Novel sulfonate-containing halogen-free flame-retardants: effect of ternary and quaternary sulfonates centered on adamantane on the properties of polycarbonate composites

Dongyu Zhu, Jianwei Guo,* Jiaxing Xian, Shuqin Fu

1.1 Characterization of 1,3,5-triphenyladamantane and 1,3,5-tri(phenyl-4-sulfonylchloride) adamantane

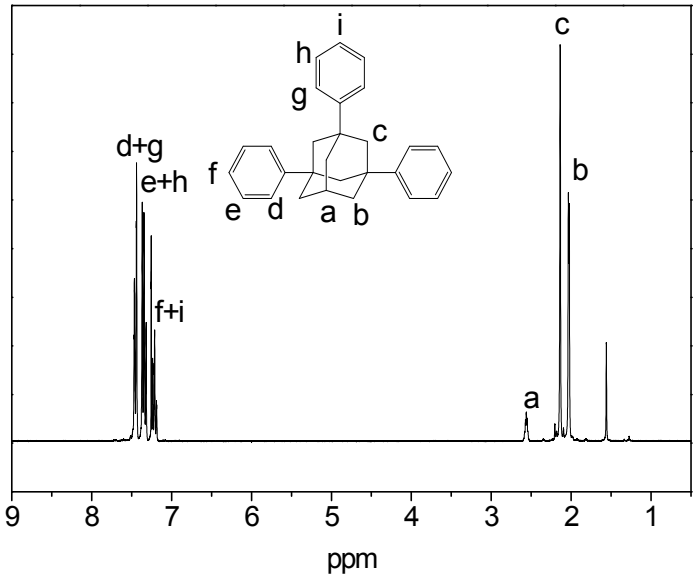


Fig. SI ^{1}H NMR spectrum of 1,3,5-triphenyladamantane with $CDCl_3$ as solvent

School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, China
E-mail address: guojw@gdut.edu.cn
† Electronic supplementary information (ESI) available.

