Supplementary Information – Revealing the flame retardancy of cotton fabrics treated with ammonium ethylenediamine tetramethylenephosphonate and trimethylol melamine

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Table S1. Accepted conformations of EDTMP molecule with total energies by using the stochastic method based on random sampling with 11 torsion angles, as depicted in Figure S1. Conformation 2 is selected as the most stable conformer with the lowest total energy.

	Torsion angle (deg)										Total	
	N8-C2	C11-N7	C9-N8	P22-C9	P21-C10	P23-C11	P24-C12	O26-P21	O25-P22	O28-P23	O27-P24	energy
Conf.	-C1-N7	-C1-C2	-C2-C1	-N8-C2	-N8-C2	-N7-C1	-N7-C1	-C10-N8	-C9-N8	-C11-N7	-C12-N7	(kcal/mol)
1	145.5587	88.5687	91.3025	-132.0731	88.3316	-84.8077	103.1009	-168.7128	156.3048	-173.6852	-161.9660	304.4787
2	144.5334	92.0433	88.4224	-124.1553	88.4636	-77.3865	110.3948	-168.6381	149.8032	-171.4053	-165.4998	290.7706
3	143.6251	97.7465	93.8686	-131.5385	81.6034	-83.1377	104.6322	-169.3228	154.7857	-175.6580	-157.5780	323.7569
4	142.1294	91.8276	91.4002	-128.5789	81.3494	-84.3777	101.7471	-165.1143	151.0602	-174.2027	-165.8418	335.7623
5	141.1943	97.0272	92.1521	-128.2407	80.2545	-76.1214	102.4363	-170.0562	156.3887	-170.2752	-165.2550	352.4175
6	140.3349	96.9212	93.3570	-130.9401	80.3715	-81.2794	105.6079	-165.7121	156.0717	-176.5418	-161.1859	365.7937
7	140.3133	92.4397	94.6899	-129.0421	80.1919	-81.2840	110.8214	-172.6188	159.0858	-170.4895	-158.4804	376.4726



Figure S1. Molecular structure of EDTMP conformer with the lowest energy determined by conformational search, as listed in Table S1.

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Table S2. Accepted conformation of TMM molecule with total energy by using the stochastic method based on random sampling with 6 torsion angles, as depicted in Figure S2. Only one conformation is accepted from the conformation search.

	Torsion angle (deg)									
Conf.	C8-N7-C6-N5	O9-C8-N7-C6	C15-N14-C2-N1	O16-C15-N14-C2	C22-N21-C4-N3	O23-C22-N21-C4	(kcal/mol)			
1	0.8252	88.1720	-177.3316	67.3261	-175.7682	-65.3077	-356.9867			



Figure S2. Molecular structure of TMM conformer with the lowest energy determined by conformational search, as listed in Table S2.

