GC-MS
APPLICATION NOTES

Analysis of organic components in lithium battery electrolyte

GC-MS

GBC

Sample preparation

The electrolyte sample is diluted to an appropriate dilution factor using ethyl acetate, and then directly injected into the machine.

Instrument conditions

Gas chromatograph conditions

Column	Equity-5 (30 m × 0.25 mm × 0.25 µm) quartz capillary column
Mode	Constant Flow Mode
Column Flow Rate	1 mL/min
Injection	Split Injection
Split Ratio	50:1
Injection volume	1 µL
Injection Port Temperature	260˚C
Column Temperature Program	Hold at 40˚C for 1 minute, then increase to 260˚C and hold for 5 minutes

Mass spectrometer conditions

Ion Source	EI Source
Ion Source Temperature	200˚C
Electron Energy	70 eV
Interface Temperature	280˚C
Scan Mode	Full Scan
Scan Mass Range	35-350 u

Results

Standard sample chromatogram

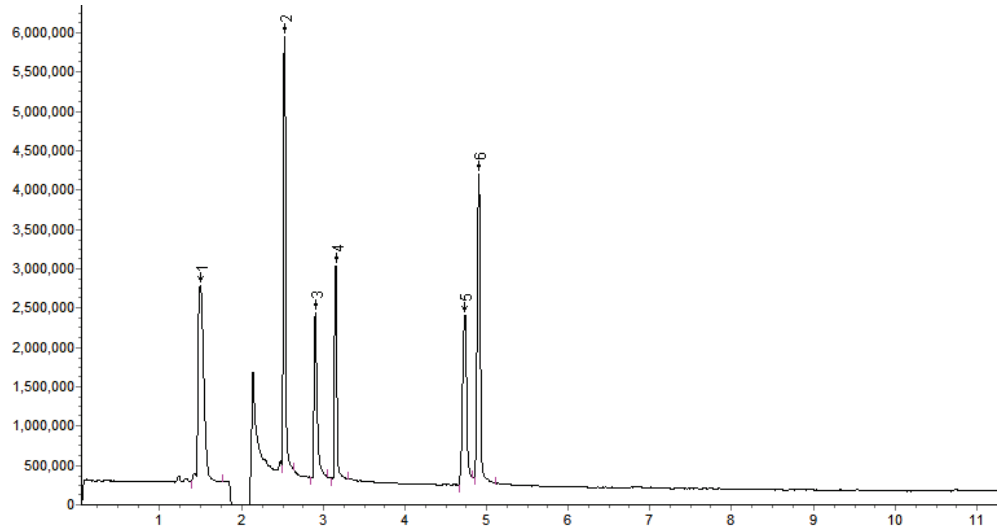

Figure 1: Full scan total ion chromatogram of the mixed standard of six target compounds

1–AN, 2–EMC, 3–VC, 4–DEC, 5–EC, 6–PC

No.	Description	Retention Period	CAS No.	Quantitative Ion	Qualitative Ion
1	Acetonitrile (AN)	1.49	75-05-8	41	40,39
2	Ethyl Methyl Carbonate (EMC)	2.53	623-53-0	77	45,59
3	Vinylene Carbonate (VC)	2.91	872-36-6	86	42,58
4	Diethyl Carbonate (DEC)	3.16	105-58-8	91	45,63
5	Ethylene Carbonate (EC)	4.73	96-49-1	88	43,58
6	Propylene Carbonate (PC)	4.90	108-32-7	57	87,102

Table 1: Relevant information of six target compounds

Preparation of the standard curve

Accurately weigh a certain amount of each target component standard, dissolve it in ethyl acetate, and prepare a mixed standard stock solution. The mixed stock solution is then gradually diluted with ethyl acetate to a series of standard solutions with different concentrations (see Table 2). According to the instrument conditions described above, the samples are measured from low concentration to high concentration to plot the standard curve. The curve equation is shown in Table 3.