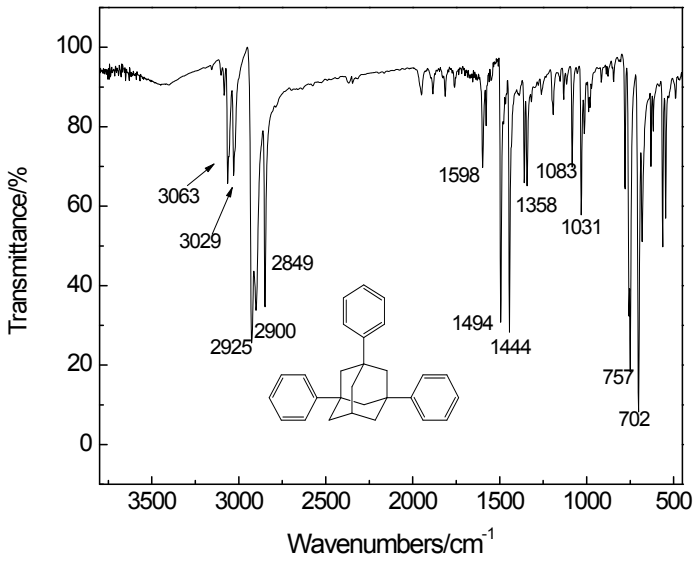


Fig. S2 FTIR spectrum of 1,3,5-triphenyladamantane

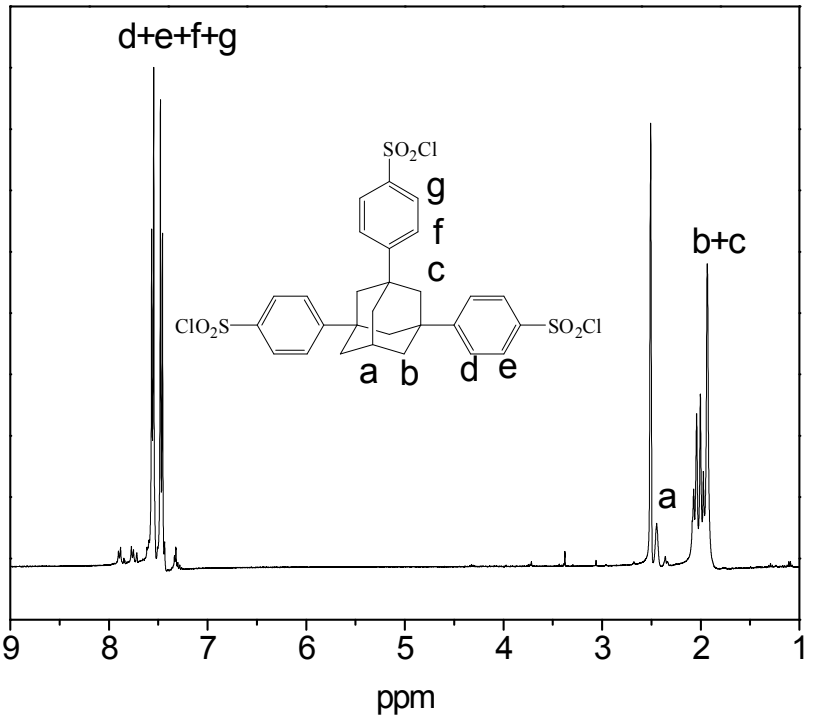


Fig. S3 ^{1}H NMR spectrum of 1,3,5-tri(phenyl-4-sulfonylchloride) adamantane with DMSO-d_6 as solvent

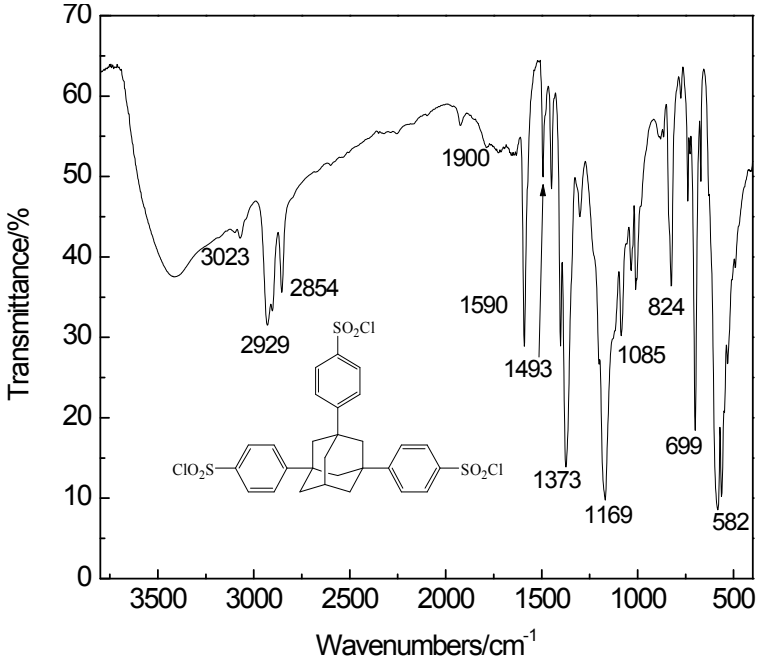


Fig. S4 FTIR spectrum of 1,3,5-tri(phenyl-4-sulfonylchloride) adamantane

1.2 **Characterization of 1,3,5,7-tetraphenyladamantane and 1,3,5,7-tetrakis(phenyl-4-sulfonylchloride)adamantane**

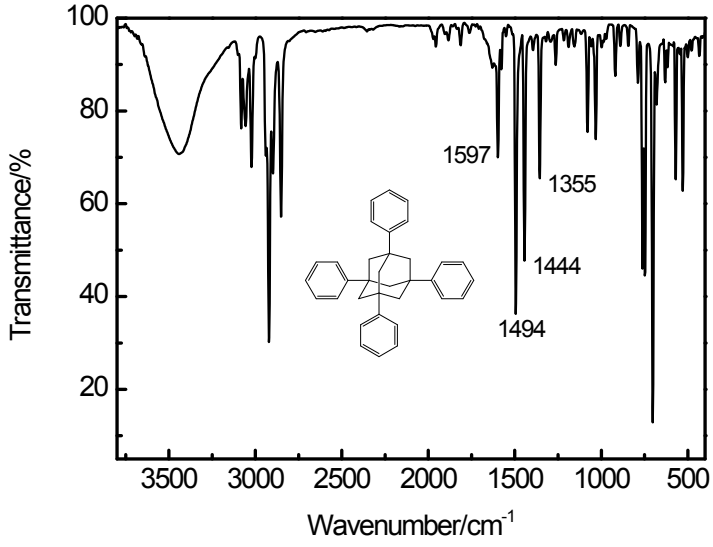


Fig. S5 FTIR spectrum of 1,3,5,7-tetraphenyladamantane

We didn't obtain the ^{1}H NMR spectrum of 1,3,5,7-tetraphenyladamantane because of its insolubility in general solvents.

