

Supporting information

Inherent flame retardation of semi-aromatic polyesters via binding small-molecule free radicals and charring

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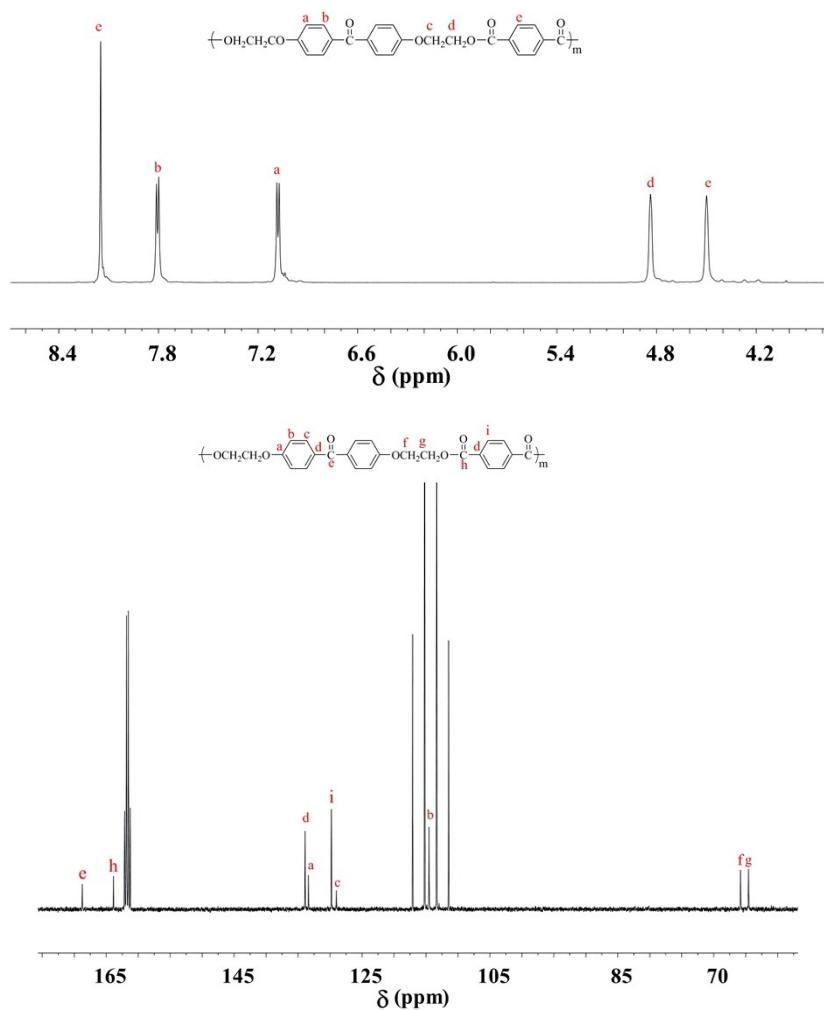
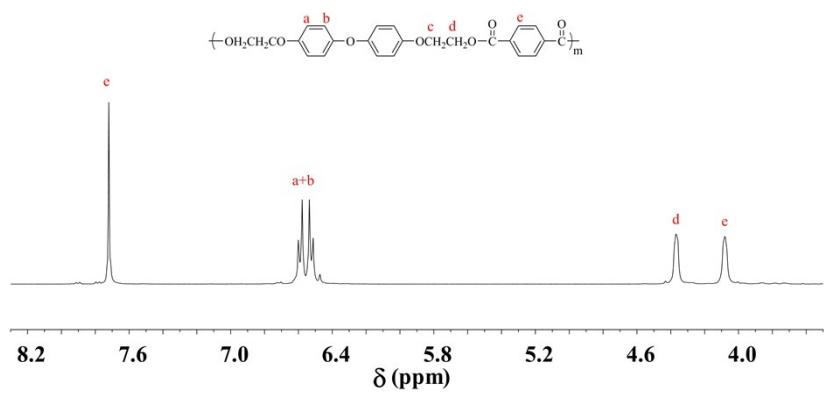


Fig. S1 ^1H NMR and ^{13}C NMR spectrum of PKT.



