Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

"Guest molecule dynamics and ferroelectric transition in a clathrate compound"

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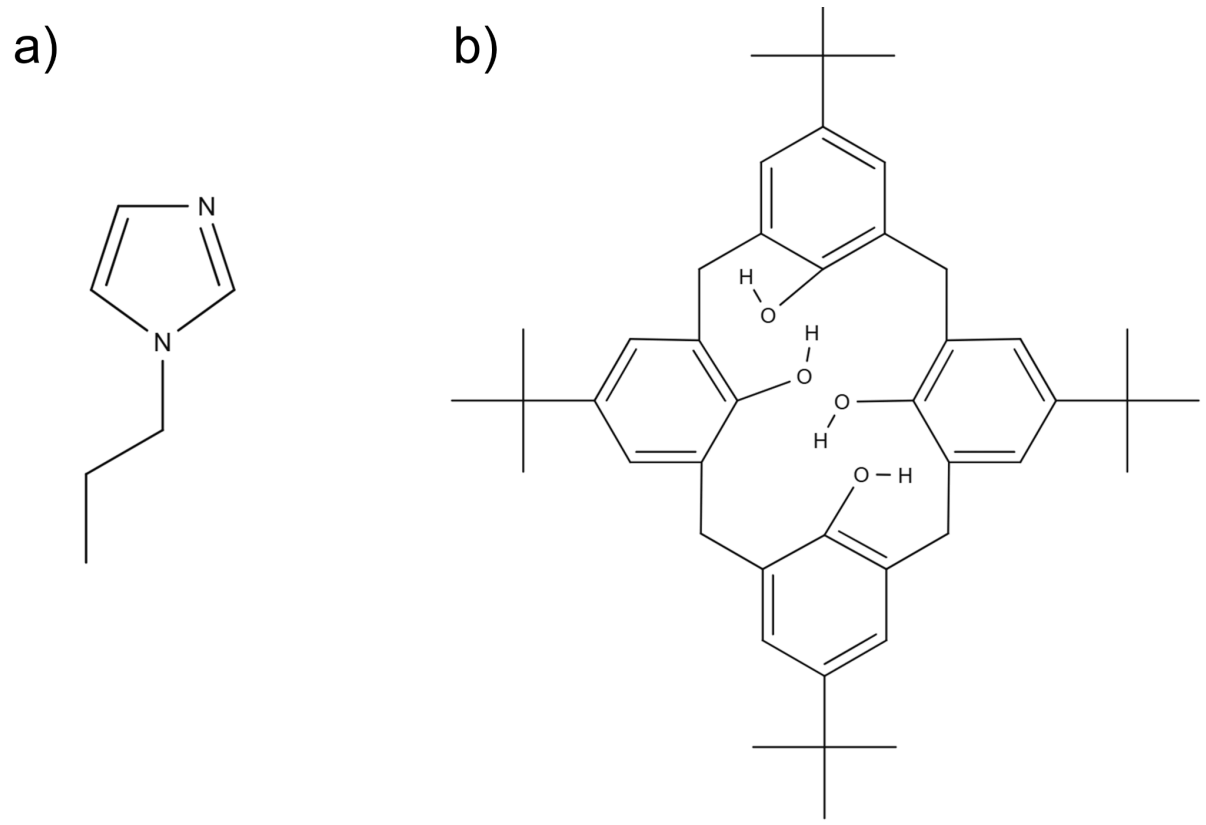

Figure S1: Chemical structures of (a) 1-propyl-1H-imidazole or **Plm** and (b) p-tert-butylcalix[4]arene or **BC**.

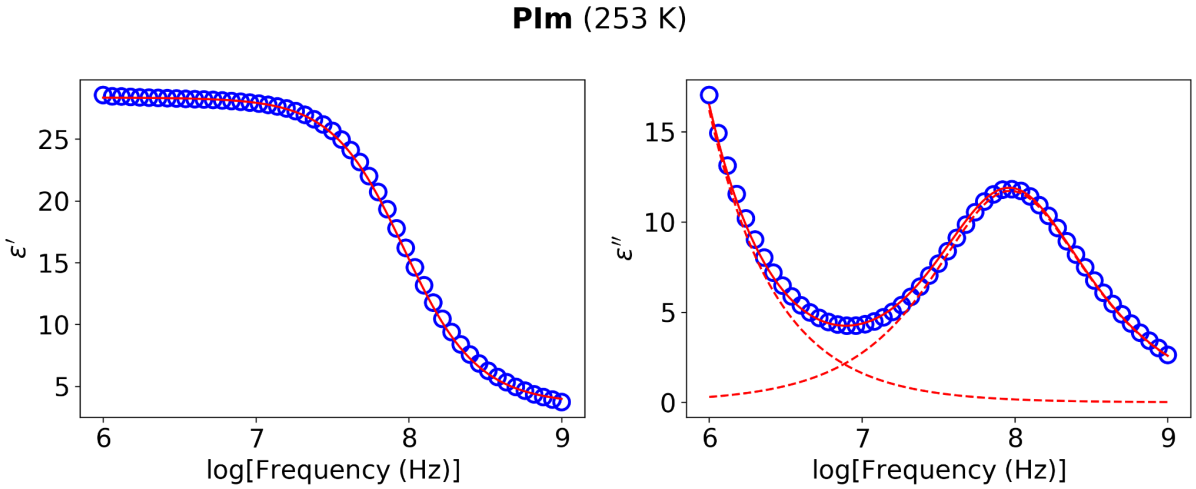

Figure S2: Real and imaginary components of the complex dielectric permittivity of **PIm** at 253 K (blue circles) and corresponding fit (solid red line). The dashed red lines correspond to the different contributions.

