Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

for

Molecular Dynamics Simulation Elucidates the Preferential Binding Affinity of Sodium and Tetramethylammonium Ions for Tetrameric Nafion Unit under Aqueous Conditions

Soumadwip Ghosh, Rajarshi Chakrabarti*

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai – 400076, India.

AUTHOR INFORMATION

*Corresponding author

Mailing Address: IIT Bombay, Department of Chemistry, Room 215, Powai, Mumbai-400076, India

Email: rajarshi@chem.iitb.ac.in

Phone: + 91-022-2576 7192

Fax : + 91-022-2576 7152

Atom Serial Number	Atom Type	Partial Charge
1	C	1.378066
2	C	-0.647428
3	C	0.875498
4	C	0.238220
5	C	0.654350
6	C	0.567950
7	C	0.431645
8	C	0.414311
9	C	0.467674
10	C	0.593316
11	C	0.484354
12	C	0.174233
13	C	0.514580
14	C	-0.154549
15	C	1.150666
16	C	0.626701
17	F	-0.188154
18	F	-0.268534
19	F	-0.201048
20	F	-0.088510
21	F	-0.241007
22	F	-0.255251
23	F	-0.250284
24	F	-0.228394
25	F	-0.244299
26	F	-0.251795
27	F	-0.249718
28	F	-0.246189
29	F	-0.245072
30	F	-0.247093
31	F	-0.249640
32	F	-0.247027
33	F	-0.240924
34	F	-0.245554
35	F	-0.252087
36	F	-0.244259
37	F	-0.249612
38	F	-0.235861
39	F	-0.224827
40	F	-0.246339
41	F	-0.243564
42	F	-0.205165
43	F	-0.115698
44	F	-0.246480
45	F	-0.241871
46	F	-0.264383
47	F	-0.272916
48	C	0.886318
49	O	-0.125358
50	F	-0.355097
51	F	-0.327390
52	F	-0.223299
53	C	0.255678
54	C	-0.506639

55	C	0.502636
56	O	-0.363030
57	O	-0.680195
58	O	-0.597246
59	F	-0.224103
60	F	-0.237333
61	F	-0.078114
62	F	0.113239
63	O	-0.622269
64	S	1.454415
65	C	1.163358
66	C	0.509542
67	C	0.579434
68	C	0.276929
69	C	0.226031
70	C	0.458194
71	C	0.619062
72	C	0.591311
73	C	0.250517
74	C	0.518002
75	C	0.747664
76	C	-0.055407
77	C	0.796310
78	C	-0.142876
79	C	1.298093
80	C	0.175741
81	F	-0.270338
82	F	-0.270656
83	F	-0.293075
84	F	-0.253273
85	F	-0.255275
86	F	-0.251069
87	F	-0.248665
88	F	-0.243646
89	F	-0.245834
90	F	-0.245977
91	F	-0.244572
92	F	-0.246153
93	F	-0.244849
94	F	-0.250757
95	F	-0.248492
96	F	-0.248753
97	F	-0.244829
98	F	-0.245876
99	F	-0.245658
100	F	-0.247359
101	F	-0.243202
102	F	-0.254236
103	F	-0.251799
104	F	-0.215788
105	F	-0.229133
106	F	-0.252570
107	F	-0.250647
108	F	-0.172969
109	F	-0.216605

110	F	-0.242963
111	F	-0.268704
112	F	-0.245001
113	C	0.943717
114	O	-0.084747
115	F	-0.243272
116	F	-0.251188
117	F	-0.196343
118	C	-0.554301
119	C	0.036908
120	C	0.843658
121	O	-0.111467
122	O	-0.704170
123	O	-0.640685
124	F	-0.238798
125	F	-0.244774
126	F	-0.207195
127	F	-0.207552
128	O	-0.609787
129	S	1.402594
130	C	1.250378
131	C	-0.487423
132	C	0.946712
133	C	0.140338
134	C	0.515593
135	C	0.549556
136	C	0.462884
137	C	0.492823
138	C	0.373033
139	C	0.567656
140	C	0.582775
141	C	0.233763
142	C	0.649950
143	C	-0.169988
144	C	1.251812
145	C	0.510477
146	F	-0.195942
147	F	-0.275177
148	F	-0.199661
149	F	-0.092878
150	F	-0.244226
151	F	-0.255965
152	F	-0.247140
153	F	-0.230384
154	F	-0.245582
155	F	-0.250783
156	F	-0.247073
157	F	-0.245934
158	F	-0.247532
159	F	-0.248031
160	F	-0.247701
161	F	-0.245266
162	F	-0.243634
163	F	-0.245748
164	F	-0.248742

165	F	-0.241014
166	F	-0.247898
167	F	-0.246035
168	F	-0.233135
169	F	-0.242153
170	F	-0.249000
171	F	-0.245231
172	F	-0.180232
173	F	-0.242548
174	F	-0.257855
175	F	-0.262775
176	F	-0.279946
177	C	0.703435
178	O	-0.183999
179	F	-0.280800
180	F	-0.298019
181	F	-0.280446
182	C	0.684443
183	C	0.226516
184	C	0.498131
185	O	-0.318751
186	O	-0.708955
187	O	-0.623234
188	F	-0.239508
189	F	-0.245589
190	F	-0.230113
191	F	-0.262875
192	O	-0.636769
193	S	1.412286
194	C	0.087437
195	C	0.220940
196	C	0.657856
197	C	0.172430
198	C	0.704320
199	C	0.338412
200	C	0.349393
201	C	0.749437
202	C	0.346982
203	C	0.383728
204	C	0.982228
205	C	-0.362025
206	C	0.787425
207	C	0.057624
208	C	1.188645
209	C	0.231276
210	F	-0.298088
211	F	-0.304325
212	F	-0.229884
213	F	0.682549
214	F	-0.252988
215	F	-0.229724
216	F	-0.192182
217	F	-0.173930
218	F	-0.249641
219	F	-0.251102

220	F	-0.241355
221	F	-0.241147
222	F	-0.246585
223	F	-0.251881
224	F	-0.247478
225	F	-0.250444
226	F	-0.252651
227	F	-0.249796
228	F	-0.243731
229	F	-0.244502
230	F	-0.254576
231	F	-0.257171
232	F	-0.211064
233	F	-0.215340
234	F	-0.258057
235	F	-0.252136
236	F	-0.175333
237	F	-0.218798
238	F	-0.252314
239	F	-0.273673
240	F	-0.253406
241	C	0.923318
242	O	-0.076326
243	F	-0.270131
244	F	-0.258869
245	F	-0.199902
246	C	-0.270795
247	C	0.049752
248	C	0.784107
249	O	-0.121046
250	O	-0.683863
251	O	-0.651359
252	F	-0.241072
253	F	-0.245779
254	F	-0.227683
255	F	-0.210843
256	O	-0.599871
257	S	1.383176
258	F	-0.335673
259	F	-0.327052
260	F	-0.304802
261	F	-0.312874
262	F	-0.274670

TABLE S1. Partial charges assigned to the different atoms constituting the 4-mer nafion according to its ground state geometry optimized using the B3LYP model of the Density Functional Theory (DFT) in combination with 6-311++G(d, p) basis set in the Gaussian-09 software. The cumulative sum of the total Mulliken charges listed above comes out to be -4.000.