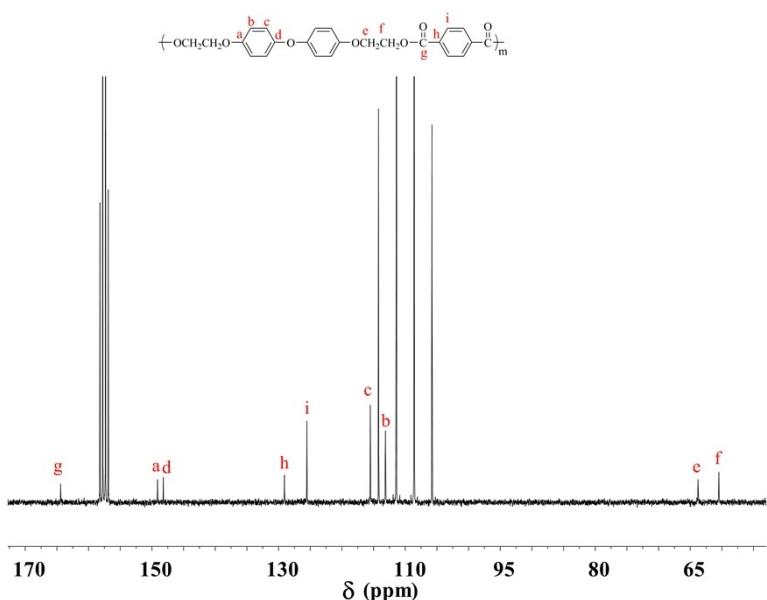


Fig. S2 ^1H NMR and ^{13}C NMR spectrum of POT.

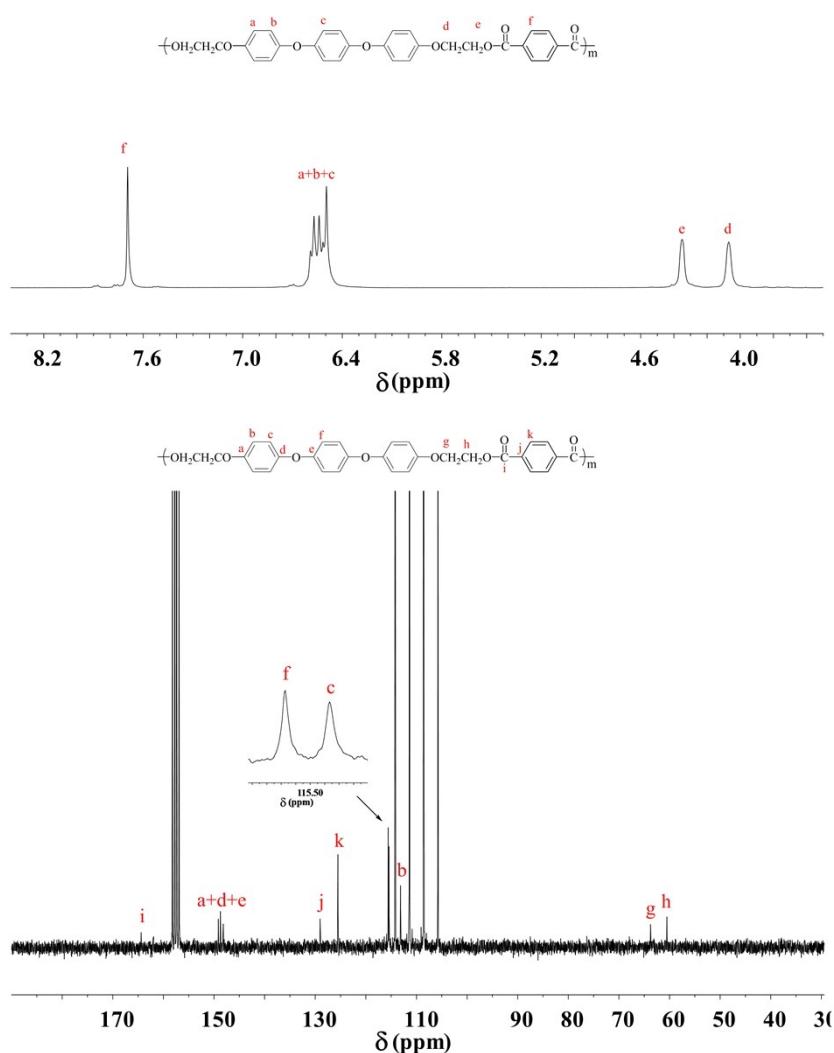


Fig. S3 ^1H NMR and ^{13}C NMR spectrum of PEET.

