10. IMPORTANT PEAKS IN THE MASS SPECTRA OF COMMON SOLVENTS

The following table gives the most important peaks that appear in the mass spectra of the most common solvents which might occur as an impurity in organic samples. The solvents are classified in ascending order of thier M^+ peaks. The highest intensity peaks are indicated with (100%).[1–3]

Important peaks in the mass spectra of common solvents

Solvents	Formula	M^+	Important peaks (*m*/*z*)
Water	H_2O	18 (100%)	17
Methanol	CH_3OH	32	31 (100%), 29, 15
Acetonitrile	CH_3CN	41 (100%)	40, 39, 38, 28, 15
Ethanol	CH_3CH_2OH	46	45, 31 (100%), 27, 15
Dimethyl ether	CH_3OCH_3	46 (100%)	45, 29, 15
Acetone	CH_3COCH_3	58	43 (100%), 42, 39, 27, 15
Acetic acid	CH_3CO_2H	60	45, 43, 18, 15
Ethylene glycol	$HOCH_2CH_2OH$	62	43, 33, 31 (100%), 29, 18, 15
Furan	C_4H_4O	68 (100%)	42, 39, 38, 37, 29, 18
Tetrahydrofuran	C_4H_8O	72	71,43, 42 (100%), 41, 40, 39, 27, 18, 15
n-Pentane	C_5H_{12}	72	57, 43 (100%), 42, 41, 39, 29, 28, 27, 15
Dimethyformamide (DMF)	$HCON(CH_3)_2$	73 (100%)	58, 44, 42, 30, 29, 28, 18, 15
Diethyl ether	$(C_2H_5)_2O$	74	59, 45, 41, 31 (100%), 29, 27, 15
Methyl acetate	$CH_3CO_2CH_3$	74	59, 43 (100%), 42, 32, 29, 28, 15
Carbon disulphide	CS_2	76 (100%)	64, 44, 38, 32
Benzene	C_6H_6	78 (100%)	77, 52, 51, 50, 39, 28
Pyridine	C_5H_5N	79 (100%)	80, 78, 53, 52, 51, 50, 39, 26
Dichloromethane	CH_2Cl_2	84	86, 51, 49 (100%), 48, 47, 35, 28
Cyclohexane	C_6H_{12}	84	69, 56, 55, 43, 42, 41, 39, 27
n-Hexane	C_6H_{14}	86	85, 71, 69, 57 (100%), 43, 42, 41, 39, 29, 28, 27
p-Dioxane	$C_4H_8O_2$	88 (100%)	87, 58, 57, 45, 43, 31, 30, 29, 28
Tetramethylsilane (TMS)	$(CH_3)_4Si$	88	74, 73, 55, 45, 43, 29
1,2-Dimethoxyethane	$(CH_3OCH_2)_2$	90	60, 58, 45 (100%), 31, 29
Toluene	$C_6H_5CH_3$	92	91 (100%), 65, 51, 39, 28
Chloroform	$CHCl_3$	118	120, 83, 81, (100%), 47, 35, 28
Chloroform-d_1	$CDCl_3$	119	121, 84, 82 (100%), 48, 47, 35, 28
Carbon tetracholoride	CCl_4	152 (not seen)	121, 119, 117 (100%), 84, 82, 58.5, 47, 35, 28
Tetrachloroethene	$CCl_2{=}CCl_2$	164 (not seen)	168, 166 (100%), 165, 164, 131, 128, 129, 95, 94, 82, 69, 59, 47, 31, 24

Reprinted from T.J. Bruno and P.D.N. Svoronos, *CRC Handbook of Basic Tables for Chemical Analysis*, CRC Press, Boca Raton, FL, 1989, p. 357.

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11. NOMENCLATURE AND TERMINOLOGY FOR ANALYTICAL PYROLYSIS (IUPAC RECOMMENDATIONS 1993)

Prepared for publication by

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Abstract

This paper defines terms and definitions used in analytical methods of pyrolysis and includes expressions for coupled systems and for the description of the temperature profiles and the products that are obtained.

Introduction

Thermal degradation under controlled conditions is often used an part of an analytical procedure, either to render a sample into a suitable form for subsequent analysis by gas chromatography, mass spectrometry or infrared spectroscopy or by direct monitoring as an analytical technique in its own right. A range of terms and expression have been used in the field and this nomenclature brings these together in a systematic manner and assigns each a specific meaning.

Analytical Pyrolysis

Analytical Pyrolysis

The characterization, in an inert atmosphere, of a material or a chemical process by a chemical degradation reaction(s) induced by thermal energy.

Catalytic Pyrolysis

A pyrolysis that is influenced by the addition of a catalyst.

Char

A solid carbonaceous pyrolysis residue.

Coil Pyrolyser

A pyrolyser in which the sample (sometimes located in a tubular vessel) is placed in a metal coil that is heated to cause pyrolysis.

Continuous Mode (Furnace) Pyrolyser

A pyrolser in which the sample is introduced into a furnace preheated to the final temperature.