Sample Name: Deuterated Polyethylene-d4

Sample #: **P41798A-dPE**

Structure:

$$\begin{array}{c} D_2 \\ C \\ D_2 \end{array}$$

Composition:

$M_n \times 10^3 \ (g/mol)$	$M_{\rm w}/M_{\rm n}$
63.0	1.04

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. The scheme of reaction is presented below:

n CD₂=CDCD=CD₂
$$\xrightarrow{\text{sec-BuLi}}$$
 CD_2 CD=CDCD₂ $\xrightarrow{\text{In CHx}}$ CD_2 CD=CDCD₂ $\xrightarrow{\text{In CHx}}$

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).

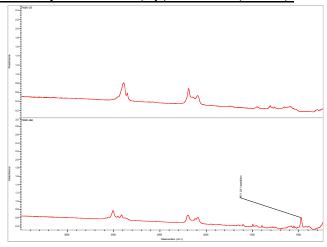
The molecular weight and polydispersity index were obtained by size exclusion chromatography (SEC) of poly(1,4-butadiene- d_6) precursor using THF as an eluent; and the molecular weight of polyethylene- d_4 was calculated accordingly.

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

Solubility:

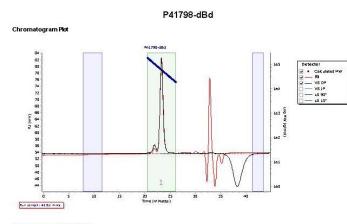
Polyethylene- d_4 is soluble in hot toluene and xylene. The obtained solution has light ivory color; this coloration is due to the presence of trace amount (we expect <5–6 ppm) of the Wilkinson catalyst used in synthesis (and which is hard to remove from the final product).

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



SEC chromatogram of dPBd precursor:

Agilent GPC/SEC Software



Peak	Mp (gimol)	Mn (gmol)	Mw (gmol)	Mz (gimol)	Mz+1 (g/mol)	Mv (g/mol)	PD
Peak 1	61831	60710	63674	67511	73211	66069	1.049

DSC thermogram:

heating (bottom) and cooling (top) scans at 10 °C/min. Sample: P41798-A_dPE (Polyethylene-d4) File: P41798A-dPE.001

2.5 85.88°C 2.0 1.5 1.0 0.5 0.0 -0.5 93.83°C 80.59J/g -1.5 -2.0 100 80 110 120 130 Temperature (°C)