

Supporting Information for

**PEG-Imidazolium-Functionalized 6FDA-Durene Polyimide
as a Novel Polymeric Membrane for Enhanced CO₂
Separation**

Irshad Kammakakam,^a SangYong Nam,^b and Tae-Hyun Kim^{*a}

^a*Organic Material Synthesis Lab. Department of Chemistry, Incheon National University, 119 Academy-ro, Songdo-dong, Yeonsu-gu, Incheon 406-772, Korea. Fax: +82-32-835-0762; E-mail: tkim@incheon.ac.kr*^{*}

^b*Department of Materials Engineering and Convergence Technology, Engineering Research Institute, Gyeongsang National University, Jinju 660-701, Korea.*

Synthesis of PEG-imidazoles having various PEG chains

All the PEG-imidazoles were synthesized by reacting imidazole with corresponding (ethylene glycol) monomethyl ether, for example monomethyl di(ethylene glycol) imidazole (**C₂PEG-Im**) was synthesized as:

In a two-necked round bottom flask equipped with a stirrer bar and condenser, di(ethylene glycol) monomethyl ether (5 g, 41.6 mmol) was dissolved in toluene (25 mL). A solution of 2.5 equiv. of sodium hydroxide in the same amount of distilled water was added portionwise to this solution, followed by addition of a catalytic amount of PTC, and the reaction mixture was allowed to stir for 30 min at room temperature. Benzene sulfonyl chloride (5.9 mL, 45.78 mmol) was then added dropwise and the solution was further stirred for 3 h at 70 °C. After this time, the reaction mixture was filtered off and filtrate was evaporated and extracted with water and DCM. The organic layer was dried over anhydrous MgSO₄, and the solvent was evaporated under reduced pressure to give the monomethyl di(ethylene glycol)-benzenesulfonate with the yield of 8.3 g (76.8%).

Imidazole (2.17 g, 31.89 mmol) was dissolved in toluene (20 mL) into a 250 mL two-necked flask equipped with a magnetic stirrer. A solution of 2.5 equiv. of sodium hydroxide in the same amount of distilled water was added portionwise to this solution, followed by the addition of a catalytic amount of PTC, and the reaction mixture was allowed to stir for 30 min at room temperature. Monomethyl di(ethylene glycol)-benzenesulfonate (8.3 g, 31.89 mmol) was then added dropwise and the solution was further stirred for 3 h at 70 °C. After this time, the reaction mixture was filtered off and filtrate was evaporated and extracted with water and DCM. The organic layer was dried over anhydrous MgSO₄, and the solvent was evaporated under reduced pressure to give the product (**C₂PEG-Im**) as pale yellow oil (4.1 g, 75.6%);

δ_H (400 MHz, $CDCl_3$) 7.47 (1 H, s, ArH), 6.95 (1H, s, ArH), 6.91 (1H, s, ArH), 4.05-4.02 (2H, t, $J = 5.1$, NCH_2), 3.66-3.64 (2H, t, $J = 5.3$, NCH_2CH_2O), 3.50-3.47 (2H, br signal, $NCH_2CH_2OCH_2$), 3.44-3.41 (2H, br signal, $NCH_2CH_2OCH_2CH_2O$) and 3.28 (3H, s, $N(CH_2CH_2O)_2CH_3$).

C₄PEG-Im; δ_H (400 MHz, $CDCl_3$) 7.54 (1 H, s, ArH), 7.04 (1H, s, ArH), 7.0 (1H, s, ArH), 4.12-4.10 (2H, t, $J = 5.1$, NCH_2), 3.76-3.73 (2H, t, $J = 5.3$, NCH_2CH_2O), 3.67-3.54 (12H, br signal, $NCH_2CH_2O(CH_2CH_2O)_3$) and 3.38 (3H, s, $N(CH_2CH_2O)_4CH_3$).

C₈PEG-Im; δ_H (400 MHz, $CDCl_3$) 7.45 (1 H, s, ArH), 6.94 (1H, s, ArH), 6.92 (1H, s, ArH), 4.04-4.01 (2H, t, $J = 5.1$, NCH_2), 3.67-3.64 (2H, t, $J = 5.3$, NCH_2CH_2O), 3.57-3.45 (28H, br signal, $NCH_2CH_2O(CH_2CH_2O)_7$) and 3.29 (3H, s, $N(CH_2CH_2O)_8CH_3$).

C₁₂PEG-Im; δ_H (400 MHz, $CDCl_3$) 7.43 (1 H, s, ArH), 6.94-6.87 (2H, broad signal, ArH), 4.01-3.98 (2H, t, $J = 5.1$, NCH_2), 3.67-3.62 (2H, t, $J = 5.3$, NCH_2CH_2O), 3.53-3.41 (44H, br signal, $NCH_2CH_2O(CH_2CH_2O)_{11}$) and 3.02 (3H, s, $N(CH_2CH_2O)_{12}CH_3$).