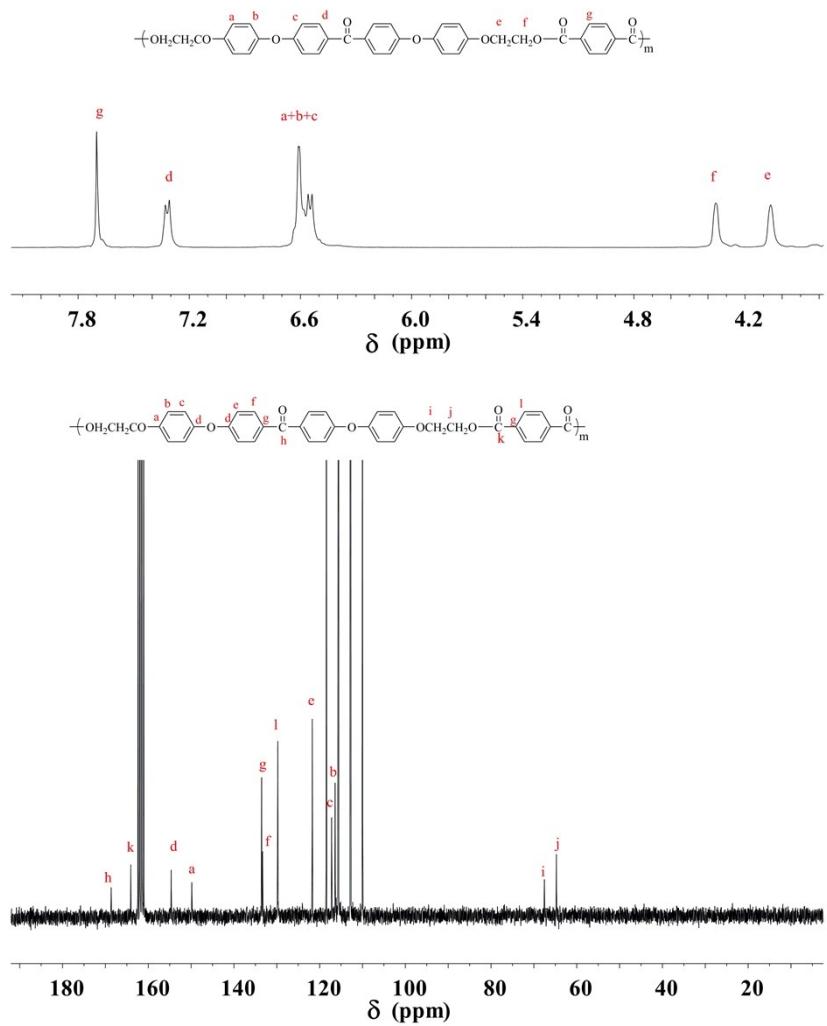


Fig. S4 ¹H NMR and ¹³C NMR spectrum of PEKET.

