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TABLE OF REDUCED MOBILITY VALUES FROM AMBIENT PRESSURE ION MOBILITY SPECTROMETRY

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CONTENTS

1 INTRODUCTION

Since 1970 when ambient pressure ion mobility spectrometry was first introduced as an analytical technique[1] the gas phase mobilities of a wide variety of organic ions have been measured and reported in the literature. Throughout the seventies ion mobility spectrometry (IMS), also called plasma chromatography or gas phase electrophoresis, was the subject of a number of investigative research publications designed to illustrate its potential as a highly sensitive analytical tool, especially useful for trace organic analysis. IMS, however, was never adopted as a routine tool by the general analytical community. Ions under atmospheric conditions could not be separated with the resolution of even a low-resolution mass spectrometer. As the expense of mass spectrometers decreased and their reliability increased at trace levels, the ion mobility spectrometer could no longer offer unique advantages for measurement.

With the development of a unidirectional flow design[2], inexpensive microprocessor control[3], a Fourier transform mode of operation[4], and a photoionization source[5], ion mobility has again become a potentially useful tool for analytical chemistry. Rather than a spectrometric technique for purified compounds it now shows promise as a versatile and tunable selective detector for capillary gas chromatography[2] and capillary supercritical fluid chromatography[6].

Selective detection of the ion mobility detector is based on selecting an arrival time window which corresponds to the drift time of a particular ion species of interest. This drift time is best determined from a standard at or near the time of analysis. However, it would be convenient to be able to look up potentially interfering compounds in a table.

Since the beginning of atmospheric pressure IMS, mobility data have been reported in terms of reduced mobility constants (K_0) using the simple equation

$$K_0 = \frac{d}{tE}\left(\frac{P}{760}\right)\left(\frac{273}{T}\right)$$

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TABLE 1

REDUCED MOBILITY VALUES FROM AMBIENT PRESSURE ION MOBILITY SPECTROMETRY

An asterisk (*) indicates mass identified ions. PI = photoionization

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
0.53	Methyl melissate	+		CO_2/CO_2	220	7
0.68	Methyl stearate	+		CO_2/CO_2	220	7
0.76	Methyl myristate	+		CO_2/CO_2	220	7
0.82	Methyl laurate	+		CO_2/CO_2	220	7
0.86	S-(1,2-dicarboxyethyl)cysteine	+	1.00, 1.08, 1.18, 1.26	N_2/N_2	200	8
0.89	Didodecylamine	+		N_2/N_2	148	9
0.89	Methyl caprate	+		CO_2/CO_2	220	7
0.90	L-Cystinyl-bis-L-alanine	+	1.00, 1.08, 1.16	N_2/N_2	200	8
0.90	Lysergic acid diethylamide	+	1.05, 1.16, 1.30, 1.40	N_2/N_2	200	8
0.91	Digitoxigenin	+	1.13, 1.18, 1.42	N_2/N_2	200	8
0.95	*n*-Octyl acetate	M_2H^+	1.42	N_2/N_2	136	10
0.97	Methyl caprylate	+		CO_2/CO_2	220	7
0.97	Triethylphosphonoacetate	M_2H^+	1.23, 1.45	N_2/N_2	150	11
0.98	1-Octanol	+	1.12, 1.21, 1.46, 1.53, 1.88	N_2/N_2	22	12
0.99	Barbital	+	1.50	Air/N_2	230	13
1.00	L-Cystinyl-bis-L-alanine	+	0.90, 1.08, 1.16	N_2/N_2	200	8
1.00	S-(1,2-Dicarboxyethyl)cysteine	+	0.86, 1.08, 1.18, 1.26	N_2/N_2	200	8
*1.01	Acenaphthalene	$(C_{12}H_8)_3H^+$	1.27, 1.84	N_2/N_2	140	14
1.01	*n*-Heptyl acetate	M_2H^+	1.50	N_2/N_2	136	10
1.02	Dibutylnitrosamine	$[(C_4H_9)_2N - NO]_2H^+$	1.56	N_2/N_2	136	15
1.02	Methyl stearate	+		N_2/N_2	150	7
*1.05	Heroin	M^+	1.15	N_2/N_2	200	16
1.05	Lysergic acid diethylamide	+	0.90, 1.16, 1.30, 1.40	N_2/N_2	200	8
1.06	1-Octanol	+	1.12, 1.19, 1.45, 1.85	N_2/N_2	100	12
1.06	Δ^9-Tetrahydrocannabinol	+		N_2/N_2	200	8
1.07	Dimethyl morpholinophosphoramidate	M_2H^+	1.14, 1.57, 1.77	N_2/N_2	150	11
1.07	Methyl caproate	+		CO_2/CO_2	220	7
1.08	1-Octanol	+	1.14, 1.22, 1.47, 1.53, 1.83	N_2/N_2	55	12
1.08	Decachlorobiphenyl	$C_{12}Cl_{10}^-$	1.16, 2.92	N_2/N_2	125	17

