Supporting Information

Dimensionally stable hexamethylenetetramine functionalized polysulfone anion exchange membranes

Wanting Chen,[a] Mengmeng Hu,[a] Haochen Wang,[b] Xuemei Wu,[a, *] Xue Gong,[a] Xiaoming Yan, [a, c] Dongxing Zhen,[a] Gaohong He[a, c, *]

[a] State Key Laboratory of Fine Chemicals, Research and Development Center of Membrane Science and Technology, School of Chemical Engineering, Dalian University of Technology, Dalian, 116024, China

[b] State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, 116023, China

[c] School of Petroleum and Chemical Engineering, Dalian University of Technology, Panjin, 124221, China

*E-mail: xuemeiw@dlut.edu.cn; hgaohong@dlut.edu.cn.

Table of Contents

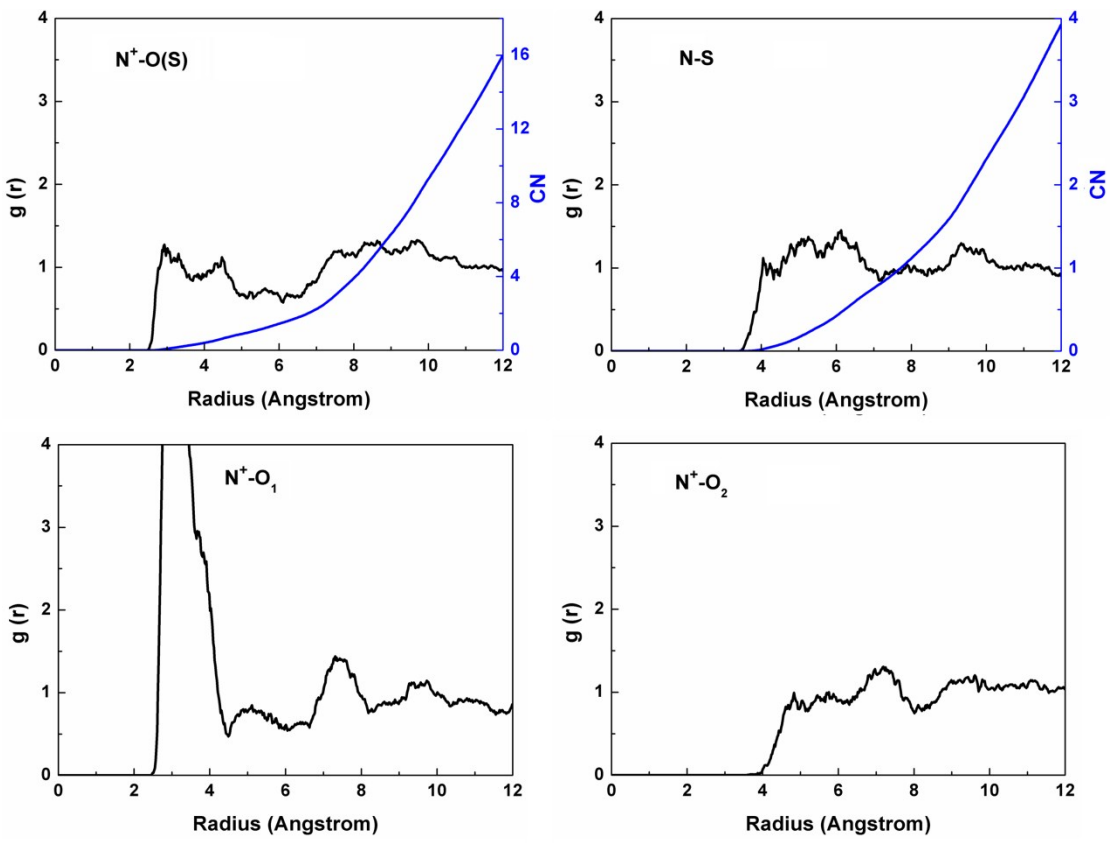

Fig. S1. RDFs and CNs of different atoms in the dry PSF-ImOH membrane.

