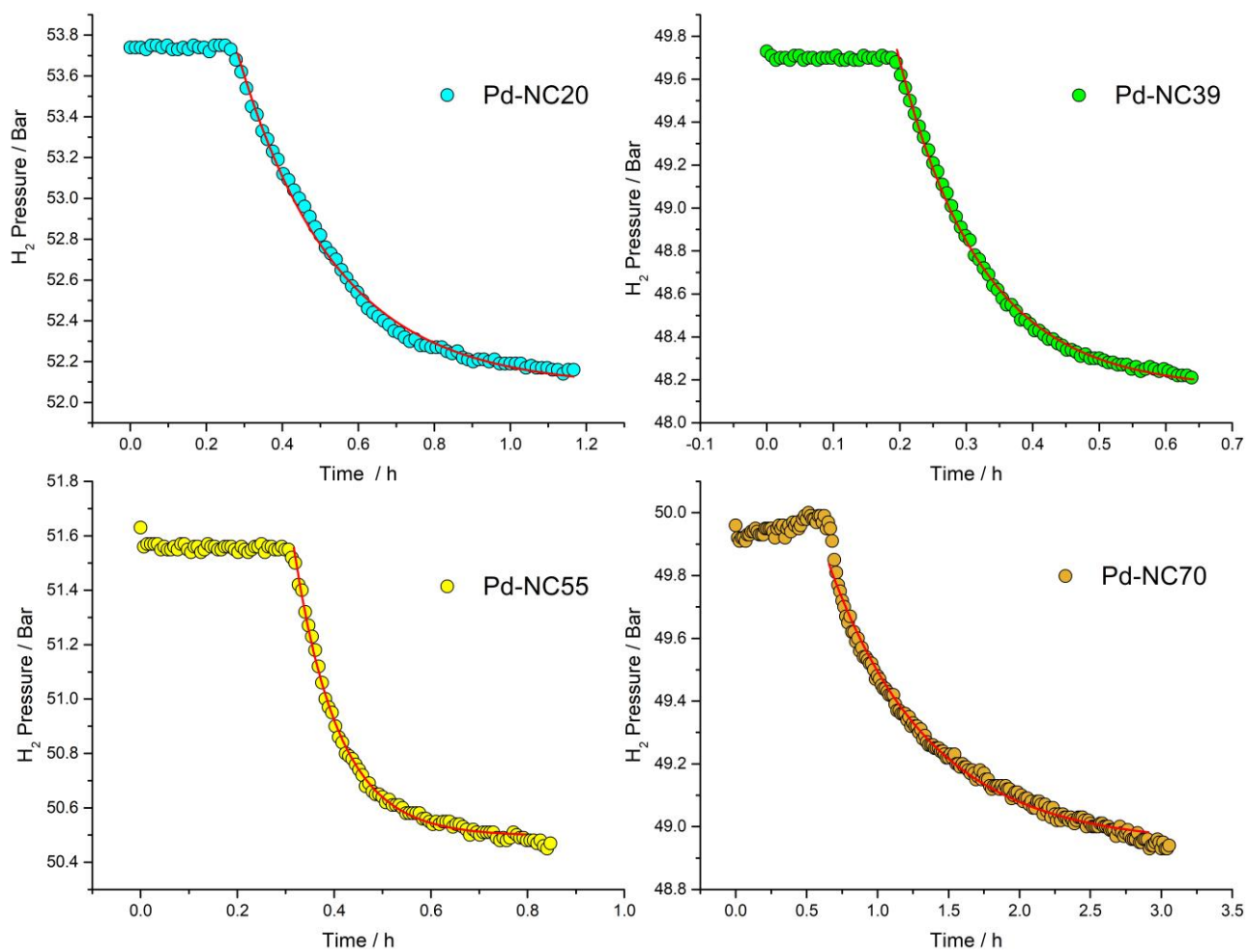


Figure S3. Kinetics profiles and first-order fitting for the ST hydrogenation by H₂ uptake with all Pd-NCs catalysts (Pd-NC85 presented no activity for this reaction).