Figure S1. Monomethyl di(ethylene glycol) imidazole, δ_H (400 MHz, $CDCl_3$)

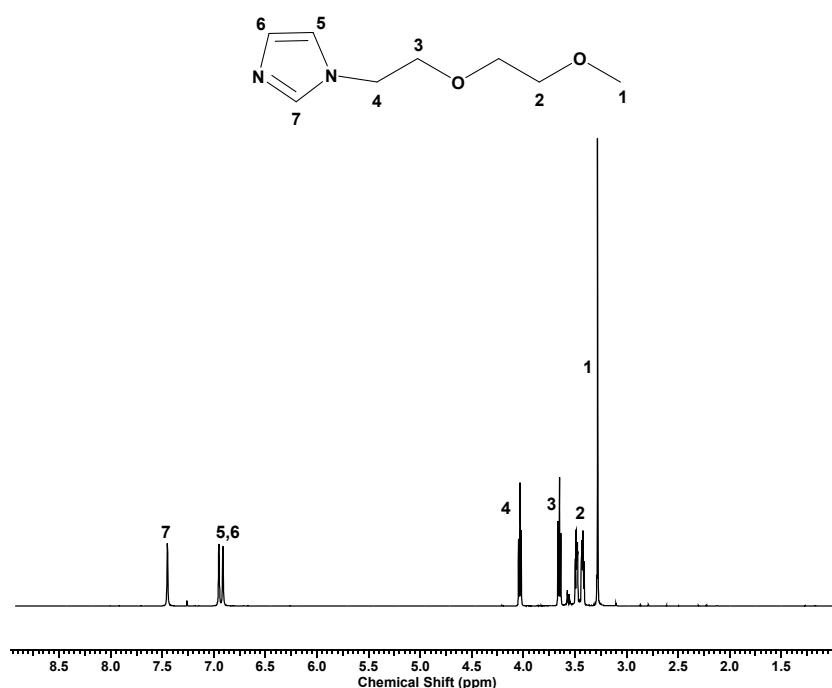


Figure S2. Monomethyl tetra(ethylene glycol) imidazole, δ_{H} (400 MHz, CDCl_3)

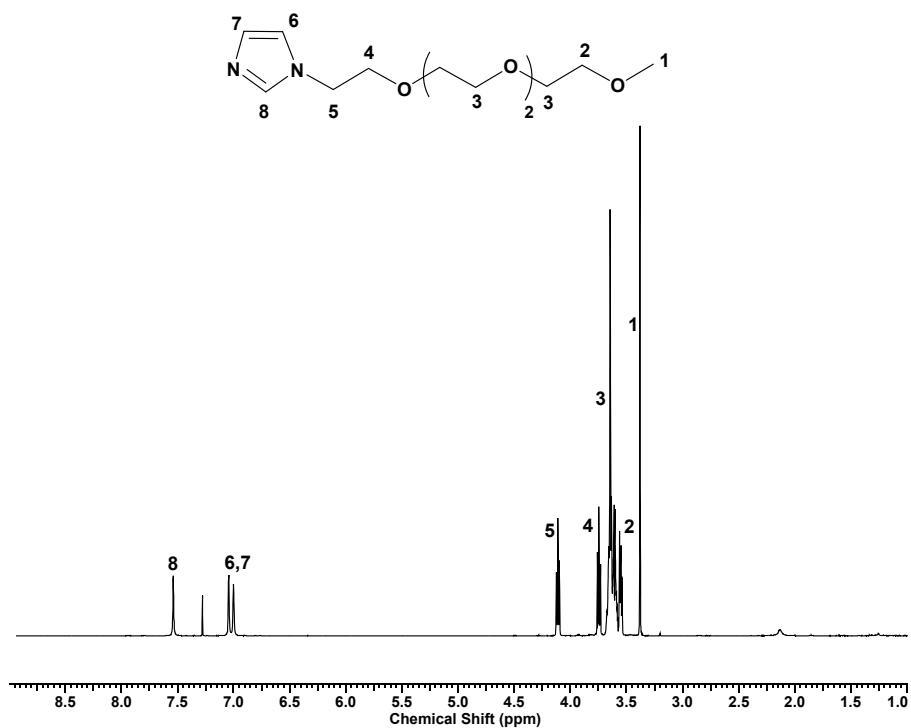


Figure S3. Poly(ethylene glycol) imidazole ($M_n \sim 350$), δ_{H} (400 MHz, CDCl_3)