Normal	A	EDTMP	•	ТММ	AED	ГМР-ТММ
Mode	-Eig. (cm ⁻¹)	Int. (Debye ² Å ⁻²)	Eig. (cm^{-1})	Int. (Debye ² Å ^{-2})	Eig. (cm^{-1})	Int (Debye ² Å ⁻²)
1	0	0	0	0	0	0.004
2	Õ	0	Õ	0	Õ	0.003
3	Õ	0.005	Õ	0	0	0.006
4	õ	0.007	Õ	0.001	Õ	0
5	Õ	0	Õ	0.001	Õ	0.003
6	õ	0.003	Õ	0	Õ	0.005
7	13 498	0.056	50.29	0.052	9.623	0.001
8	24.87	0.002	55,101	0.028	11.897	0.019
9	33,114	0.003	65.506	0.113	14 326	0.007
10	45.212	0.069	81.129	0.099	20.177	0.012
11	51.073	0.11	86 818	0.026	26 348	0.047
12	55.898	0.506	111.572	0.019	31.476	0.029
13	66 454	0.125	156 154	0.029	40 364	0.04
14	68.56	0.279	175.092	0.021	52.115	0.064
15	83.015	0.12	202 434	0.186	54 299	0.121
16	83.892	0.181	209.488	0.083	58 429	0.023
17	91 894	0.183	225 404	0.121	59 199	0.025
18	93 571	0.04	268 569	0.163	63 418	0.089
10	104 816	0.18	323 071	0.133	66 834	0.033
20	107.757	0.18	367 329	2 184	71 501	0.023
20	119 796	0.021	402.91	0.133	75 269	0.116
21	121 442	0.257	471 726	0.071	79.896	0.025
22	135.03	0.017	521.085	2 278	83 857	0.023
23	143.65	0.052	535 735	0.882	07 100	0.105
24	145.05	0.032	557 274	0.082	100.034	0.195
25	155 435	0.105	566 57	1 305	100.034	0.023
20	159 262	0.507	572 251	1.595	115 177	0.233
21	150.202	0.011	509.27	1.560	121.26	0.024
20	102.004	0.105	508 870	2.308	121.50	0.097
29	102.210	0.088	590.019	3.138	130.611	0.571
50 21	195.219	0.52	040.287	1.028	140.118	0.081
22	213.314	0.103	670 124	2.474	144.188	0.025
32	221.807	0.301	0/0.124	2.588	149.040	0.001
33 24	223.202	0.251	740.700	0.025	155.825	0.175
54 25	224.227	0.755	151.258	0.26	101./11	0.214
35	239.077	0.144	/5/./8	0.324	100.587	0.174
36	243.275	0.279	829.599	2.891	1/3.334	0.224
3/	253.227	0.964	937.144	2.213	181.681	0.261
38	269.024	0.811	944.505	0.292	188.168	0.4/3
39	282.269	1.095	959.26	0.23	198.639	0.302
40	315.853	0.074	9/8.143	6.66	209.627	0.54
41	323.799	0.592	996.34	0.432	211.662	0.274
42	334.916	0.371	1002.884	5.788	215.829	0.105
43	336.917	1.453	1036.631	0.682	221.417	0.159
44	342.931	0.315	1053.495	0.873	226.139	0.391
45	346.711	0.119	1088.389	0.982	231.018	0.2
46	348.968	0.723	1102.128	0.248	242.882	0.022
47	355.624	0.13	1150.679	0.745	248.745	0.325
48	363.509	0.233	1159.964	5.796	259.815	0.236
49	365.648	0.303	1261.178	0.352	264.018	0.054
50	368.665	0.722	1270.143	0.356	266.036	0.977
51	374.35	1.082	1285.78	0.343	269.402	0.132
52	392.053	0.048	1320.567	0.009	279.375	0.519
53	398.839	0.573	1379.042	0.031	285.981	1.112
54	413.796	2.138	1390.88	0.984	303.146	0.813
55	426.904	1.323	1401.362	0.149	308.577	0.131
56	428.062	0.374	1407.477	0.365	315.407	0.031
57	429.716	1.412	1429.66	8.245	320.892	0.034
58	432.066	0.027	1435.309	5.137	332.309	0.105
59	437.74	0.56	1444.679	0.512	336.936	0.462
60	450.995	1.558	1456.947	0.183	346.88	0.418
61	471.207	4.902	1492.274	1.48	357.749	0.046
62	476.168	0.55	1520.504	1.491	365.659	0.364
63	487.276	2.122	1527.146	2.318	375.369	2.106
64	497.366	2.238	1534.095	0.355	381.315	0.351
65	503.664	1.215	1547.211	1.276	390.387	1.154
66	521.802	8.739	1574.997	22.84	392.477	2.975
67	524.836	9.51	1589.861	1.518	400.962	3.539
68	549.077	6.353	1612.331	30.203	409.912	1.038
69	567.925	0.953	1671.813	1.31	413.366	0.455
70	601.973	0.152	3065.129	1.195	416.985	0.343
71	627.967	0.094	3066.553	1.219	419.09	0.309
72	633.336	0.119	3108.152	0.784	424.339	0.779
73	637.128	0.333	3174.489	0.792	434.542	1.072
74	687.319	0.068	3176.937	0.717	435.501	0.14

Table S3. Calculated FTIR wavenumbers of AEDTMP, TMM molecules and AEDTMP-TMM molecular complex. Eig. and Int. mean the eigenvalue and intensity.

