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Structural and Conformational Properties of Polybenzimidazoles in Melt and Phosphoric Acid Solution: A Polyelectrolyte Membrane for Fuel cell

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Table SI1. Dihedral parameter values for PBI and ABPBI

Dihedral	C_0 (kJ/mol)	C_1 (kJ/mol)	C_2 (kJ/mol)	C_3 (kJ/mol)	C_4 (kJ/mol)	C_5 (kJ/mol)
C-C-C-N (PBI)	23.6855	1.5774	-40.0972	-1.2647	17.7090	0.9971
C-C-C-C (PBI)	9.1038	-0.1848	-35.7188	-1.8278	35.7281	1.8779
C-C-C-N (ABPBI)	19.3584	2.6036	-38.1289	-0.6441	17.6170	0.6493

Table SI2. Bonded force field parameters for PBI

Bond description	b_0 (nm)	K_b (kJ/mol/nm^2)
$C_{benzene}$-$C_{benzene}$	0.140	392459.2
$C_{benzene}$-$N_{attached\ with\ hydrogen}$	0.138	357313.6
$C_{benzene}$-$N_{without\ hydrogen}$	0.139	346435.2
$C_{benzene}$-$H_{benzene}$	0.108	307105.6
$N_{attached\ with\ hydrogen}$-H	0.101	363171.2
$C_{benzimidazole}$-$H_{terminal}$	0.108	307105.6
$C_{benzimidazole}$-$N_{attached\ with\ hydrogen}$	0.134	399153.6
$C_{benzimidazole}$-$N_{without\ hydrogen}$	0.133	408358.4
$C_{benzimidazole}$-$C_{benzene}$	0.140	392459.2

Angle description	**θ_0 (nm)**	**K_θ (kJ/mol/rad^2)**
$C_{benzene}$-$C_{benzene}$-$C_{benzene}$	120.00	527.184
$C_{benzene}$-$C_{benzene}$-$C_{benzimidazole}$	120.00	527.184
$C_{benzene}$-$C_{benzene}$-$N_{attached\ with\ hydrogen}$	108.70	585.760
$C_{benzene}$-$Cbenzene$-$N_{without\ hydrogen}$	108.70	585.760
$Cbenzene$-$N_{attached\ with\ hydrogen}$-$C_{benzimidazole}$	109.80	585.760
$C_{benzene}$-$N_{without\ hydrogen}$-$C_{benzimidazole}$	109.80	585.760
$N_{attached\ with\ hydrogen}$-$C_{benzimidazole}$-$N_{without\ hydrogen}$	120.00	585.760
$C_{benzene}$-$C_{benzene}$-$H_{benzene}$	120.00	292.880
$C_{benzene}$-$N_{attached\ with\ hydrogen}$-$H_{attached\ with\ nitrogen}$	118.00	292.880
$C_{benzimidazole}$-$N_{attached\ with\ hydrogen}$-$H_{attached\ with\ nitrogen}$	120.00	292.880
$N_{attached\ with\ hydrogen}$-$C_{benzimidazole}$-$H_{terminal}$	120.00	292.880
$N_{without\ hydrogen}$-$C_{benzimidazole}$-$H_{terminal}$	120.00	292.880

Table SI3: Charges for the atoms of PBI. See Figure SI2 for atom numbers.

Atom number	Atom name	Charge	Atom number	Atom name	Charge
1	H	0.00	20	C	-0.04
2	C	0.35	21	H	0.20
3	N	-0.49	22	C	-0.17
4	C	-0.09	23	H	0.20
5	C	0.40	24	N	-0.51
6	N	-0.95	25	C	0.46
7	H	0.40	26	N	-1.03
8	C	-0.04	27	H	0.40
9	H	0.20	28	C	0.08
10	C	-0.04	29	C	-0.11
11	C	-0.17	30	H	0.17
12	H	0.20	31	C	-0.17
13	C	-0.02	32	H	0.17
14	H	0.18	33	C	-0.12
15	C	-0.04	34	C	-0.16
16	C	-0.04	35	H	0.18
17	H	0.19	36	C	-0.10
18	C	0.39	37	H	0.21
19	C	-0.09	38	H	0.00

Table SI4: Charges for the atoms of ABPBI. See Figure SI3 for atom numbers.