PIm	
Parameter	**Value range**
$\Delta\varepsilon$	13–165*
α	0.9–1
β	0.7–1.1

Table S1: Fit parameters for the main mode of **PIm**. The ranges correspond to values obtained at different temperatures. The asterisk indicates that a clear tendency is observed (from high to low temperatures).

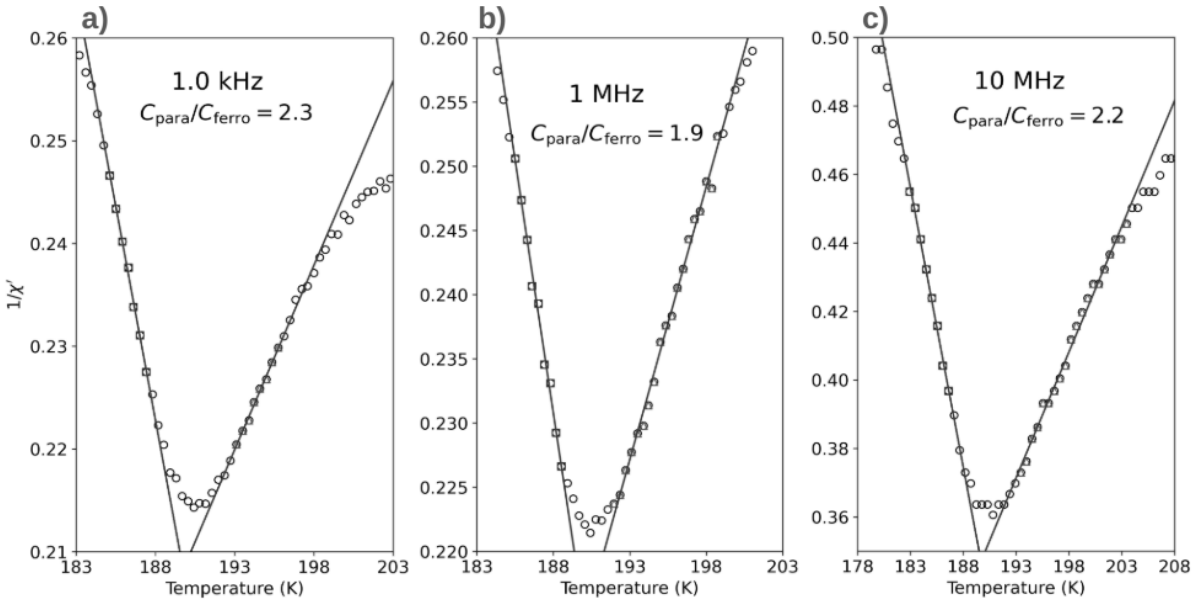

Figure S3: Inverse susceptibility as a function of temperature for a) 1 kHz, b) 1 MHz and c) 10 MHz. The continuous lines indicate Curie-Weiss fits in the ferroelectric $\chi' = C_{ferro}/(T_0 - T)$ and paraelectric phases $\chi' = C_{para}/(T - T'_0)$. The obtained ratio C_{para}/C_{ferro} is also displayed.

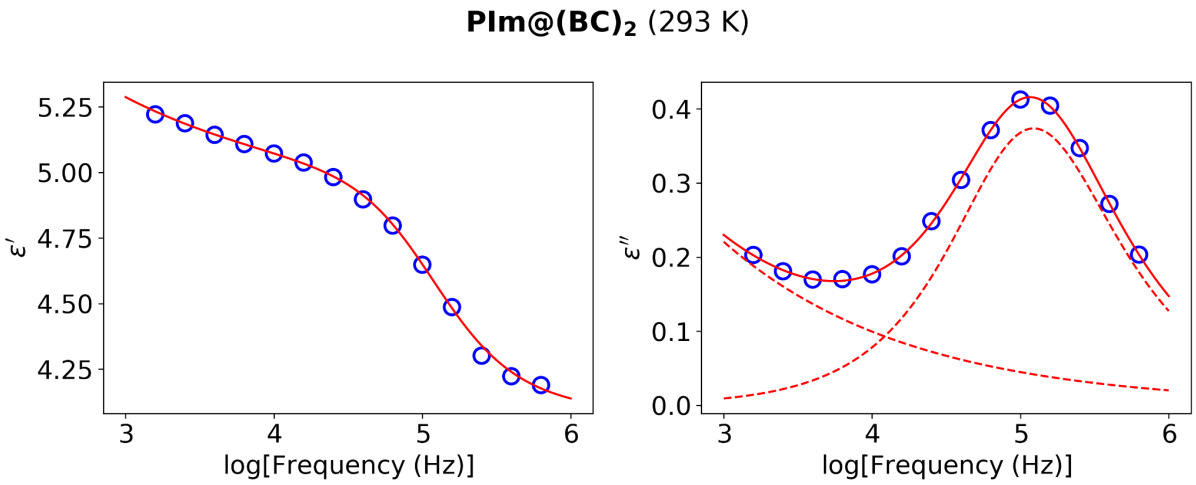

Figure S4: Real and imaginary components of the complex dielectric permittivity of **PIm@(BC)$_2$** at 293 K (blue circles) and corresponding fit (solid red line). The dashed red lines correspond to the different contributions.

PIm@(BC)$_2$	
Parameter	**Value range**
$\Delta\varepsilon_L$	0.8–1
α_L	0.8–1
β_L	0.6–1.1
$\Delta\varepsilon_H$	1–1.7*
α_H	0.7–0.9
β_H	0.2–0.9

Table S2: Fit parameters for the two modes of **PIm@(BC)$_2$**. The ranges correspond to values obtained at different temperatures. The asterisk indicates that a clear tendency is observed (from high to low temperatures).