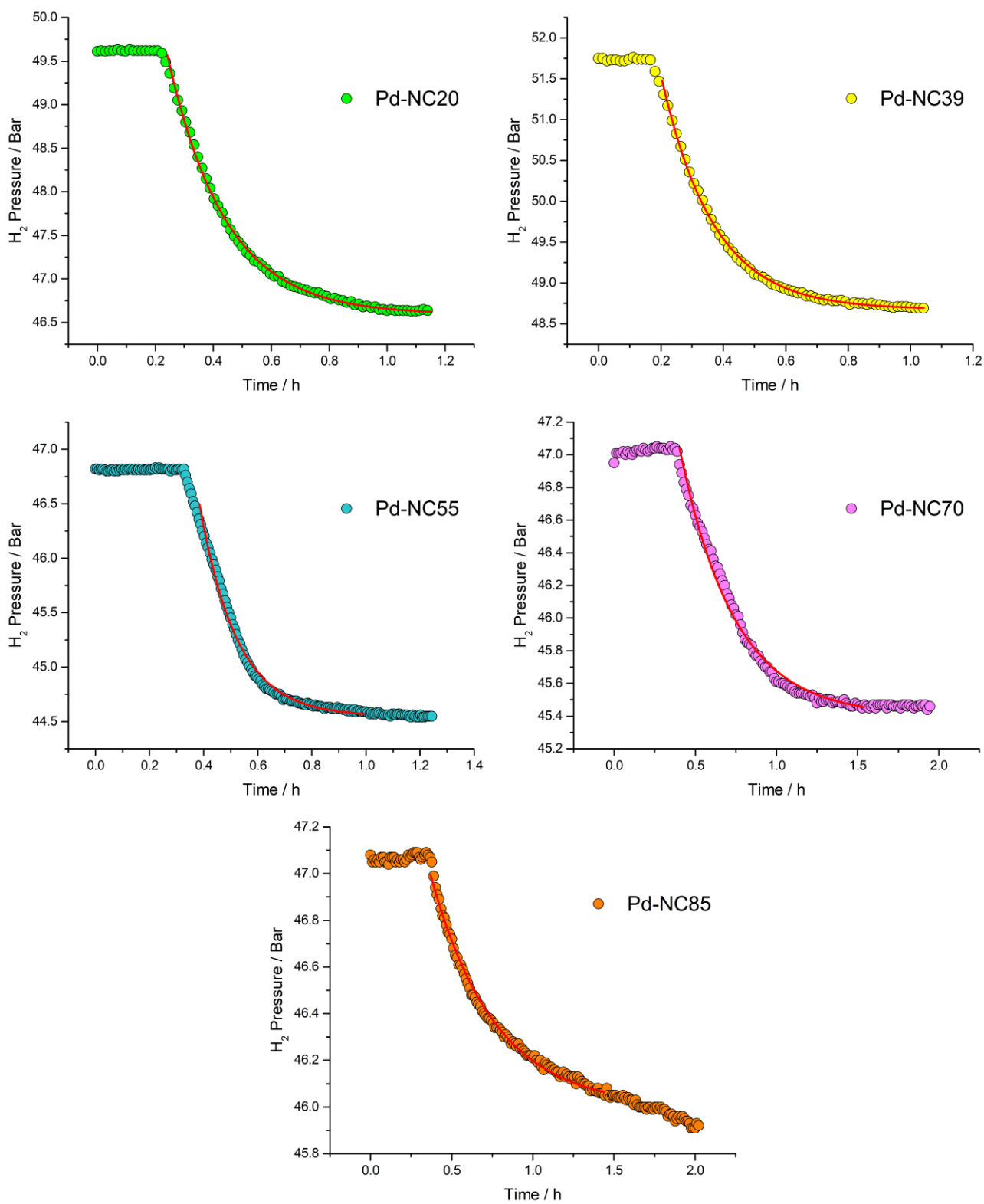


Figure S4. Kinetics profiles and first-order fitting for the PA hydrogenation by H_2 uptake with all Pd-NCs catalysts.