Compound Name	Concentration 1 mg/mL	Concentration 2 mg/mL	Concentration 3 mg/mL	Concentration 4 mg/mL	Concentration 5 mg/mL
Acetonitrile (AN)	0.035	0.07	0.175	0.35	0.7
Ethyl Methyl Carbonate (EMC)	0.108	0.216	0.54	1.08	2.16
Vinylene Carbonate (VC)	0.066	0.132	0.33	0.66	1.32
Diethyl Carbonate (DEC)	0.052	0.104	0.26	0.52	1.04
Ethylene Carbonate (EC)	0.1	0.2	0.5	1	2
Propylene Carbonate (PC)	0.122	0.244	0.61	1.22	2.44

Table 2: Standard series concentrations of six target compounds

No.	Compound Name	Retention Period	Curve Equation	Correlation Coefficient
1	Acetonitrile	1.49	Y = 1.768674e+007 X -105158.255922	0.99982
2	Ethyl Methyl Carbonate	2.53	Y = 844960.315553 X -56882.740345	0.99703
3	Vinylene Carbonate	2.91	Y = 5.251620e+006 X -115124.407312	0.99912
4	Diethyl Carbonate	3.16	Y = 3.869839e+006 X -42555.048146	0.99908
5	Ethylene Carbonate	4.73	Y = 3.118548e+006 X -87042.295829	0.99929
6	Propylene Carbonate	4.90	Y = 3.440776e+006 X -156791.896241	0.99879

Table 3: Linear equations and linear correlation coefficients of six target compounds

Electrolyte sample analysis

The electrolyte Sample D and Electrolyte Sample 04 are each diluted to an appropriate dilution factor with ethyl acetate. Then, 1 µL is taken using a microsyringe and injected for analysis. The chromatograms and detection results are as follows.