Normal	A 1	EDTMD		тмм		TMD TMM
Mode	$\frac{A}{Fig.(om^{-1})}$	$\frac{\text{EDTMP}}{\text{Int} (\text{Dabya}^2 \text{ Å}^{-2})}$	Fig. (am ⁻¹)	$\frac{1}{1} \frac{1}{1} \frac{1}$	Eig (om ⁻¹)	$\frac{1 \text{ MP-1 MW}}{\text{Int} (\text{Dabya}^2 \text{ Å}^{-2})}$
75	680 706	0.250	2170.882		452.766	6 071
75	605 778	0.339	2572 441	0.448	452.700	0.071
70	702.41	0.073	2507 251	0.012	433.731	1.078
70	725.41	0.100	2628 226	0.477	470.398	0.545
/8	760.215	1.54/	3628.226	0.134	4/5.812	2.24
/9	/61.053	1.986	3644.505	1.269	482.365	1.402
80	772.784	0.228	3656.691	2.142	495.99	0.143
81	/85.398	0.392	3657.318	0.683	505.484	2.861
82	/90.906	2.119			510.3	2.694
83	808.105	0.127			513.384	1.907
84	814.438	3.815			514.811	1.525
85	821.768	3.337			519.952	2.684
86	839.934	1.075			527.907	0.638
87	856.807	7.047			531.939	0.291
88	861.219	1.337			537.948	1.138
89	886.195	2.193			548.243	0.599
90	900.452	5.568			561.887	1.754
91	906.416	2.295			569.806	1.676
92	910.076	1.906			574.644	0.005
93	920.817	14.57			609.186	1.25
94	928.902	3.817			628.083	1.038
95	938.669	8.799			631.179	3.665
96	947.812	3.574			659.26	2.424
97	961.994	5.081			675.853	0.038
98	965.331	3.505			678.849	5.42
99	969.932	4 753			685 473	0.986
100	1019 699	5.01			688 975	1 047
101	1030 152	0.905			704 997	5 283
102	1084 717	0.469			705 326	1 117
102	1150 59	2 473			732 777	/ 10
103	1158.056	0.62			736 422	0.858
104	1184 636	2 506			730.422	0.058
105	1224 400	2.590			740.66	0.007
100	1224.409	0.03			749.00	0.201
107	1247.902	2.924			776.415	0.718
108	1204.957	0.739			7/0.415	0.038
109	1280.372	0.982			780.094	0.004
110	1301.934	0.047			/82.309	0.117
111	1319.479	0.179			/91.65	0.741
112	1333.48	0.844			805.385	0.585
113	1335.91	0.221			825.682	0.434
114	1347.253	0.785			847.018	2.963
115	1354.103	0.626			873.368	0.929
116	1357.826	0.452			885.049	0.928
117	1373.754	1.563			889.247	3.14
118	1379.543	6.316			906.594	0.262
119	1390.222	0.996			912.512	0.591
120	1393.546	1.138			920.428	0.7
121	1401.139	0.448			924.731	0.273
122	1413.624	0.728			929.897	0.804
123	1418.176	2			948.24	0.829
124	1441.126	0.642			954.025	2.925
125	1447.947	2.094			960.353	5.732
126	1465.828	0.2			964.153	15.524
127	1488.173	0.295			975.632	0.918
128	1491.109	0.335			980.939	18.746
129	1492.251	0.175			986.701	1.455
130	1496.98	0.257			1002.231	0.187
131	1531.284	0.211			1006.237	0.58
132	1536	0.883			1025.18	2.99
133	1628.826	10.655			1031.777	0.896
134	1630.501	12.392			1036.193	4.162
135	1631.348	3 999			1045 93	2.418
136	1641 609	3 129			1052 402	12 486
137	1673.66	13 561			1060 955	2.779
138	1705 326	1 969			1064 674	4 021
130	1710.067	2 835			1072 858	0.539
1/0	1712 622	2.035			1082.85	1 1
140	172.055	-1.307 0.786			1002.05	4. 4 0.016
141	1725.719	0.780			1075.959	11 /05
142	1726 922	0.502			1100.334	11.47J 2 402
143	1/20.822	0.043			1130.114	2.405
144	1/51.95/	55.//			1145.0/1	0.951
145	1/4/.869	18.22			1152.819	2.216
146	1/49.189	55.12			1157.097	0.51
147	1/58.886	6.59			1172.823	0.812
148	1813.432	3.233			1188.298	1.153
149	2096.397	6.719			1219.692	0.137
150	2102.468	6.213			1224.773	0.232
151	2105.168	11.915			1265.73	7.688
152	2247.347	4.791			1274.429	0.725
153	2370.207	49.188		S 4	1280.371	1.094
				54		