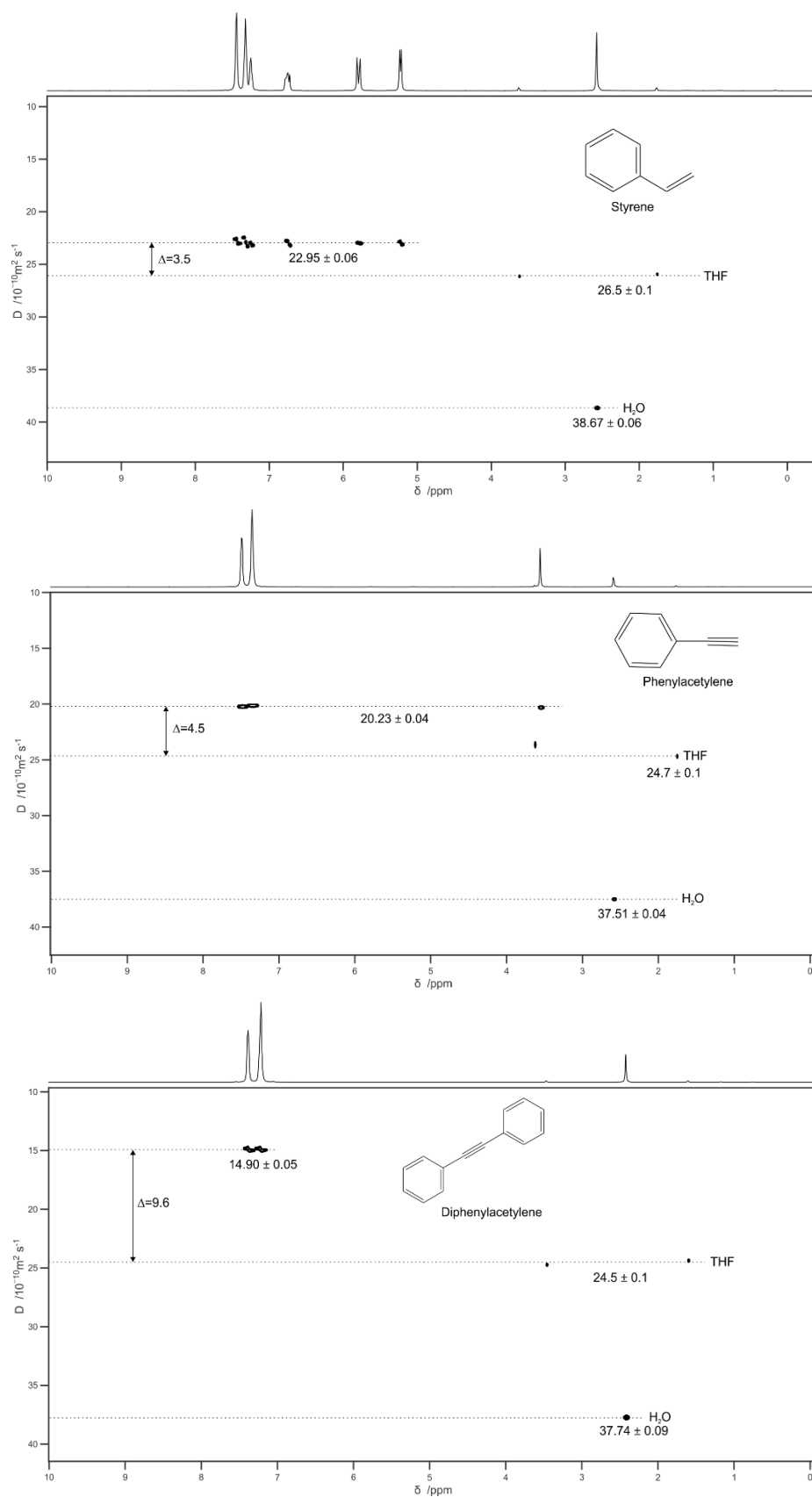


Figure S5. ^1H NMR DOSY analysis of (top) styrene (ST), (middle) phenylacetylene (PA) and (bottom) diphenylacetylene (DPA) for the diffusion coefficients determination (D).

Table S3. Parameters used for the DaII calculation

Reaction	k / s^{-1}	$c_{\text{substrate}} / (\text{mol L}^{-1})$	$n-1$	β	$D / (\text{m}^2 \text{s}^{-1})$	δ / m	a / m^{-1}	DaII
ST20	1.18×10^{-3}	0.5	0	82.06×10^{-4}	3.50×10^{-10}	4.27×10^{-8}	11439.4	1.26×10^{-5}
ST39	2.25×10^{-3}	0.5	0	47.52×10^{-4}	3.50×10^{-10}	7.37×10^{-8}	11715.5	4.04×10^{-5}
ST55	2.51×10^{-3}	0.5	0	46.08×10^{-4}	3.50×10^{-10}	7.60×10^{-8}	11148.6	4.89×10^{-5}
ST70	6.07×10^{-4}	0.5	0	8.13×10^{-3}	3.50×10^{-10}	4.31×10^{-8}	11148.6	6.70×10^{-6}
ST85	0	0.5	0	64.04×10^{-4}	3.50×10^{-10}	5.47×10^{-8}	11439.4	0.00
PA20	1.25×10^{-3}	0.5	0	105.51×10^{-4}	4.50×10^{-10}	4.27×10^{-8}	11439.4	1.04×10^{-5}
PA39	1.69×10^{-3}	0.5	0	6.11×10^{-3}	4.50×10^{-10}	7.37×10^{-8}	11715.5	2.36×10^{-5}
PA55	1.87×10^{-3}	0.5	0	59.25×10^{-4}	4.50×10^{-10}	7.60×10^{-8}	11148.6	2.83×10^{-5}
PA70	1.06×10^{-3}	0.5	0	104.53×10^{-4}	4.50×10^{-10}	4.31×10^{-8}	11148.6	9.10×10^{-6}
PA85	7.28×10^{-4}	0.5	0	82.34×10^{-4}	4.50×10^{-10}	5.47×10^{-8}	11439.4	7.73×10^{-6}
DPA20	4.39×10^{-4}	0.5	0	225.09×10^{-4}	9.60×10^{-10}	4.27×10^{-8}	11439.4	3.88×10^{-3}
DPA39	9.39×10^{-5}	0.5	0	130.35×10^{-4}	9.60×10^{-10}	7.37×10^{-8}	11715.5	65.48×10^{-4}
DPA55	4.86×10^{-5}	0.5	0	12.64×10^{-3}	9.60×10^{-10}	7.60×10^{-8}	11148.6	70.96×10^{-4}
DPA70	6.39×10^{-5}	0.5	0	2.23×10^{-2}	9.60×10^{-10}	4.31×10^{-8}	11148.6	40.22×10^{-4}
DPA85	3.33×10^{-5}	0.5	0	175.66×10^{-4}	9.60×10^{-10}	5.47×10^{-8}	11439.4	49.76×10^{-4}

k: rate constant; c: concentration; n: reaction order; β : mass transport coefficient; D: diffusion coefficient; δ : length scale; a: total area of the interface; DaII: Damkohler number.