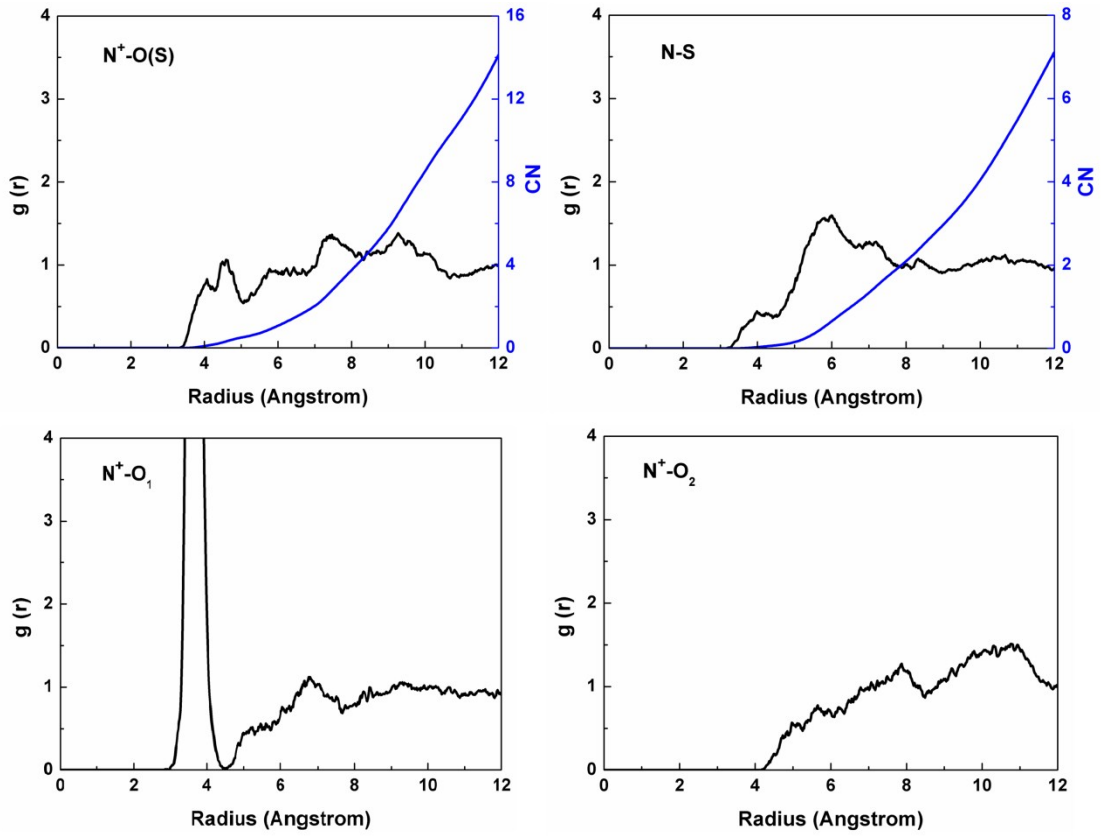

Fig. S2. RDFs and CNs of different atoms in the dry PSF-QuOH membrane.

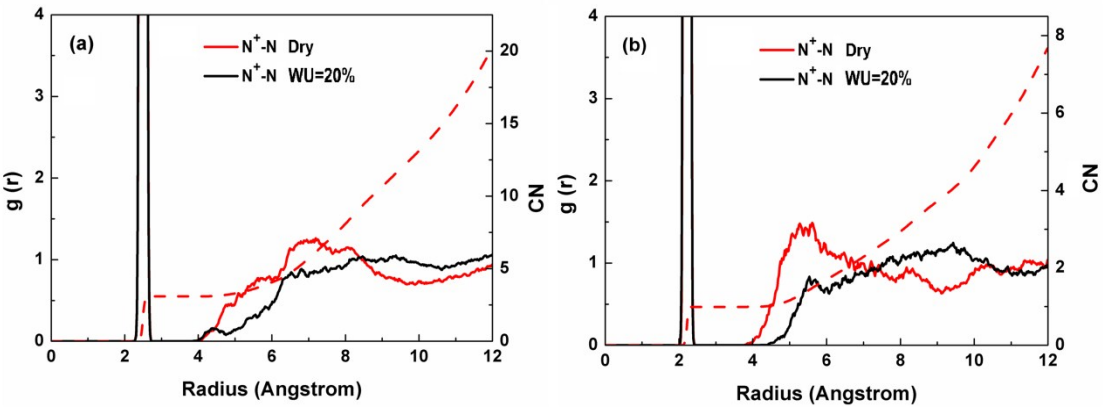

Fig. S3. RDFs (solid lines) and CNs (dashed lines) of N^+-N in the dry and hydrated (a) PSF-QuOH and (b) PSF-ImOH membranes. (WU: water uptake)

Table S1 Coordination Numbers of different atoms.

AEMs	N^+-O_1		N^+-O_2		N^+-O(S)		N-S		N^+-N	
	r^a (Å)	CN(O_1)	r^a (Å)	CN(O_2)	r^a (Å)	CN(O(S))	r^a (Å)	CN(S)	r^a (Å)	CN(N)
PSF-ImOH	-[b]	0	-[b]	0	4.9	0.8	7.1	0.8	9.0	2.7[c]
PSF-QuOH	-[b]	0	-[b]	0	5.0	0.5	7.9	2.0	9.6	9.1[d]

[a] Upper boundary for integration of the first shell.