Normal	А	EDTMP		ТММ	AED	TMP-TMM
Mode	Eig. (cm ⁻¹)	Int. (Debye ² Å ⁻²)	Eig. (cm ⁻¹)	Int. (Debye ² Å ⁻²)	Eig. (cm ⁻¹)	Int. (Debye ² Å ⁻²)
154	2416.167	60.572			1282.732	11.72
155	2433.249	26.308			1284.317	1.305
150	2435.939 2466 827	27.80			1305.76	0.517
158	2721.61	34.023			1312.749	3.151
159	2961.676	14.515			1322.239	1.034
160	3008.95	1.376			1328.566	0.211
161	3029.321	1.477			1332.886	1.316
162	3048.595	0.345			1358.206	2.212
164	3055.131	1.369			1362.894	7.412
165	3059.475	0.252			1373.242	0.929
166	3091.546	15.164			1381.179	2.255
167	3130.15	2.623			1390.279	1.575
169	3142.076	0.085			1394.813	0.314
170	3146.995	0.081			1398.617	4.193
171	3148.634	0.183			1405.481	18.858
172	3158.373	0.008			1407.938	0.755
173	3510.682	0.978			1413.783	2.267
175	3512.552	0.859			1421.208	0.586
176	3513.64	0.986			1426.682	3.484
177	3582.895	0.885			1430.751	3.825
178	3607.013	0.788			1457.520	21.285
180	3610.313	0.772			1466.779	4.955
181					1474.077	1.38
182					1485.242	1.482
183					1485.729	4.982
184					1498.771	0.2
186					1499.39	2.503
187					1510.445	3.422
188					1513.295	16.924
189					1517.872	0.519
190					1541.263	4.798
192					1552.467	3.563
193					1558.999	7.762
194					1564.03	0.107
195					1576.262	16.701
197					1581.223	0.195
198					1634.306	28.069
199					1640.407	1.989
200					1650.747	2.106
202					1676.271	8.401
203					1694.778	5.022
204					1717.984	15.962
205					1/53.716	3.775
200					1775.144	0.644
208					1775.228	0.895
209					1800.799	14.075
210					1817.084	16.751
211					1883.603	17.422
213					2034.811	3.841
214					2367.003	10.102
215					2425.53	6.279
210					2034.931 2704 702	47.352 9.872
218					2732.174	29.333
219					2778.786	43.565
220					2821.627	11.449
221					2947.09 2083.006	11.149
223					2994.787	1.181
224					3009.321	1.57
225					3015.105	13.247
226					3043.771	0.282
227					3043.22 3046 849	0.398
229					3051.431	0.555
230					3081.873	0.787
231					3108.741	0.064