1 08	L-Cystinyl-bis-L-alanine	+	0 90, 1.00, 1.16	N_2/N_2	200	8
*1 08	*n*-Hexyl acetate	M_2H^+	1 58	N_2/N_2	136	10
1 08	S-(1,2-Dicarboxyethyl)cysteine	+	0.86, 1.00, 1.18, 1 26	N_2/N_2	200	8
1 09	2,4,4′-Di-*sec* -butylchlorodiphenyl oxide	+		Air/Air	206	18
1.11	Tri-*n*-hexylamine	+		N_2/N_2	149	9
*1 12	"Tolan"	$(C_{14}H_{10})_2H^+$	1.67	N_2/N_2	140	14
1.12	1-Octanol	+	0 98, 1 21, 1.46, 1 53, 1 88	N_2/N_2	22	12
1 12	1-Octanol	+	1.06, 1.19, 1.45, 1 85	N_2/N_2	100	12
1.12	2,4,2′-Di-*sec*.-Butylchlorodiphenyl oxide	+		Air/Air	206	18
1 13	1-Hexanol	+	1.36, 1.66, 1 74	N_2/N_2	22	12
1 13	Diethyl cyanomethyl phosphonate	M_2H^+	1 39, 1 48, 1.58, 1.82	N_2/N_2	150	11
1 13	Digitoxigenin	+	0 91, 1.18, 1 42	N_2/N_2	200	8
1.14	1-Octanol	+	1 08, 1 22, 1 47, 1.53, 1.83	N_2/N_2	55	12
1.14	Dimethyl morpholinophosphoramidate	$(M_2 - CH_3OCH_3)H^+$	1 07, 1.57, 1.77	N_2/N_2	150	11
1 15	Diethyl-2-bromo-5					
*1.15	Heroin	$(M - CH_3CO_2)^+$	1 05	N_2/N_2	200	16
*1 15	Isophthalic acid	$[(C_8H_6O_4)_2 - H_2O]^-$	1.58	N_2/N_2	150	19
1.15	Methyl myristate	+		N_2/N_2	150	7
1 15	Trimethylphosphonoacetate	M_2H^+	1.26, 1 54, 1 68, 1 92	N_2/N_2	150	11
1.16	1-Octanol	+	1 46	N_2/N_2	140	2
*1 16	Cocaine	M^+	1 50, 1.84	N_2/N_2	153	16
1 16	Decacholorobiphenyl	$C_{12}Cl_{10}^-$	1 08, 2 92	N_2/N_2	125	17
1 16	L-Cystinyl-bis-L-alanine	+	0.90, 1.00, 1.08	N_2/N_2	200	8
1.16	Lysergic acid diethylamide	+	0 90, 1 05, 1 30, 1.40	N_2/N_2	200	8
1 16	Octachlorobiphenyl	$(C_{12}H_2Cl_8)H^+$		N_2/N_2	125	17
1 16	Octachlorobiphenyl	$C_{12}H_2Cl_8^-$	2.92	N_2/N_2	125	17
1 18	1-Hexanol	+	1 65, 1.81	N_2/N_2	140	2
1 18	1-Iodobutane	+	1 37, 1 57, 1 67, 1 98, 2.2, 2.33	N_2/N_2	135	20
1 18	Digitoxigenin	+	0 91, 1 13, 1.42	N_2/N_2	200	8
1 18	Methyl butyrate	+		CO_2/CO_2	220	7
1.18	*n*-Pentyl acetate	M_2H^+	1 85	N_2/N_2	136	10
1 18	S-(1,2-Dicarboxyethyl)cysteine	+	0.86, 1.00, 1 08, 1 26	N_2/N_2	200	8
1.19	1-Octanol	+	1 06, 1 12, 1.45, 1.85	N_2/N_2	100	12
*1 20	7-Methylhexahelicene	$(C_{27}H_{18})H^+$		N_2/N_2	140	14
1.20	*n*-Tetradecylamine	+		N_2/N_2	148	9
1.20	Tribenzylamine	+		N_2/N_2	145	9