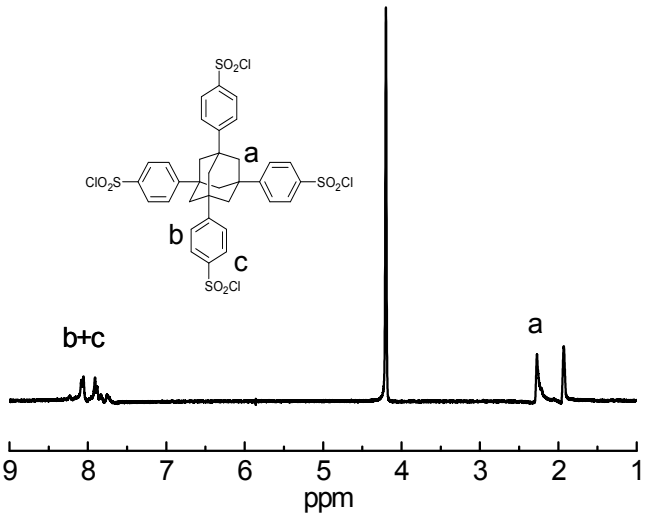


Fig. S6 ^{1}H NMR spectrum of 1,3,5,7- tetrakis(phenyl-4-sulfonylchloride)adamantane with DMSO-d_6 as solvent

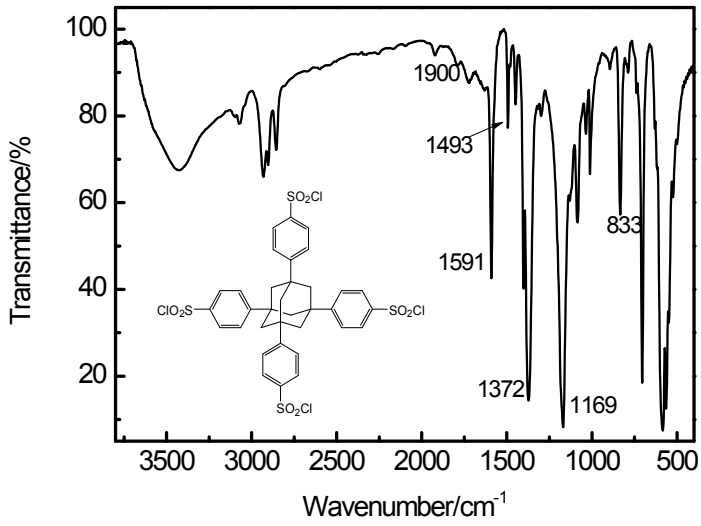


Fig. S7 FTIR spectrum of 1,3,5,7- tetrakis(phenyl-4-sulfonylchloride)adamantane

2. Thermal degradation kinetics

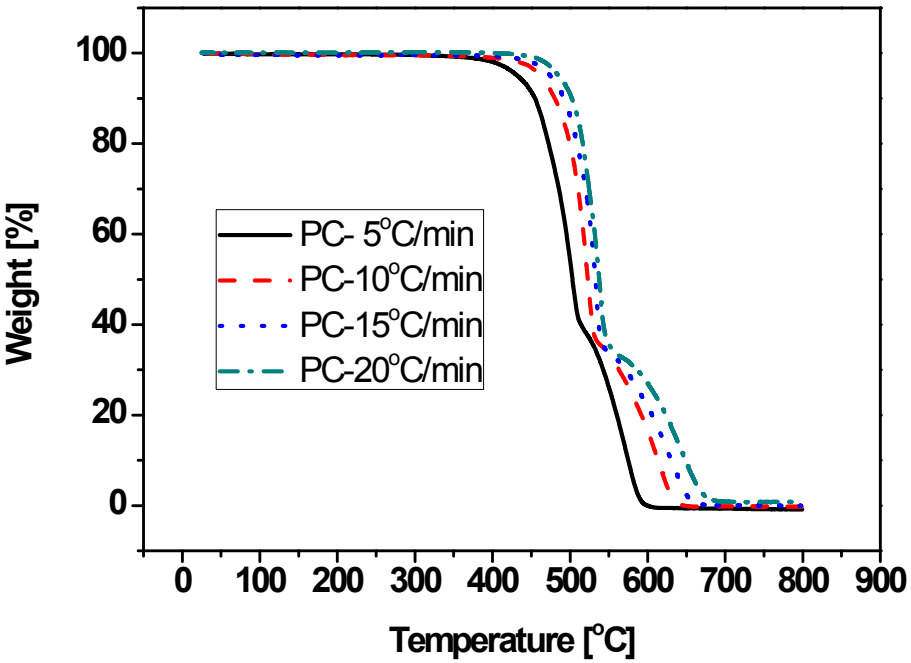


Fig. S8 TG curves of PC under different heating flow rates. PC/AS_4(0.08%)