Normal	A	EDTMP		TMM	AED	AEDTMP-TMM		
Mode	Eig. (cm^{-1})	Int. (Debye ² Å ⁻²)	Eig. (cm^{-1})	Int. (Debye ² Å ^{-2})	Eig. (cm^{-1})	Int. (Debye ² Å ⁻²)		
232					3117.273	10.151		
233					3118.346	0.324		
234					3128.763	0.74		
235					3131.072	0.113		
236					3134.792	0.061		
237					3141.658	1.238		
238					3142.261	0.07		
239					3155.664	0.671		
240					3167.339	9.86		
241					3203.283	0.022		
242					3325.747	2.586		
243					3438.742	0.511		
244					3450.162	0.958		
245					3481.067	0.138		
246					3481.224	0.765		
247					3484.375	0.713		
248					3519.142	0.158		
249					3526.792	0.286		
250					3556.414	1.036		
251					3559.208	1.512		
252					3571.884	1.405		



Figure S3. Frontier molecular orbitals including HOMO-1 and LUMO+1 with their energy levels (unit: eV) of AEDTMP and TMM molecules.

Table S4. Fukui indices for electrophilic (f^{-}) , nucleophilic (f^{+}) , radical attack (f^{0}) and dual descriptor
$(\Delta f = f^+ - f^-)$ based on assigned Fukui charges in Mulliken and Hirshfeld approaches for AEDTMP
molecule