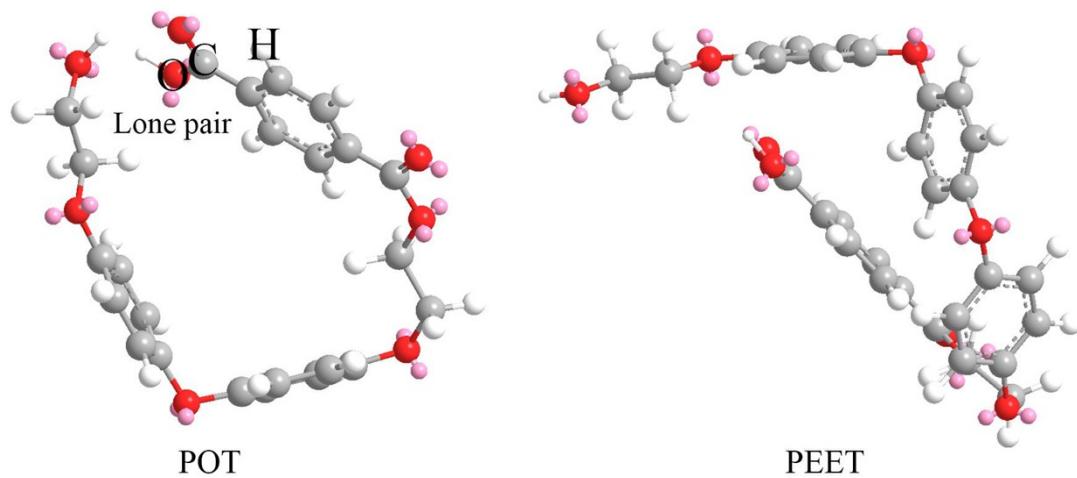


Fig. S5 3D structure for POT and PEET structure units simulated by Chembio 3D

MM2 Minimize Energy

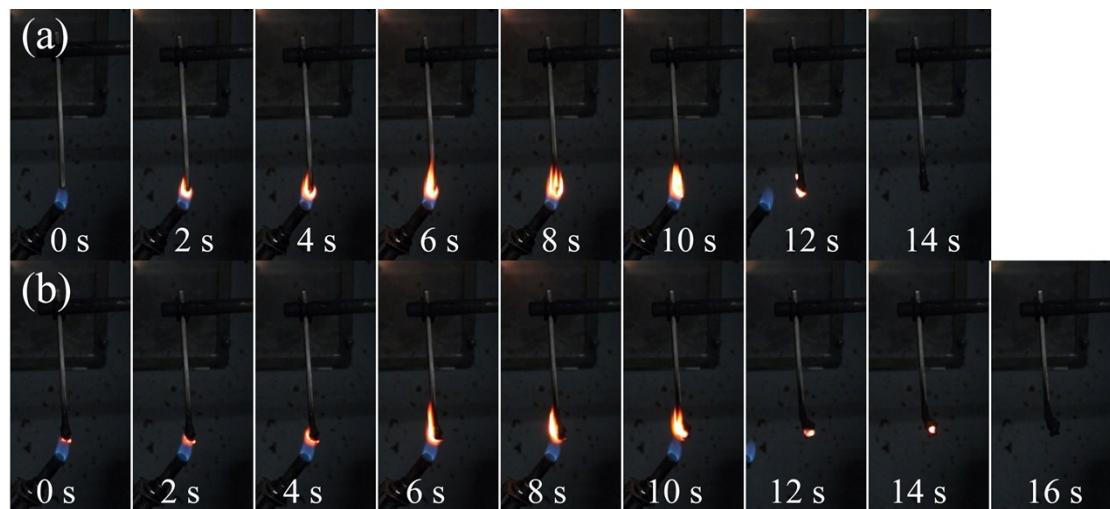
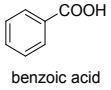
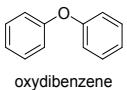
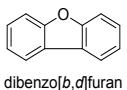
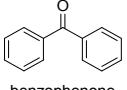
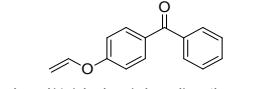
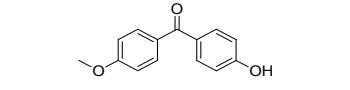
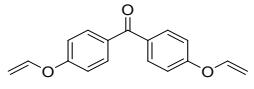
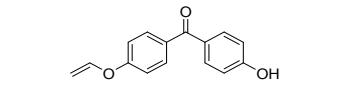
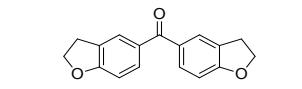
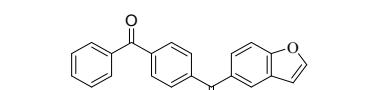
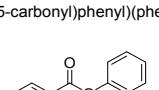
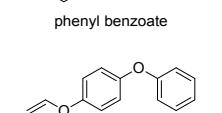
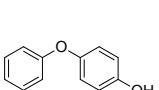


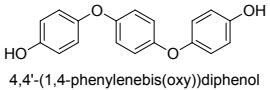
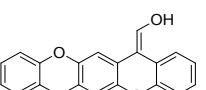
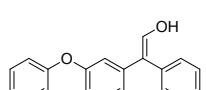
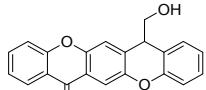
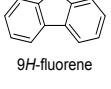
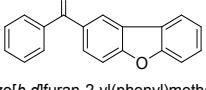
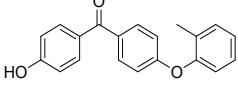
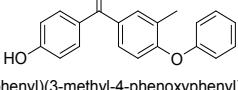
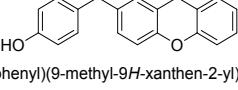
Fig. S6 UL-94 test for PEET: (a) the first ignition and (b) the second ignition.