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TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
1 21	1-Octanol	+	0 98, 1.12, 1.46, 1.53, 1 88	N_2/N_2	22	12
1.22	"Endrin"	+		N_2/N_2	124	21
1 22	"Parathion"	$M(H_2O)H^+$	1 27, 1 78	N_2/N_2	150	11
1 22	1-Octanol	+	1 08, 1 14, 1 47, 1 53, 1 83	N_2/N_2	55	12
1 22	Hydantoin-5-propionic acid	+	1 38, 1 50	N_2/N_2	200	8
*1 23	Hexahelicene	$(C_{26}H_{16})H^+$		N_2/N_2	140	14
1 23	Triethylphosphonoacetate	$(M_2-C_2H_5OC_2H_5)H^+$	0 97, 1 45	N_2/N_2	150	11
1 24	Methyl laurate	+		N_2/N_2	150	7
1 24	Methyl propionate	+		CO_2/CO_2	220	7
*1 25	*trans,trans*-1,4-Distryrylbenzene	$(C_{22}H_{18})H^+$		N_2/N_2	140	14
1 26	"Fenitrothion"	$M(H_2O)H^+$	1 31, 1 40, 1 72, 1 80	N_2/N_2	150	11
*1 26	Butylated hydroxytoluene	$(M-H)^+$		N_2/N_2	210	22
1.26	DDT	+	1 45	N_2/N_2	124	21
1 26	*n*-Dodecylamine	+		N_2/N_2	148	9
1.26	S-(1,2-Dicarboxyethyl)cysteine	+	0 86, 1 00, 1 08, 1.18	N_2/N_2	200	8
1 26	Trimethylphosphonoacetate	$(M_2-CH_3OCH_3)H^+$	1 15, 1 54, 1 68, 1 92	N_2/N_2	150	11
1.27	"Dieldrin"	+		N_2/N_2	124	21
1 27	"Parathion"	MH^+	1 22, 1 78	N_2/N_2	150	11
1.27	4,4′-*sec* -Butylchlorodiphenyl oxide	+		Air/Air	206	18
1 28	2,4′-*sec* -Butylchlorodiphenyl oxide	+		Air/Air	206	18
1 28	Butabarbital	+	1 35	Air/N_2	230	13
1 28	Butabarbital	–	1 34	Air/N_2	230	13
1 28	CO_2 reactant ion	+		CO_2/CO_2	220	7
1.28	*n*-Butyl acetate	M_2H^+	2.00	N_2/N_2	136	10
1 28	*n*-Pentadecane	$C_{15}H_{31}{}^+$	1 34, 1 40, 1 47, 1.54, 1.62, 1 72, 1 86, 1 93, 2.04	N_2/N_2	135	23
1 30	4,2′-*sec*.-Butylchlorodiphenyl oxide	+		Air/Air	206	18
1.30	Amobarbital	–	1.64	Air/N_2	230	13
1 30	Ethyl-S-2-diisopropylaminoethylmethyl-phosphonothiolate	MH^+		N_2/N_2	150	11