	Electrophil	ic attack (f^-)	Nucleophil	ic attack (f^+)	Radical a	ttack (f^0)	Dual descr	riptor (Δf)
Atom	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld
C1	-0.013	0.021	-0.011	0.004	-0.012	0.013	0.002	-0.017
C2	-0.024	0.024	0.000	0.002	-0.012	0.013	0.024	-0.022
HI	0.019	0.011	0.011	0.005	0.015	0.008	-0.008	-0.006
н2	0.046	0.021	0.024	0.005	0.035	0.000	-0.022	-0.010
112	0.040	0.021	0.024	0.005	0.035	0.010	-0.022	-0.010
H3 114	0.060	0.030	0.013	0.005	0.036	0.018	-0.047	-0.025
H4	0.038	0.016	-0.013	-0.002	0.013	0.007	-0.051	-0.018
NI	0.033	0.037	0.003	0.008	0.018	0.023	-0.030	-0.029
N2	0.134	0.133	-0.001	0.000	0.066	0.066	-0.135	-0.133
C3	-0.043	0.018	-0.010	0.002	-0.026	0.010	0.033	-0.016
C4	-0.040	0.020	-0.001	0.002	-0.021	0.011	0.039	-0.018
C5	-0.024	0.006	-0.014	0.004	-0.019	0.005	0.010	-0.002
C6	-0.019	0.005	0.000	0.023	-0.009	0.014	0.019	0.018
H5	0.027	0.013	0.030	0.014	0.028	0.013	0.003	0.001
H6	0.032	0.016	0.008	0.004	0.020	0.010	-0.024	-0.012
H7	0.003	0.002	0.016	0.009	0.010	0.006	0.013	0.007
H8	0.039	0.019	0.039	0.009	0.039	0.010	0.000	0.000
110	0.032	0.017	0.057	0.017	0.035	0.015	0.000	0.000
П9 1110	0.073	0.045	0.010	0.007	0.043	0.025	-0.037	-0.050
HIU	0.043	0.019	0.006	0.003	0.024	0.011	-0.037	-0.016
HII	0.059	0.031	-0.004	-0.001	0.027	0.015	-0.063	-0.032
H12	0.050	0.024	0.016	0.007	0.033	0.016	-0.034	-0.017
P1	0.015	0.026	0.003	0.004	0.009	0.015	-0.012	-0.022
P2	0.016	0.022	0.007	0.006	0.012	0.014	-0.009	-0.016
P3	0.002	0.007	0.002	0.006	0.002	0.006	0.000	-0.001
P4	0.005	0.007	0.058	0.034	0.031	0.020	0.053	0.027
01	0.045	0.042	0.010	0.012	0.028	0.027	-0.035	-0.030
O2	0.058	0.052	0.010	0.010	0.034	0.031	-0.048	-0.042
03	0.016	0.015	-0.019	0.023	-0.001	0.019	-0.035	0.008
04	0.030	0.026	0.017	0.015	0.023	0.021	-0.013	-0.011
05	-0.004	0.020	0.012	0.013	0.004	0.007	0.015	0.012
05	-0.004	0.001	0.012	0.015	0.004	0.007	0.022	0.012
00	0.017	0.010	-0.005	0.015	0.000	0.015	-0.022	-0.001
07	0.009	0.009	-0.011	0.003	-0.001	0.007	-0.020	-0.004
08	-0.003	0.002	0.009	0.028	0.003	0.015	0.012	0.026
09	0.037	0.031	0.009	0.010	0.023	0.021	-0.028	-0.021
010	0.005	0.008	-0.005	0.000	0.000	0.004	-0.010	-0.008
011	0.029	0.026	0.006	0.008	0.018	0.017	-0.023	-0.018
012	0.023	0.018	-0.013	-0.006	0.005	0.006	-0.036	-0.024
H13	0.009	0.005	0.022	0.007	0.016	0.006	0.013	0.002
H14	0.013	0.010	0.008	0.005	0.011	0.007	-0.005	-0.005
N3	-0.002	0.008	-0.009	0.009	-0.005	0.009	-0.007	0.001
H15	0.013	0.008	0.024	0.013	0.018	0.011	0.011	0.005
H16	0.003	0.003	0.006	0.004	0.004	0.004	0.003	0.001
H17	0.008	0.006	0.006	0.005	0.007	0.005	-0.002	-0.001
H18	0.014	0.009	0.020	0.011	0.017	0.010	0.006	0.002
N/	-0.001	0.008	-0.227	0.101	-0.114	0.055	-0.226	0.002
ц10	0.001	0.004	0.056	0.044	0.021	0.033	0.220	0.075
1120	0.005	0.004	0.050	0.044	0.031	0.024	0.051	0.040
П20 1121	0.015	0.009	0.304	0.178	0.190	0.094	0.349	0.109
H21	0.006	0.004	0.024	0.034	0.015	0.019	0.018	0.030
H22	0.013	0.008	0.340	0.168	0.176	0.088	0.327	0.160
N5	-0.001	0.011	-0.024	0.013	-0.013	0.012	-0.023	0.002
H23	0.017	0.011	0.043	0.021	0.030	0.016	0.026	0.010
H24	0.010	0.008	0.005	0.005	0.007	0.007	-0.005	-0.003
H25	0.019	0.012	0.041	0.021	0.030	0.017	0.022	0.009
H26	0.004	0.003	0.004	0.004	0.004	0.004	0.000	0.001
N6	-0.001	0.012	-0.012	0.005	-0.007	0.008	-0.011	-0.007
H27	0.025	0.015	0.023	0.011	0.024	0.013	-0.002	-0.004
H28	0.011	0.009	0.009	0.005	0.010	0.007	-0.002	-0.004
H20	0.007	0.005	0.009	0.004	0.008	0.005	0.002	-0.001
H30	0.007	0.005	0.002	0.007	0.000	0.003	_0.002	-0.003
LI30	0.007	0.003	0.005	0.002	0.005	0.005	0.004	0.005
1122	0.005	0.005	0.040	0.019	0.022	0.011	0.035	0.010
<u>п</u> 32	0.007	0.004	0.005	0.001	0.000	0.003	-0.002	-0.003

