

Supplementary Information

Anomalies in the Low Frequency Vibrational Density of States for a Polymer with Intrinsic Microporosity – The Boson Peak of PIM-1

Reiner Zorn¹, Huajie Yin², Wiebke Lohstroh³, Wayne Harrison⁴, Peter M. Budd⁴, Brian R.
Pauw², Martin Böhning², Andreas Schönhals^{2,*}

¹Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS,
Forschungszentrum Jülich, 52425 Jülich, Germany

²Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205
Berlin, Germany.

³Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße
1, 85748 Garching, Germany

⁴The University of Manchester, School of Chemistry, Manchester M13 9PL, United Kingdom

Calculation of the neutron cross sections per monomer

Table S1. Calculation of the neutron cross sections per monomer (coherent scattering, incoherent scattering and absorption) for PIM-1. 1 barn = 10^{-24} cm². The first column of each type of cross section contains the tabulated bound cross section for a single nucleus. The second column shows the contribution of all atoms of that type in the monomer. Absorption cross sections are scaled to the wavelength actually used, 5 Å, from the tabulated reference, 1.8 Å.

Atom	Number	σ_{coh} [barn]		σ_{inc} [barn]		σ_{abs} [barn]	
C	29	5.551	160.98	0.001	0.03	0.0035	0.28
H	22	1.7568	38.65	80.26	1765.72	0.3326	20.33
O	4	4.232	16.93	0.0008	0.003	0.00019	0.002
N	2	11.01	22.02	0.50	1.00	1.90	10.56
Monomer			238.58		1766.75		31.17

Table S2. Calculation of the macroscopic neutron cross sections (coherent scattering, incoherent scattering and absorption) for PIM-1.

Mass density [g/cm ³]	1.210
Monomer mass [g/mol]	462.51
Monomer density [nm ⁻³]	1.5755
Σ_{coh} [mm ⁻¹]	0.0376
Σ_{inc} [mm ⁻¹]	0.2783
Σ_{sca} [mm ⁻¹]	0.3159
Σ_{abs} [mm ⁻¹]	0.0049
Σ_{tot} [mm ⁻¹]	0.3208

Table S3. Calculation of the neutron cross sections per monomer (coherent scattering, incoherent scattering and absorption) for Matrimid. 1 barn = 10^{-24} cm². The first column of each type of cross section contains the tabulated bound cross section for a single nucleus. The second column shows the contribution of all atoms of that type in the monomer. Absorption cross sections are scaled to the wavelength actually used, 5 Å, from the tabulated reference, 1.8 Å.

Atom	Number	σ_{coh} [barn]		σ_{inc} [barn]		σ_{abs} [barn]	
C	35	5.551	194.29	0.001	0.04	0.0035	0.34
H	26	1.7568	45.68	80.26	2086.76	0.3326	24.02
O	5	4.232	21.16	0.0008	0.004	0.00019	0.003
N	2	11.01	22.02	0.50	1.00	1.90	10.56
Monomer			238.14		2087.80		34.92

Table S4. Calculation of the macroscopic neutron cross sections (coherent scattering, incoherent scattering and absorption) for Matrimid.

Mass density [g/cm ³]	1.240
Monomer mass [g/mol]	554.61
Monomer density [nm ⁻³]	1.3464
Σ_{coh} [mm ⁻¹]	0.0381
Σ_{inc} [mm ⁻¹]	0.2811
Σ_{sca} [mm ⁻¹]	0.3192
Σ_{abs} [mm ⁻¹]	0.0047
Σ_{tot} [mm ⁻¹]	0.3239

Photograph of a cast PIM-1 film

Figure S1. Photograph of a cast PIM-1 film (approx. 70mm diameter, 200 μm thickness)



The color of a cast PIM-1 film is yellowish and not completely transparent. Furthermore the yellow color indicates that PIM-1 absorbs in the blue wave length range of the light spectrum. These properties of PIM-1 prevent Brillouin scattering experiments to measure the transverse sound velocity. Such measurements require a fully transparent sample with no absorption or fluorescence.