1 30	Lysergic acid diethylamide	+	0 90, 1 05, 1.16, 1 40	N_2/N_2	200	8
1 31	"Fenitrothion"	MH^+	1.26, 1 40, 1 72, 1.80	N_2/N_2	150	11
1 31	"Methyl parathion"	$M(H_2O)H^+$	1 36, 1 80	N_2/N_2	150	11
1 31	Pentobarbital	–	1.46, 1 53, 1 59	Air/N_2	230	13
1 31	Secobarbital	+	1 48, 1.55	Air/N_2	230	13
1.32	1-Hexanol	+	1.62, 1 76, 2 10	N_2/N_2	100	12
1 32	1-Hexanol	+	1.63, 1 72	N_2/N_2	55	12
1.32	2,2'-*sec.*-Butyl-chlorodiphenyl oxide	+		Air/Air	206	18
1.32	Amobarbital	+	1 36, 1 53	Air/N_2	230	13
*1.32	Coronene	$(C_{24}H_{12})H^+$		N_2/N_2	140	14
1 32	Dimethyl terephthalate	+	1 51, 1 69	N_2/N_2	150	24
1 34	"Disyston"	MH^+	2 09	N_2/N_2	150	11
1 34	Butabarbital	–	1.28	Air/N_2	230	13
1 34	Di-*n*-hexylamine	+		N_2/N_2	145	9
1 34	*n*-Pentadecane	$C_{14}H_{29}^+$	1 28, 1 40, 1 47, 1.54, 1 62, 1 72, 1.86, 1 93, 2.04	N_2/N_2	135	23
1 34	*n*-Tetradecane	$C_{14}H_{29}^+$	1.46, 1 54, 1 62, 1.72, 1 85, 1 92, 2.04	N_2/N_2	135	23
1.35	Butabarbital	+	1.28	Air/N_2	230	13
1 35	*n*-Decylamine	+		N_2/N_2	149	9
1 36	"Methyl parathion"	MH^+	1.31, 1 80	N_2/N_2	150	11
1 36	1-Hexanol	+	1.13, 1 66, 1.74	N_2/N_2	22	12
1.36	Amobarbital	+	1.32, 1 53	Air/N_2	230	13
1 36	Methyl caprate	+		N_2/N_2	150	7
1 37	"Thimet"	MH^+		N_2/N_2	150	11
1 37	1-Butanol	+	1 61, 1 76, 1.87, 1.97	N_2/N_2	22	12
1 37	1-Iodobutane	+	1 18, 1.57, 1.67, 1 98, 2 20, 2.33	N_2/N_2	135	20
1 37	4-Chlorobenzophenone	+		N_2/N_2		25
1 38	Barbital	–	1 54	Air/N_2	230	13
1 38	Hydantoin-5-propionic acid	+	1 22, 1 50	N_2/N_2	200	8
1 38	Pentobarbital	+		Air/N_2	230	13
*1 39	1,2,5,6-Dibenzanthracene	$(C_{12}H_{14})H^+$		N_2/N_2	140	14
1 39	Aprobarbital	+	1 56, 1.64, 1 75	Air/N_2	230	13
1 39	Aprobarbital	–	1.61	Air/N_2	230	13
1.39	Diethyl cyanomethyl phosphonate	MNO^+	1 13, 1.48,1.58,1 82	N_2/N_2	150	11
1 39	Lutidine	+		N_2/N_2	85	26
1 40	"Fenitrothion"	$(M-CH_2O)H^+$	1 26, 1 31, 1.72, 1.80	N_2/N_2	150	11
1.40	1-Chloropentane	+	1 88, 1 99, 2 20, 2 31	N_2/N_2	135	20

(Continued on p 146)

