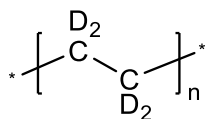


Sample Name: Deuterated Polyethylene-d₄

Sample #: P40244-dPE

Structure:



Composition:

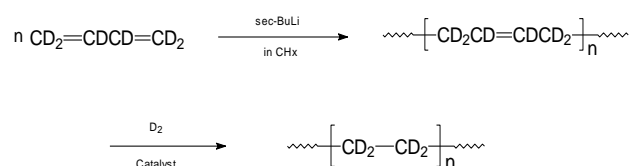
$M_n \times 10^3$ (g/mol)	M_w/M_n
175.0	1.34

Thermal properties:

Melting point, T_m	Crystallization point, T_{cr}
101 °C	87 °C

Synthesis procedure:

The polyethylene-d₄ was obtained by deuteration of poly(1,4-butadiene-d₆), which was synthesized by living anionic polymerization of butadiene-d₆ in non-polar solvent. The scheme of reaction is presented below:



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).

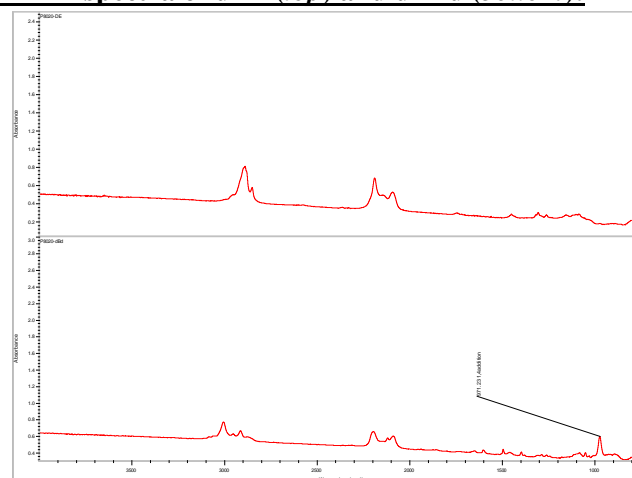
The molecular weight and polydispersity index were obtained by size exclusion chromatography (SEC) of poly(1,4-butadiene-d₆) precursor using THF as an eluent; and the molecular weight of polyethylene-d₄ was calculated accordingly.

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).

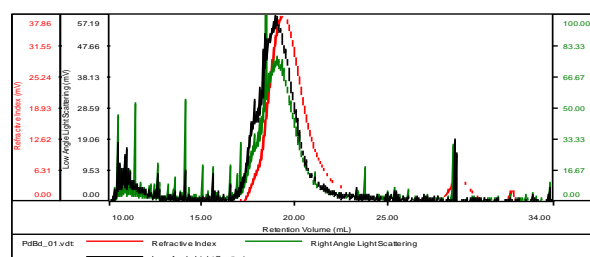
FT-IR spectra of dPE (top) and dPBd (bottom):



SEC chromatogram of dPBd precursor:

P5912A-dBd

Concentration (mg/mL)	1.7790
Sample dn/dc (mL/g)	0.1270
Method File	PS80K-Nov2016-6-0000.vcm
Column Set	3x PL 1113-6300
Solvent	THF



Sample	Mn (Da)	Mw (Da)	Mw/Mn	IV (dL/g)	Mp (Da)
PdBd_01.vdt	167,765	225,355	1.343	3.1278	205,110

DSC thermograms of the dPE product:

1st cooling (upper) and 2nd heating (lower) scans, both performed at a rate 10 °C/min.:

Sample: P40244_dPE (d4; Mn=175k)
Size: 9.7000 mg

File: P40244_dPE.002