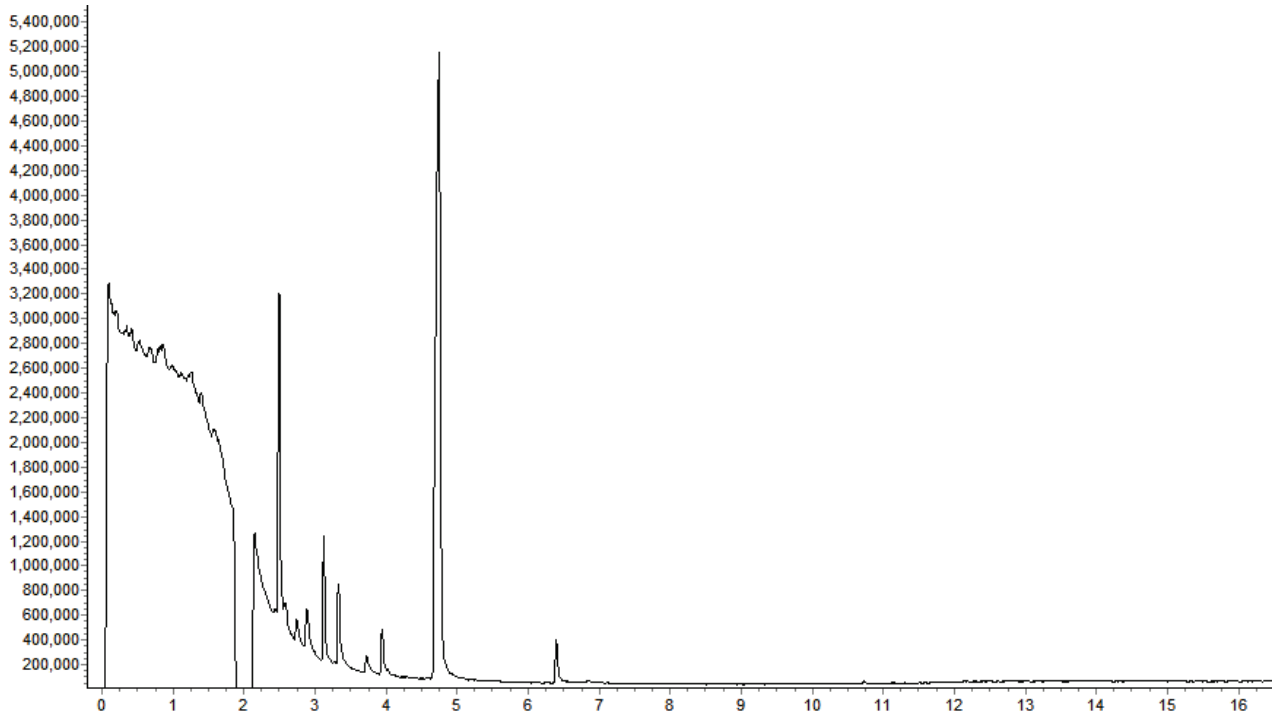

Figure 2: Total ion chromatogram of electrolyte sample D

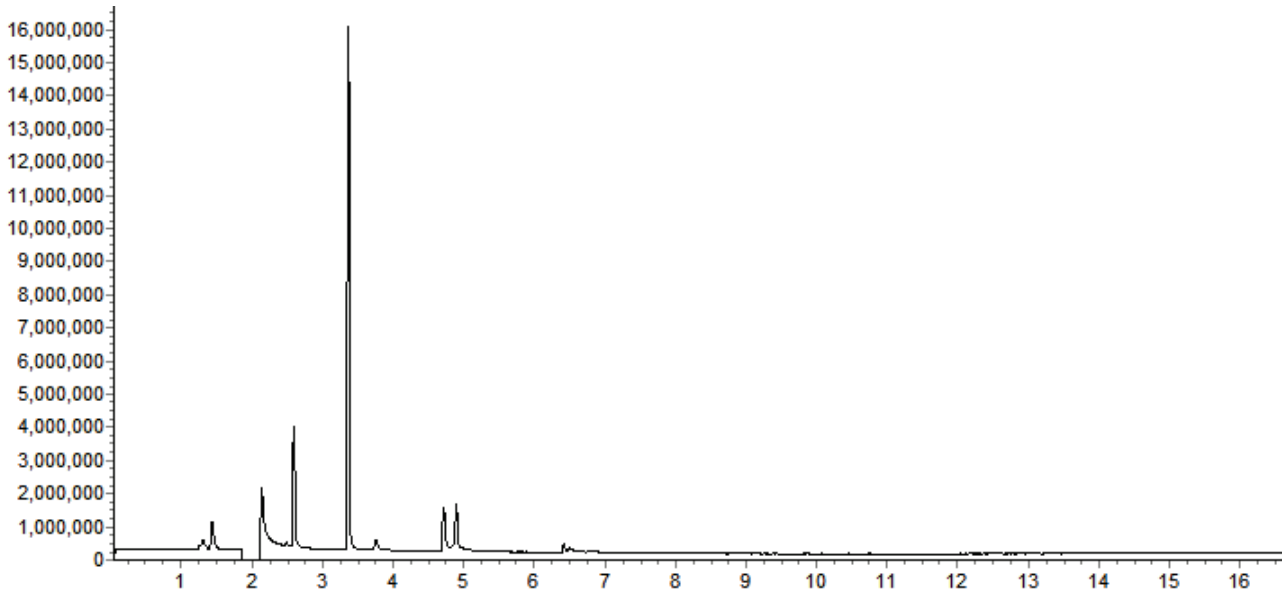

Figure 3: Total ion chromatogram of electrolyte sample 04

No.	Compound Name	Concentration (%)	
		Electrolyte Sample No. 4	Electrolyte Sample D
1	Acetonitrile (AN)	ND	ND
2	Ethyl Methyl Carbonate (EMC)	0.06	2.96
3	Vinylene Carbonate (VC)	ND	0.79
4	Diethyl Carbonate (DEC)	ND	0.88
5	Ethylene Carbonate (EC)	12.02	22.14
6	Propylene Carbonate (PC)	8.17	ND

Table 4: Determination results of lithium battery electrolyte samples ***Note: ND indicates not detected***

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