TABLE I *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
1.40	Benzaldehyde	+	1 84, 1.91, 2.03	N_2/N_2	150	24
1 40	Diethylnitrosamine	$[(C_2H_5)_2N-NO]_2H^+$	1 96	N_2/N_2	136	15
1 40	Dimethyl methylphosphonate	M_2H^+	2.06	N_2/N_2	150	11
1 40	Lysergic acid diethylamide	+	0 90, 1 05, 1 16, 1 30	N_2/N_2	200	8
1 40	*n*-Pentadecane	$C_{13}H_{27}^+$	1.28,1.34,1.47,1.54, 1.62, 1.72, 1 86, 1 93, 2 04	N_2/N_2	135	23
1 40	*n*-Tridecane	$C_{13}H_{27}^+$	1.46, 1.54,1.67,1.72, 1 82, 1 92, 2 04	N_2/N_2	135	23
1 40	Secobarbital	−	1 46	Air/N_2	230	13
1 41	2,4,6-Trinitrotoluene	$(M+NO)^+$	1 48	N_2/N_2	193	27
1 41	3,4-Dimethyl benzophenone	+		N_2/N_2		25
1 41	*n*-Propyl acetate	M_2H^+	2 02	N_2/N_2	136	10
1 42	2,4,6-Trinitrotoluene	$(M+NO)^+$	1.49	Air/N_2	193	27
1 42	Digitoxigenin	+	0 91, 1 13, 1 18	N_2/N_2	200	8
1.42	Mephobarbital	−	1.66	Air/N_2	230	13
1.42	*n*-Octyl acetate	MH^+	0 95	N_2/N_2	136	10
1.42	Tri-*n*-butylamine	+		N_2/N_2	147	9
1.43	Dibenzylamine	+		N_2/N_2	145	9
1 43	Phenobarbital	−	1 63	Air/N_2	230	13
1 44	4-Aminobenzophenone	+		N_2/N_2		25
1 44	Dicyclohexylamine	+		N_2/N_2	149	9
1 44	Mephobarbital	+	1.81	Air/N_2	230	13
1 44	Phenobarbital	+		Air/N_2	230	13
1 45	1-Octanol	+	1.06, 1.12, 1.19, 1.85	N_2/N_2	100	12
1.45	DDT	+	1 26	N_2/N_2	124	21
1 45	*m*-Phthalic acid methyl ester	+		Air/N_2	230	28
*1.45	Perylene	$(C_{20}H_{12})H^+$		N_2/N_2	140	14
1 45	Triethylphosphonoacetate	MH^+	0 97, 1 23	N_2/N_2	150	11
1.46	1-Octanol	+	0.98, 1 12, 1 21, 1.53, 1.88	N_2/N_2	22	12
1 46	1-Octanol	+	1 16	N_2/N_2	140	2
1.46	*n*-Dodecane	$C_{12}H_{25}^+$	1.54, 1.62, 1.72, 1.83, 1 92, 2.04	N_2/N_2	135	23