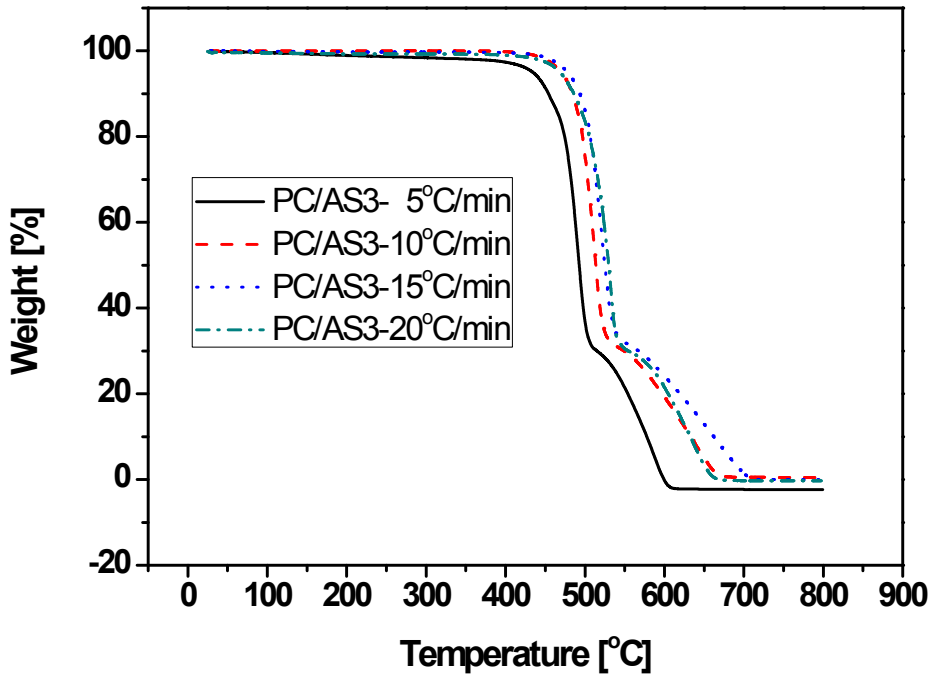


Fig. S9 TG curves of PC/AS_3(0.1%) under different heating flow rates.

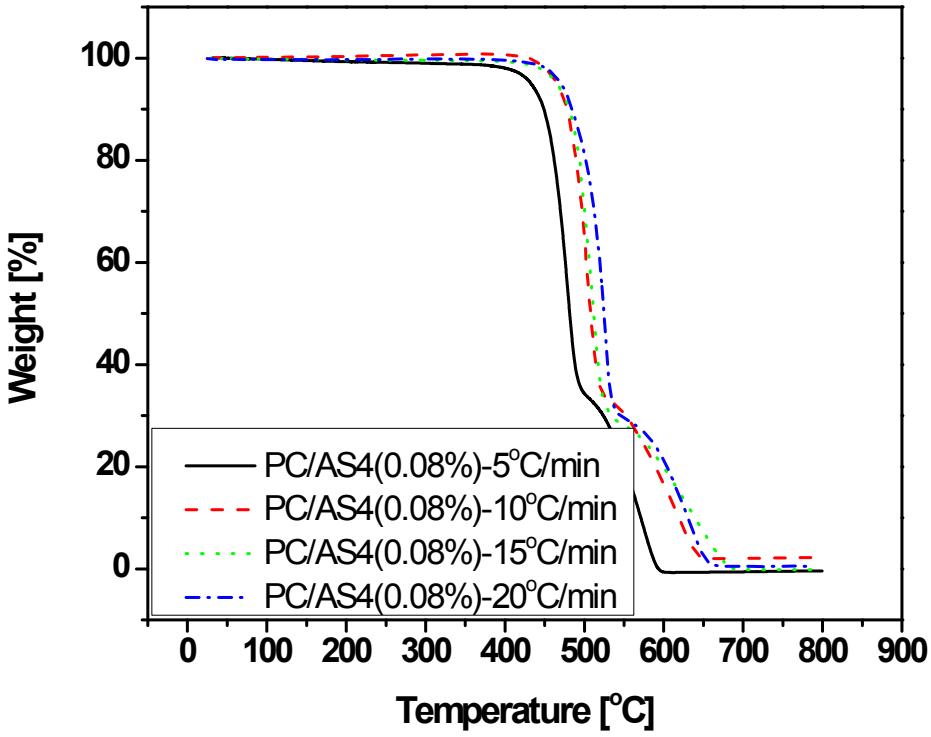


Fig. S10 TG curves of PC/AS_4(0.08%) under different heating flow rates.