[b]The first peaks of the RDFs (except for the first strong peaks (<4 Å)) are very weak. This indicates the atoms are uniform distribution in the AEMs and the corresponding CNs are close to zero.

[c, d]CN(N)=CN(total)-CN(one repeat unit), CN(total) is the integration of the RDFs; CN(one repeat unit) is the numbers of N atoms around N^+ ion in one repeat unit, and equal to 1 for PSF-ImOH and 3 for PSF-QuOH, respectively.

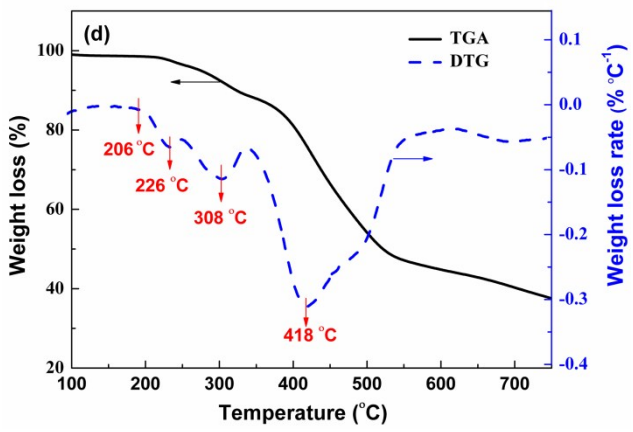

Fig. S4. TGA and DTG curves of the PSF-QuOH 1.67 membrane.

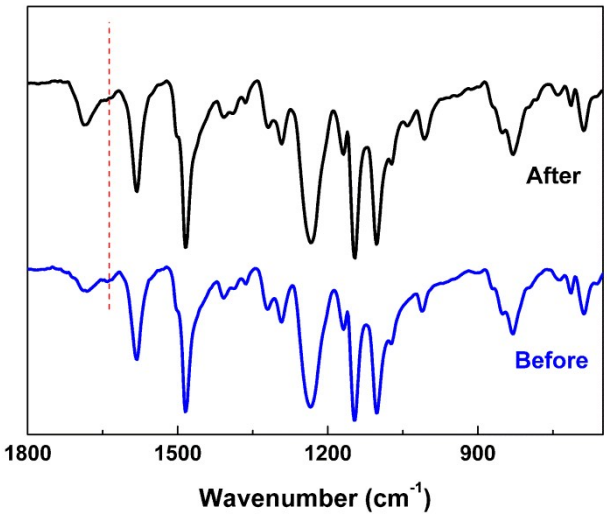

Fig. S5. FTIR of the PSF-QuOH 1.94 membrane before and after 1 M KOH immersion at 60 °C for 168 h.

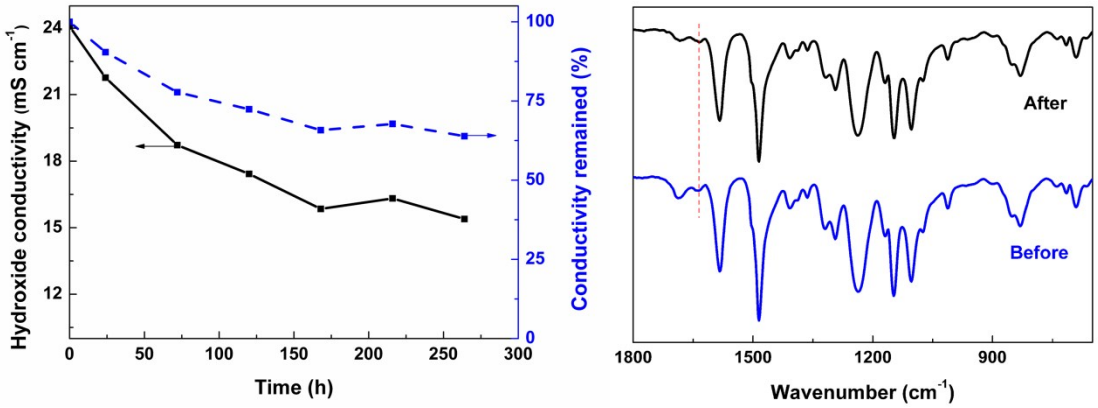

Fig. S6. Alkaline stability of the PSF-QuOH 1.39 after 4 M NaOH immersion at 80 °C for 264 h.