1.46	*n*-Tetradecane	$C_{12}H_{25}^+$	1.34, 1 54, 1 62, 1 72, 1 85, 1 92, 2 04	N_2/N_2	135	23
1.46	*n*-Tridecane	$C_{12}H_{25}^+$	1 40, 1 54, 1 62, 1 72, 1.82, 1 92,2.04	N_2/N_2	135	23
1 46	Pentobarbital	–	1 31,1 53,1 59	Air/N_2	230	13
1 46	Secobarbital	–	1 40	Air/N_2	230	13
1.47	"Dimethoate"	MH^+		N_2/N_2	150	11
1 47	1-Octanol	+	1 08, 1.14, 1.22, 1.53, 1 83	N_2/N_2	55	12
1.47	*n*-Pentadecane	$C_{12}H_{25}^+$	1.28,1.34, 1 40, 1.54, 1.62,1.72, 1 86, 1.93, 2.04	N_2/N_2	135	23
1 47	*p*-Phthalic acid methyl ester	+		Air/N_2	230	28
1 48	2,4,6-Trinitrotoluene	MH^+	1 41	N_2/N_2	193	27
*1.48	3,4-Benzopyrene	$(C_{20}H_{12})H^+$		N_2/N_2	140	14
1.48	Diethyl cyanomethyl phosphonate	$M(H_2O)H^+$	1 13, 1.39, 1 58, 1.82	N_2/N_2	150	11
1.48	*m*-Phthalic acid methyl ester	–		Air/N_2	230	28
1 48	Secobarbital	+	1 31, 1 55	Air/N_2	230	13
1.49	1-Chlorohexane	+	1.72, 1 81, 1 90, 2.06	N_2/N_2	135	20
1 49	2,4,6-Trinitrotoluene	–	1 54, 1.59	Air/N_2	200	29
*1.49	2,4,6-Trinitrotoluene	M^-	1.54, 1 59	Air/N_2	166	30
*1 49	2,4,6-Trinitrotoluene	M^-	1 54, 1.59	N_2/N_2	166	30
1.49	2,4,6-Trinitrotoluene	MH^+	1.42	Air/N_2	193	27
1 50	2,4,6-Trinitrotoluene	M^-	1 57	Air/N_2	193	27
1.50	2,4,6-Trinitrotoluene	M^-	1.60	N_2/N_2	193	27
1 50	Barbital	+	0 99	Air/N_2	230	13
*1.50	Cocaine	$(M-C_6H_5CO_2)^+$	1.16, 1 84	N_2/N_2	153	16
1.50	Hydantoin-5-propionic acid	+	1 22, 1.38	N_2/N_2	200	8
1.50	*n*-Heptyl acetate	MH^+	1.01	N_2/N_2	136	10
1.50	*n*-Octylamine	+		N_2/N_2	149	9
1 50	*p*-Phthalic acid methyl ester	–		Air/N_2	230	28
*1 50	Terephthalic acid	$(C_8H_6O_4)NO^+$	1 57, 1.77, 1 91	N_2/N_2	150	19
*1 51	Benzo[*c*]phenanthrene	$(C_{18}H_{12})H^+$		N_2/N_2	140	14
1 51	Benzophenone	+		N_2/N_2		25
1 51	Dibromonitrobenzene	$(C_6H_3Br_2NO_2)H^+$		N_2/N_2	148	31
1 51	Dimethyl terephthalate	+	1 32, 1.69	N_2/N_2	150	24
1.52	1-Bromo-2-chlorobenzene	+		N_2/N_2	220	26
*1 52	Isophthalic acid	$(C_8H_6O_4)NO^+$	1 57, 1 77, 1.91	N_2/N_2	150	19
1 52	Isophthalic acid	+	1.57, 1 76, 1 91, 2.14	N_2/N_2	150	24
1.52	Methyl benzoate	+	1 82, 2.05	N_2/N_2	150	24

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TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
1.52	Methyl caprylate	+		N_2/N_2	150	7
*1.52	Phthalic acid	$(C_8H_6O_4)NO^+$	1.64, 1.77	N_2/N_2	150	19
1.52	Phthalic acid	+	1.64, 1.77, 2.15	N_2/N_2	150	24
1.52	Terephthalic acid	+	1.57, 1.76, 1.91, 2.14	N_2/N_2	150	24
1.53	1-Bromo-2-chlorobenzene	+		N_2/N_2	175	26
1.53	1-Octanol	+	0.98, 1.12, 1.21, 1.46, 1.88	N_2/N_2	22	12
1.53	1-Octanol	+	1.08, 1.14, 1.22, 1.47, 1.83	N_2/N_2	55	12
1.53	Amobarbital	+	1.32, 1.36	Air/N_2	230	13
1.53	Dimethyl terephthalate	–		N_2/N_2	150	24
1.53	*o*-Phthalic acid methyl ester	–		Air/N_2	230	28
1.53	Pentobarbital	–	1.31, 1.46, 1.59	Air/N_2	230	13
*1.54	1,2-Benzanthracene	$(C_{18}H_{12})H^+$		N_2/N_2	140	14
1.54	1-Bromo-2-chlorobenzene	+		N_2/N_2	140	26
*1.54	2,4,6-Trinitrotoluene	$(M-H)^-$	1.49, 1.59	Air/N_2	166	30
*1.54	2,4,6-Trinitrotoluene	$(M-H)^-$	1.49, 1.59	N_2/N_2	166	30
1.54	2,4,6-Trinitrotoluene	–	1.49, 1.59	Air/N_2	200	29
1.54	Barbital	–	1.38	Air/N_2	230	13
1.54	Fluoranthene	+		N_2/N_2	85	26
1.54	*n*-Dodecane	$C_{11}H_{23}^+$	1.46, 1.62, 1.72, 1.83, 1.92, 2.04	N_2/N_2	135	23
1.54	*n*-Pentadecane	$C_{11}H_{23}^+$	1.28, 1.34, 1.40, 1.47, 1.62, 1.72, 1.86, 1.93, 2.04	N_2/N_2	135	23
1.54	*n*-Tetradecane	$C_{11}H_{23}^+$	1.34, 1.46, 1.62, 1.72, 1.85, 1.92, 2.04	N_2/N_2	135	23
1.54	*n*-Tridecane	$C_{11}H_{23}^+$	1.40, 1.46, 1.62, 1.72, 1.82, 1.92, 2.04	N_2/N_2	135	23
1.54	*n*-Undecane	$C_{11}H_{23}^+$	1.67, 1.71, 1.84, 1.92, 2.04	N_2/N_2	135	23
1.54	*o*-Chlorodiphenyl oxide	+		Air/Air	206	18
1.54	*o*-Phthalic acid methyl ester	+		Air/N_2	230	28
1.54	*p*-Chlorodiphenyl oxide	+		Air/Air	206	18
1.54	Trimethylphosphonoacetate	MNO^+	1.15, 1.26, 1.68, 1.92	N_2/N_2	150	11
1.55	1-Bromo-2-chlorobenzene	+		N_2/N_2	220	26