Atom number	Atom name	Charge	Atom number	Atom name	Charge
1	H	0.00	9	C	-0.27
2	C	-0.15	10	H	0.16
3	C	-0.05	11	N	-0.77
4	H	0.11	12	C	0.72
5	C	-0.33	13	N	-0.74
6	H	0.18	14	H	0.43
7	C	0.30	15	H	0.00
8	C	0.41			

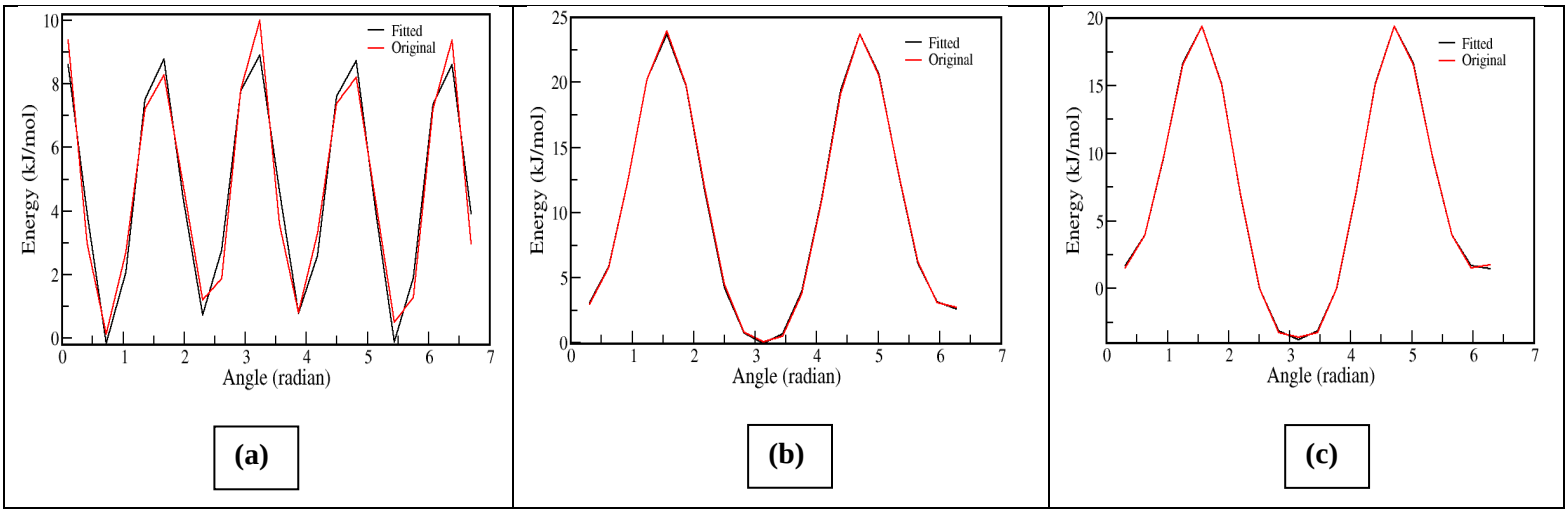

Figure SI1. Fitting of dihedral potential energy of a) C_b-C_b-C_b-C_b b) C_b-C_b-C_{im}-N_{im} dihedral for PBI and c) C_b-C_b-C_{im}-N_{im} for ABPBI

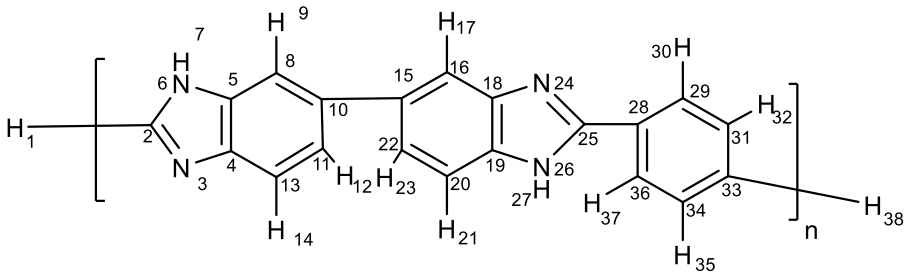

Figure SI2. Chemical structure of PBI

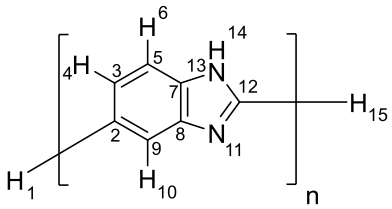

Figure SI3. Chemical structure of ABPBI