Table S1. Peak numbers, retention time, molecular weight and major mass fragments for pyrolysis products.

Peak numbers	Retention time (min)	M	Compounds	Major mass fragments
1	1.48	92	 toluene	92, 91, 65
2	2.62	106	 ethylbenzene	106, 91, 77, 65, 51
3	3.04	104	 styrene	104, 103, 78, 77, 63, 51
4	3.64	120	 (vinyloxy)benzene	120, 94, 91, 77, 66, 65, 51
5	4.30	94	 phenol	94, 66, 65
6	5.25	120	 acetophenone	120, 105, 77, 51
7	5.55	136	 methyl benzoate	136, 105, 77, 51
8	5.99	148	 4-(vinyloxy)benzaldehyde	148, 105, 77, 51

9	6.70	122		benzoic acid	122, 105, 77, 51
10	8.34	154		1,1'-biphenyl	155, 154, 153, 152, 151, 150, 77, 76
11	8.52	170		oxydibenzene	170, 168, 142, 141, 115, 77, 51
12	9.51	168		dibenzo[b,d]furan	168, 139, 70, 51
13	10.39	182		benzophenone	182, 105, 77, 51
14	12.46	224		phenyl(4-vinyloxy)phenyl)methanone	224, 181, 147, 121, 105, 91, 77, 65
15	13.92	228		(4-hydroxyphenyl)(4-methoxyphenyl)methanone	227, 105, 77, 51
16	14.27	266		bis(4-vinyloxyphenyl)methanone	266, 223, 147, 121, 91
17	14.88	240		(4-hydroxyphenyl)(4-vinyloxyphenyl)methanone	241, 240, 197, 147, 121, 93, 91, 65
18	15.53	266		bis(2,3-dihydrobenzofuran-5-yl)methanone	266, 223, 147, 119, 91, 65
19	18.58	326		(4-(benzofuran-5-carbonyl)phenyl)(phenyl)methanone	326, 105, 77, 51
20	10.59	198		phenyl benzoate	198, 105, 77, 51
21	10.69	212		1-phenoxy-4-(vinyloxy)benzene	212, 183, 129, 91, 77
22	11.18	186		4-phenoxyphenol	186, 158, 129, 77

23	11.39	210		210, 182, 181, 154, 153, 152, 77
24	12.56	254		254, 225, 119, 91, 65
25	13.01	228		228, 199, 91, 65
26	13.07	240		240, 228, 211, 210, 183, 119, 91, 77
27	13.22	252		252, 223, 195, 169, 141, 91, 89
28	13.71	226		226, 197, 169
29	13.79	254		254, 91, 65
30	15.74	316		315, 285, 284, 283, 105, 77
31	17.17	316		316, 105, 77
32	17.81	316		316, 105, 77
33	14.16	262		262, 246, 185, 141, 115, 77
34	15.72	298		298, 273, 185, 182, 141, 115, 91, 77
35	16.14	276		276, 275, 185, 141, 115, 77

36	16.35	294	 4,4'-(1,4-phenylenebis(oxy))diphenol	294, 293, 181, 141, 115, 77
37	17.14	328	 (E)-(14-methylchromeno[2,3-b]xanthen-7(14H)-ylidene)methanol	328, 183, 182, 181, 155, 154, 153
38	17.74	326	 (E)-(14-methylenechromeno[2,3-b]xanthen-7(14H)-ylidene)methan	326, 183, 182, 181, 155, 154, 153
39	18.25	328	 (14-methylene-7,14-dihydrochromeno[2,3-b]xanthen-7-yl)methan	328, 183, 182, 181, 155, 154, 153, 91
40	10.04	166	 9H-fluorene	166, 165, 164, 163, 139, 115, 83
41	15.66	272	 dibenzo[b,d]furan-2-yl(phenyl)methanone	273, 272, 197, 141, 115, 105, 77
42	17.11	304	 (4-hydroxyphenyl)(4-(o-tolyl)oxy)phenylmethanone	305, 304, 211, 168, 157, 105
43	17.20	304	 (4-hydroxyphenyl)(3-methyl-4-phenoxyphenyl)methanone	304, 197, 126, 72
44	17.75	316	 (4-hydroxyphenyl)(9-methyl-9H-xanthen-2-yl)methanone	315, 303, 302, 239, 238, 237