	Electrophili	ic attack (f^-)	Nucleophili	c attack (f^+)	Radical a	ttack (f^0)	Dual desc	riptor (Δf)
Atom	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld
N1	0.140	0.140	0.048	0.054	0.094	0.097	-0.092	-0.086
C1	0.019	0.033	0.125	0.115	0.072	0.074	0.106	0.082
N2	0.057	0.051	0.035	0.047	0.046	0.049	-0.022	-0.004
C2	0.020	0.026	0.051	0.051	0.035	0.039	0.031	0.025
N3	0.042	0.033	0.081	0.071	0.061	0.052	0.039	0.038
C3	0.023	0.034	0.052	0.056	0.038	0.045	0.029	0.022
N4	0.065	0.074	0.022	0.037	0.043	0.055	-0.043	-0.037
C4	-0.011	0.021	-0.005	0.020	-0.008	0.020	0.006	-0.001
01	0.052	0.053	0.025	0.040	0.039	0.047	-0.027	-0.013
H1	0.014	0.015	0.038	0.025	0.026	0.020	0.024	0.010
H2	0.046	0.032	0.041	0.026	0.043	0.029	-0.005	-0.006
H3	0.049	0.026	0.048	0.026	0.048	0.026	-0.001	0.000
H4	0.028	0.016	0.021	0.014	0.024	0.015	-0.007	-0.002
N5	0.051	0.060	0.039	0.064	0.045	0.062	-0.012	0.004
C5	-0.015	0.020	-0.010	0.024	-0.012	0.022	0.005	0.004
O2	0.050	0.050	0.032	0.041	0.041	0.045	-0.018	-0.009
H5	0.014	0.013	0.021	0.015	0.017	0.014	0.007	0.002
H6	0.035	0.021	0.044	0.024	0.040	0.022	0.009	0.003
H7	0.048	0.025	0.052	0.028	0.050	0.027	0.004	0.003
H8	0.043	0.029	0.053	0.038	0.048	0.033	0.010	0.009
N6	0.069	0.077	0.024	0.038	0.047	0.058	-0.045	-0.039
C6	-0.016	0.019	-0.012	0.018	-0.014	0.019	0.004	-0.001
O3	0.045	0.044	0.025	0.037	0.035	0.041	-0.020	-0.007
H9	0.009	0.010	0.035	0.023	0.022	0.017	0.026	0.013
H10	0.047	0.024	0.046	0.025	0.046	0.025	-0.001	0.001
H11	0.035	0.020	0.030	0.017	0.033	0.019	-0.005	-0.003
H12	0.044	0.033	0.039	0.026	0.042	0.030	-0.005	-0.007

Table S5. Fukui indices for electrophilic (f^-) , nucleophilic (f^+) , radical attack (f^0) and dual descriptor $(\Delta f = f^+ - f^-)$ based on assigned Fukui charges in Mulliken and Hirshfeld approaches for TMM molecule.



Figure S4. EDX spectra of the treated cotton fabric samples with 5% AEDTMP FR solution as increasing the treating times from (a) 1 to (e) 5, and (f) the single-treated sample with denser 25% AEDTMP FR solution.

Table S6. Testing result such as LOI value and char length for flame retardancy and durability of cotton samples, treated with 5% AEDMTP FR solution and 5% TMM binder solution as increasing the treating times (5FR-*N*) and treated once with 25% AEDMTP FR solution (25FR-1), before washing and after 10 and 20 times washing.

	AEDTMP portion	Before washing		10 times washing		20 ti	20 times washing	
Sample	(%)	LOI (%)	Char length (cm)	LOI (%)	Char length (cm)	LOI (%)	Char length (cm)	
5FR-1	8.6	26.2	13.5	23.4	17.2	19.1	00	
5FR-2	11.2	29.5	11.2	26.3	14.1	23.2	16.2	
5FR-3	14.4	32.1	9.1	28.6	13.4	25.5	14.9	
5FR-4	17.9	37.5	8.6	33.4	10.1	29.7	11.6	
5FR-5	21.5	42.4	6.2	38.7	7.8	34.6	8.9	
25FR-1	21.5	42.6	5.9	32.1	9.4	26.5	11.1	