Electronic Supporting Information

Characterization of polyalphaolefins using halogen anion attachment in atmospheric pressure photoionization coupled to ion mobility spectrometry - mass spectrometry†

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Experimental

Instrumentation

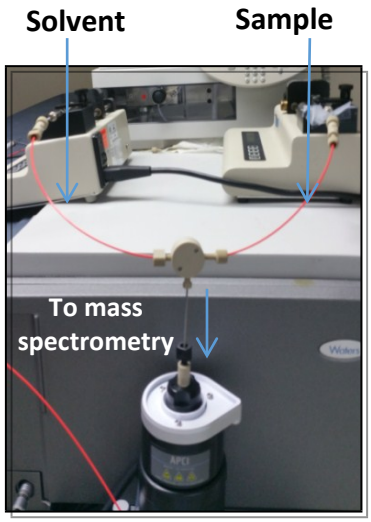

Figure S1. Introduction system for the polyalphaolefins analysis.

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Table S1. NMR results for the studied mPAO and PAO.

		mPAO-A	PAO-B	mPAO-C	PAO-D	mPAO-E
Proportion (%)	CH saturated	12.8	9.7	12.1	10.2	12.7
	CH_2 saturated	74.3	79.5	75.8	78.2	74.1
	CH_3 saturated	12.8 (12.3^a/0.5^b)	10.7 (10.4^a/0.3^b)	11.9 (11.6^a/0.3^b)	11.3 (9.2^a/2.2^b)	13.1 (12.5^a/0.6^b)
	Chain length	C8	-	C9	-	C8

[a] long chains, [b] short chains

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Table S2. Alpha olefin combinations that can explain the ions observed for the main series of the mPAO-C.

m/z	Chemical formula of $[M+Cl]^-$ ions	Monomers combination
821.9	$C_{56}H_{114}Cl$	$7C_8$ or $4C_{12}+C_8$ or $2C_{12}+4C_8$
877.9	$C_{60}H_{122}Cl$	$5C_{12}$ or $6C_8+1C_{12}$ or $3C_{12}+3C_8$
934.0	$C_{64}H_{130}Cl$	$4C_{12}+2C_8$ or $8C_8$ or $2C_{12}+5C_8$
990.0	$C_{68}H_{138}Cl$	$5C_{12}+C_8$ or $7C_8+1C_{12}$ or $3C_{12}+4C_8$

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Table S3. Alpha olefin combinations that can explain the ions observed for the minor series of the mPAO-C.

m/z	Chemical formula of $[M+Cl]^-$ ions	Monomers combination
1018.1	$C_{70}H_{142}Cl$	$5C_{12}+C_{10}$ or $8C_8+C_6$ or $7C_{10}$
1074.2	$C_{74}H_{150}Cl$	$7C_8+3C_6$ or $2C_{12}+5C_{10}$ or $5C_{10}+3C_8$
1130.2	$C_{78}H_{158}Cl$	$6C_{12}+C_6$ or $9C_8+C_6$ or $6C_{10}+3C_6$

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APPI-MS

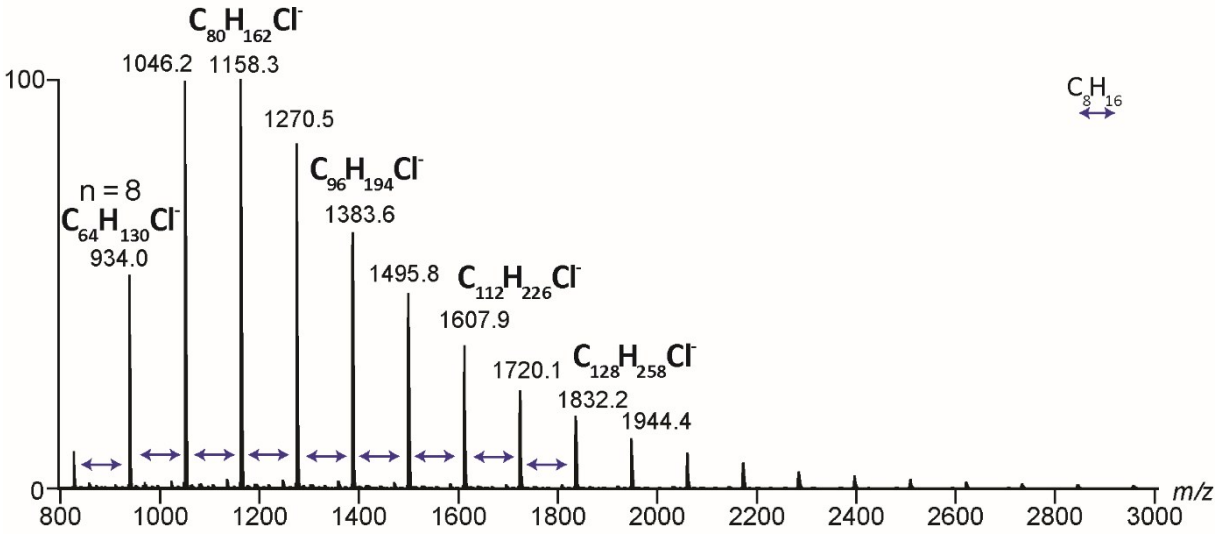

Figure S2. APPI(−)-MS mass spectrum of the mPAO-E (grade 100) using CH_2Cl_2 and toluene.