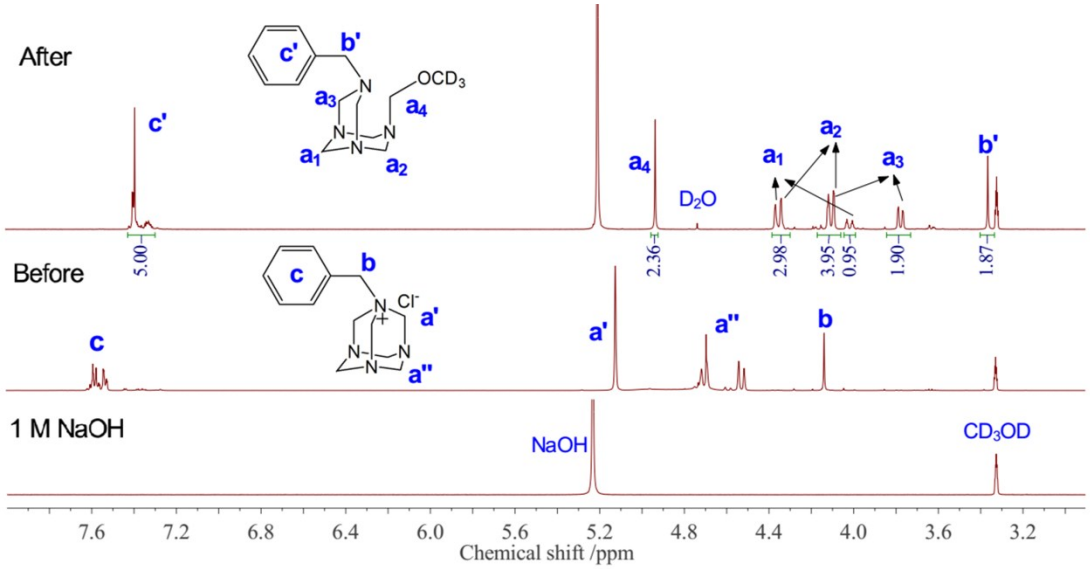

Fig. S7. ^{1}H NMR spectra of BHMTA degradation in 1 M NaOH CD_3OD/D_2O (3:1).

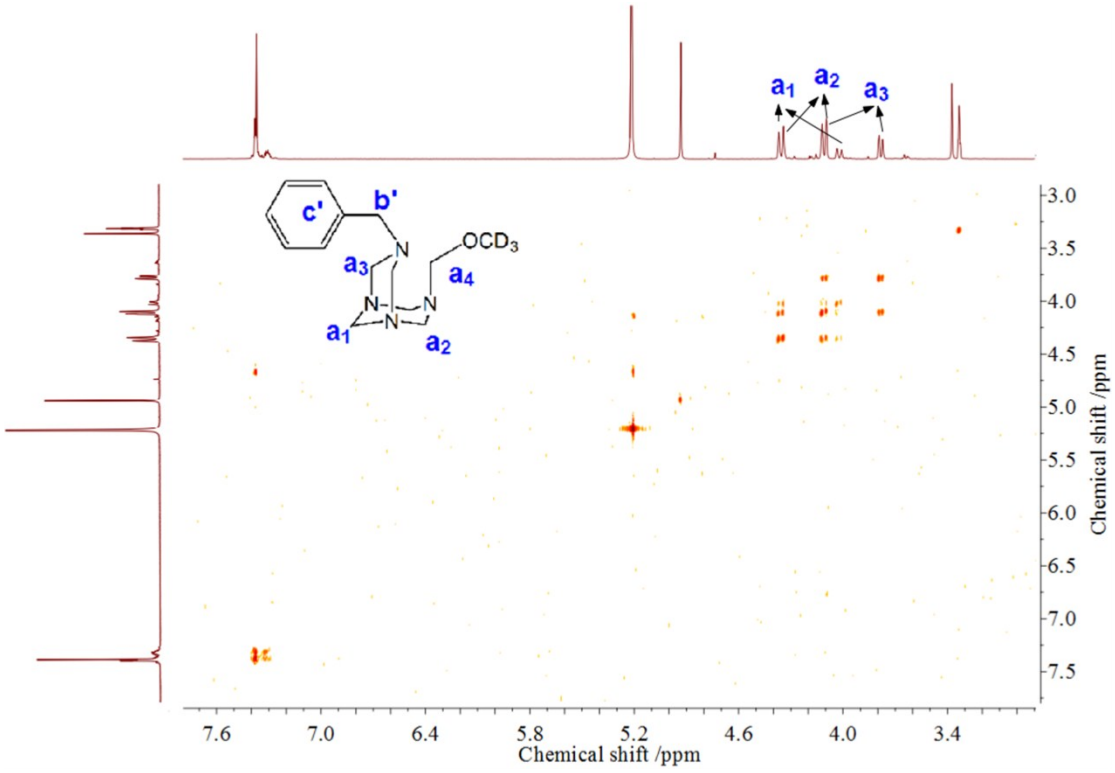

Fig. S8. Chemical shift correlated spectroscopy (COSY) of BHMTA degradation products