Table S1. The calculated activation energy data of PC

PC								
α/%	β/(°C/min)				Slop	r	E/(KJ/mol)	Ë/ (KJ/mol)
	5	10	15	20				
10	454.87	479.85	491.51	501.64	-6.9789	0.9905	126.9641	
20	472.07	497.56	508.31	515.84	-7.9648	0.9946	144.9001	
30	484.87	508.10	519.91	524.44	-8.8328	0.9922	160.6912	
40	495.27	516.15	527.31	531.44	-9.8866	0.9931	179.8626	176.9138
50	502.87	521.24	532.31	537.04	-10.7647	0.9968	195.8375	
60	514.07	527.83	536.71	542.64	-13.4846	0.9999	245.3194	
70	542.67	561.49	570.71	585.24	-10.1592	0.9914	184.8219	

a: conversion rate, □β: heating rate, r: correlation coefficient, E: activation energy, Ë: Average activation energy.

Table S2. The calculated activation energy data of PC/AS_3(0.1%)

PC/AS_3(0.1%)								
α/%	β/(°C/min)				Slop	r	E/(KJ/mol)	Ë/ (KJ/mol)
	5	10	15	20				
10	456.63	484.08	493.36	486.01	-6.9789	0.9905	126.9641	
20	475.43	496.88	507.16	505.21	-8.6703	0.9982	157.7349	
30	483.23	503.28	513.56	516.21	-9.2803	0.9991	168.8324	
40	488.43	508.68	519.56	523.81	-9.9528	0.9938	181.0669	160.7523
50	493.23	513.48	524.96	529.81	-9.8185	0.9957	178.6236	
60	498.43	518.88	531.16	534.41	-9.8923	0.9917	179.9663	
70	523.03	549.08	567.16	554.41	-7.26	0.9995	132.0779	

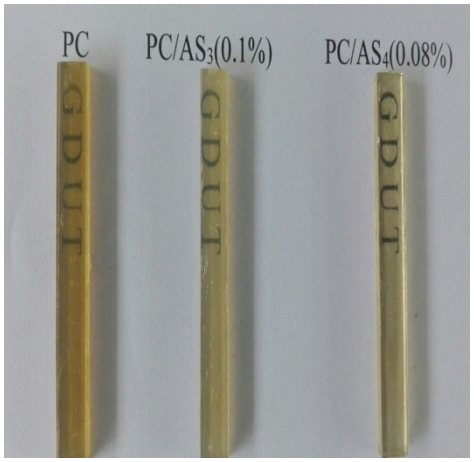
a: conversion rate, □β: heating rate, r: correlation coefficient, E: activation energy, Ë: Average activation energy.

Table S3. The calculated activation energy data of PC/AS_4(0.08%)

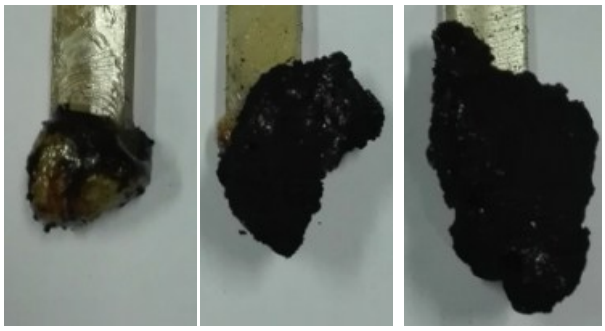
PC/AS_4(0.08%)								
α/%	β/(°C/min)				Slop	r	E/(KJ/mol)	Ë/ (KJ/mol)
	5	10	15	20				
10	456.63	484.08	493.36	486.01	-8.2313	0.9417	149.7484	
20	475.43	496.88	507.16	505.21	-8.3440	0.9750	151.7987	
30	483.23	503.28	513.56	516.21	-8.2700	0.9769	150.4525	
40	488.43	508.68	519.56	523.81	-8.3095	0.9816	151.1711	153.4673
50	493.23	513.48	524.96	529.81	-8.4625	0.9814	153.9545	
60	498.43	518.88	531.16	534.41	-8.9970	0.9766	163.6785	
70	523.03	549.08	567.16	554.41	-8.7055	0.92897	158.3753	

a: conversion rate, □β: heating rate, r: correlation coefficient, E: activation energy, Ë: Average activation energy.

3、Transparency



4、Digital photos of char residue



PC PC/AS_3(0.1%) PC/AS_4(0.08%)