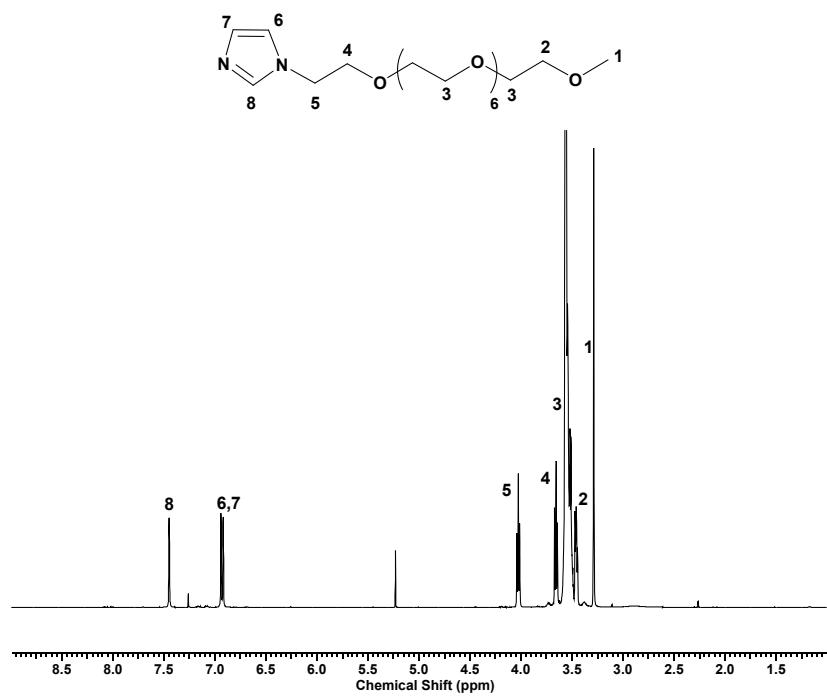


Figure S4. Poly(ethylene glycol) imidazole ($M_n \sim 550$), δ_H (400 MHz, $CDCl_3$)

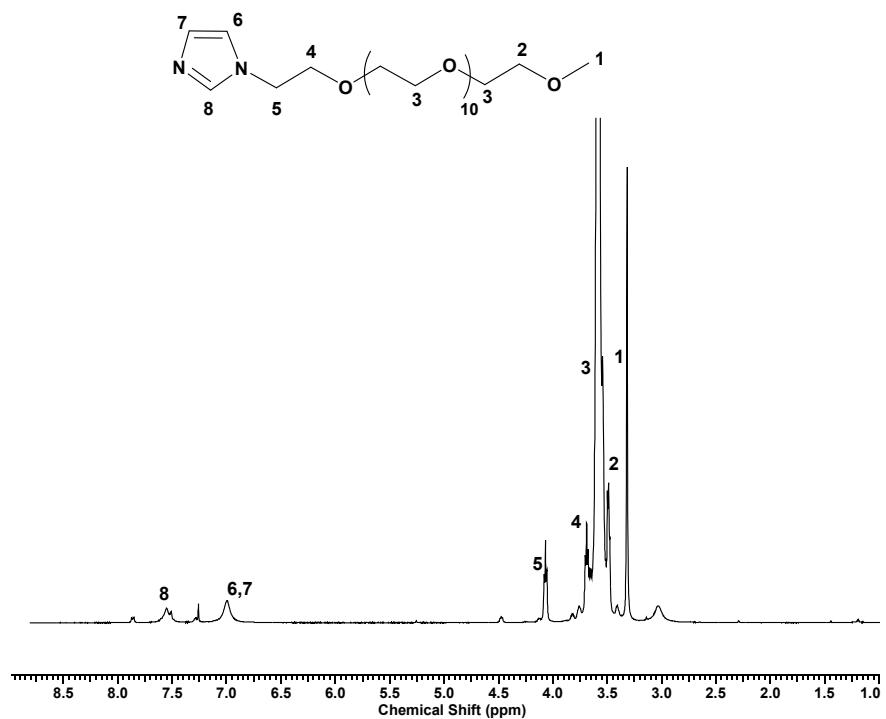


Figure S5. ^1H NMR spectra of 6FDA-Durene PI **2** (a) and brominated PI **3** (b).

