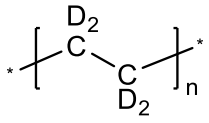
Sample Name: **Deuterated Polyethylene-d_4**

Sample #: **P40901-dPE**

Structure:



Composition:

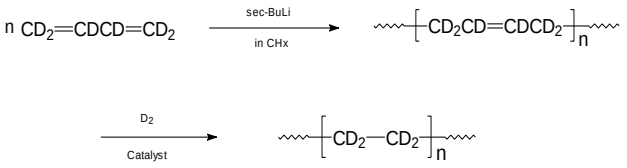
$M_n \times 10^3$ (g/mol)	M_w/M_n
88.0	1.04

Thermal properties:

Melting point, T_m	Crystallization point, T_{cr}
92 °C	81 °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:



Characterization:

Deuterium NMR spectroscopy was used to confirm the structure of polybutadiene-d_6 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}).

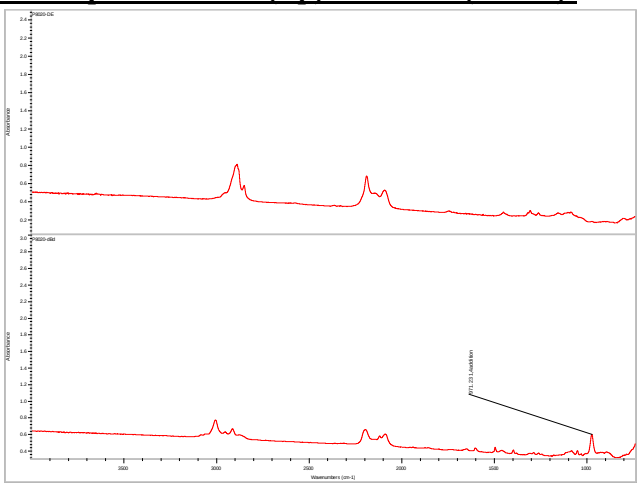
The molecular weight and polydispersity index were obtained by size exclusion chromatography (SEC) of poly(1,4-butadiene-d_6) precursor using THF as an eluent; and the molecular weight of polyethylene-d_4 was calculated accordingly.

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).

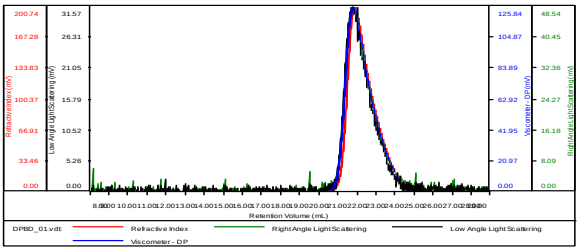
FT-IR spectra of dPE (*top*) and dPBd (*bottom*):



SEC chromatogram of dPBd precursor:

P40901-dBD

Concentration (mg/mL)	5.0000
Sample dn/dc (mL/g)	0.1250
Method File	PS80K_2017-12-21_new-0000.vcm
Column Set	3x PL 1113-6300
Solvent	THF



Sample	Mn (Da)	Mw (Da)	Mw/Mn	IV (dL/g)	Mp (Da)
DPBD_01.vdt	85,008	88,782	1.044	1.1083	84,913

DSC thermograms of the dPE product:

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