Sample Name: Deuterated Poly(ethylene-d4)

<u>Sample #:</u> **P42252A-dPE**

Structure:



Composition:

$M_n imes 10^3 \ (g/mol)$	M_w/M_n
48.0	1.01

Thermal properties:

Melting point, T _m	Crystallization point, T _{cr}
102 °C	86 °C

Synthesis procedure:

The polyethylene- d_4 was obtained by deuteration of poly(1,4-butadiene- d_6), which was synthesized by living anionic polymerization of butadiene- d_6 in non-polar solvent.

Characterization:

Deuterium NMR spectroscopy was used to confirm the structure of polybutadiene-d₆ rich in 1,4-addition.

The complete deuteration of the product was confirmed by FT-IR spectroscopy analysis by disappearance of alkene double bond (C=C at 971 cm⁻¹).

The molecular weight and polydispersity index were obtained by size exclusion chromatography (SEC) of poly(1,4-butadiene-d₆) precursor using THF as an eluent; and the molecular weight of polyethylene-d₄ was calculated accordingly.

Thermal analysis was performed on TA Instruments Q100 differential scanning calorimeter (DSC) under a nitrogen atmosphere at a scan rate 10 °C/min.

Solubility:

Polyethylene-d₄ is soluble in hot toluene and xylene. The obtained solution has light ivory color; this coloration is due to the presence of trace amount (we expect <5-6 ppm) of the Wilkinson catalyst used in synthesis (and which is hard to remove from the final product).

H NMR spectrum of dPBd precursor:



80 85 80 75 70 85 60 55 50 <u>45</u> 40 35 30 25 20 15 10 65 00



<figure>

FT-IR spectra of dPE (top) and dPBd (bottom):



DSC thermogram:

heating (bottom) and cooling (top) scans at 10 °C/min.

