Sample Name: Deuterated Polyethylene-d4

Sample #: **P42213-dPE** 

#### **Structure:**

#### **Composition:**

$M_n \times 10^3 \ (g/mol)$	$M_{\rm w}/M_{\rm n}$
57.0	1.02

## Thermal properties:

Melting point, T <sub>m</sub>	Crystallization point, $T_{cr}$
102 °C	86 °C

#### **Synthesis procedure:**

The polyethylene-d<sub>4</sub> was obtained by deuteration of poly(1,4-butadiene-d<sub>6</sub>), which was synthesized by living anionic polymerization of butadiene-d<sub>6</sub> in non-polar solvent.

#### **Characterization:**

Deuterium NMR spectroscopy was used to confirm the structure of polybutadiene-d<sub>6</sub> 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<sup>-1</sup>).

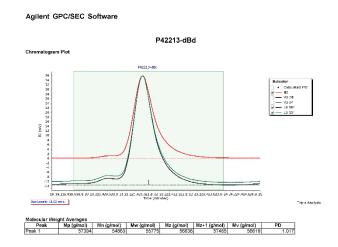
The molecular weight and polydispersity index were obtained by size exclusion chromatography (SEC) of poly(1,4-butadiene-d<sub>6</sub>) precursor using THF as an eluent; and the molecular weight of polyethylene-d<sub>4</sub> was calculated accordingly.

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

#### **Solubility:**

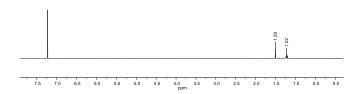
Polyethylene- $d_4$  is soluble in hot toluene and xylene. The obtained solution has light ivory color; this coloration is due to the presence of trace amount (we expect <5–6 ppm) of the Wilkinson catalyst used in synthesis (which is hard to remove from the final product).

## SEC chromatogram of dPBd precursor:

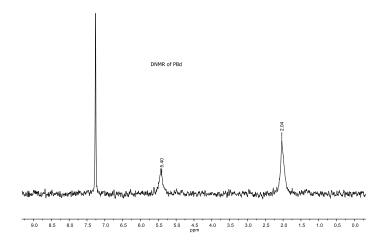


# **H NMR spectrum of dPBd precursor:**

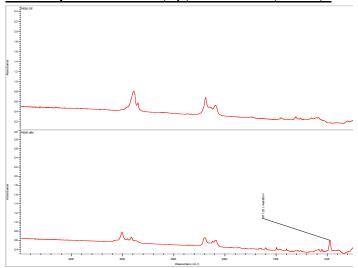
dBd HNMR spectrum



# **D NMR spectrum of PBd precursor:**



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



# DSC thermogram:

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