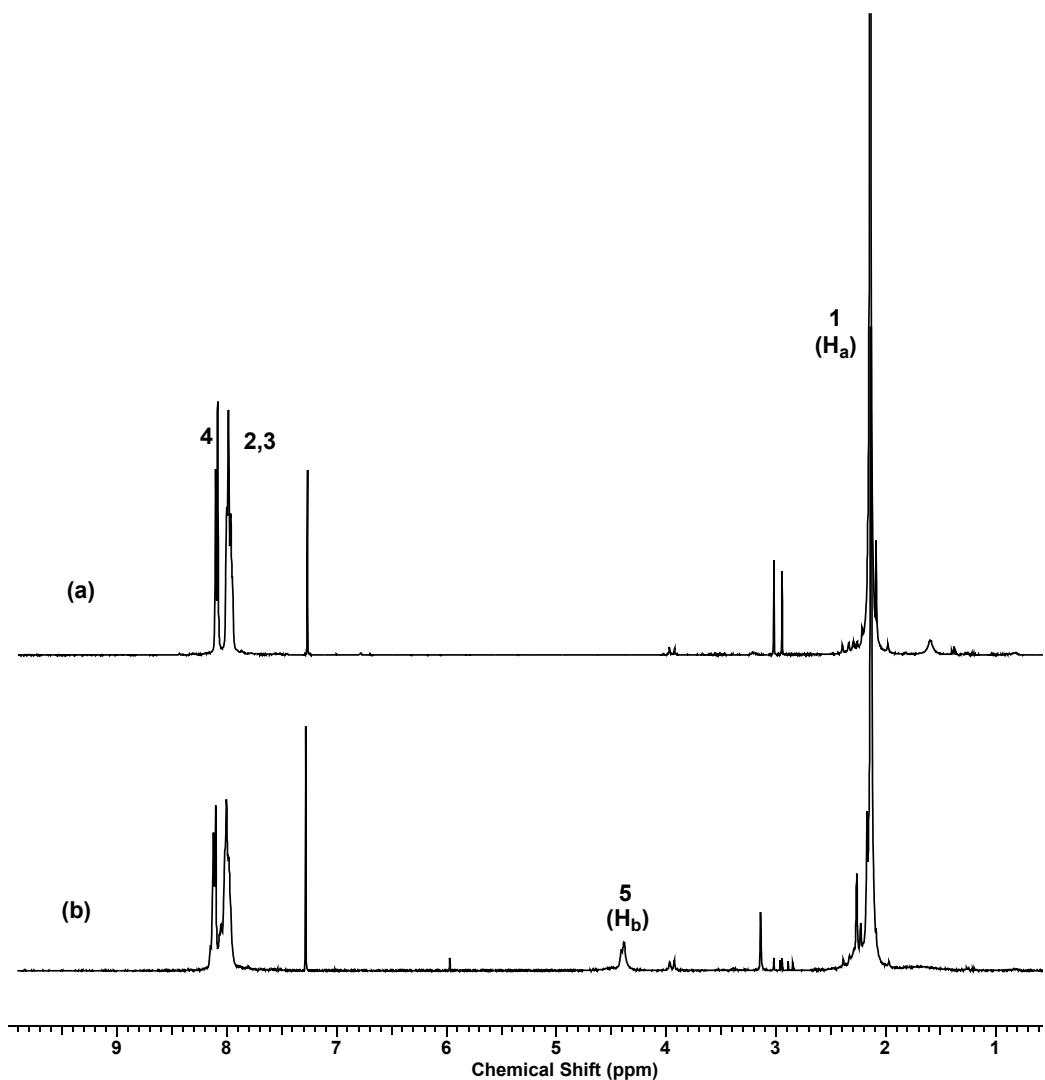


Figure S6. FT-IR spectra (4000-600 cm⁻¹) of the PEG-Im-PI and 6FDA-durene PI polymers.

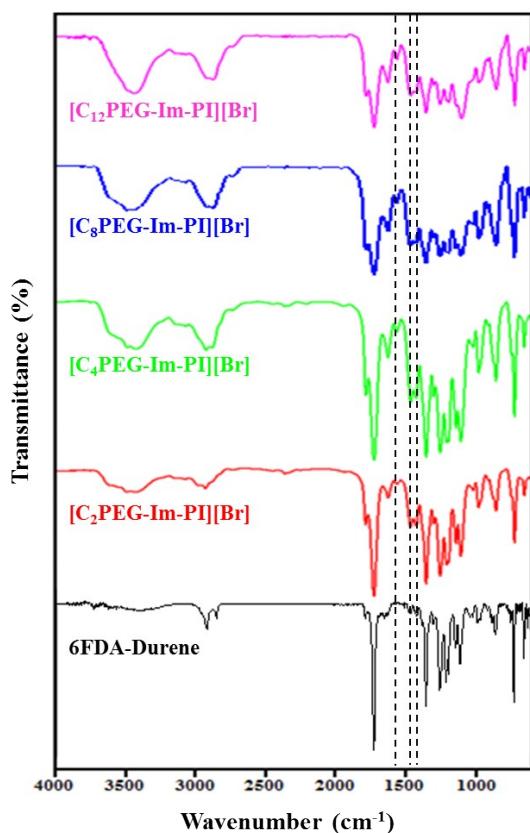


Figure S7. Stress-strain behavior of the Pristine and PEG-Im-PI membranes