1 55	1-Bromo-2-chlorobenzene	+		N_2/N_2	175	26
1 55	2,4-Dinitrotoluene	MNO^+	1.62	N_2/N_2	193	27
*1 55	Chrysene	$(C_{18}H_{12})H^+$		N_2/N_2	140	14
1 55	Fluoranthene	+		N_2/N_2	175	26
1.55	Fluoranthene	+		N_2/N_2	140	26
1 55	Fluoranthene	+		N_2/N_2	110	26
1 55	Secobarbital	+	1 31, 1 48	Air/N_2	230	13
1 56	1-Bromo-2-chlorobenzene	+		N_2/N_2 (PI)	140	26
1.56	1-Bromo-2-chlorobenzene	+		N_2/N_2	110	26
1 56	1-Bromo-2-chlorobenzene	+		N_2/N_2	85	26
1.56	2,4-Dinitrotoluene	MNO^+		Air/N_2	193	27
1.56	Aprobarbital	+	1.39, 1.64, 1.75	Air/N_2	230	13
1.56	Bromochloronitrobenzene	$(C_6H_3BrClNO_2)H^+$		N_2/N_2	148	31
1 56	Dibutylnitrosamine	$[(C_4H_9)N-NO]H^+$	1.02	N_2/N_2	136	15
1.57	1-Butanol	+	1.61, 1 73, 1.84, 1 96	N_2/N_2	55	12
1 57	1-Iodobutane	+	1.18, 1.37, 1 67, 1 98, 2 20, 2 33	N_2/N_2	135	20
1.57	2,4,6-Trinitrotoluene	$(M-NO_2)$	1 50	Air/N_2	193	27
1 57	3-Chloropropiophenone	+		N_2/N_2		25
1 57	Dimethyl morpholinophosphoramidate	MH^+	1 07, 1 14, 1 77	N_2/N_2	150	11
1 57	Ethyl acetate	M_2H^+	2.06	N_2/N_2	136	10
1 57	Fluoranthene	+		N_2/N_2 (PI)	220	26
1 57	Fluoranthene	+		N_2/N_2	220	26
1 57	Fluoranthene	+		N_2/N_2 (PI)	175	26
1.57	Fluoranthene	+		N_2/N_2 (PI)	140	26
1 57	Fluoranthene	+		N_2/N_2 (PI)	85	26
*1.57	Isophthalic acid	$(C_8H_6O_4)H^+$	1.52, 1 77, 1.91	N_2/N_2	150	19
1 57	Isophthalic acid	+	1.52, 1 76, 1 91, 2.14	N_2/N_2	150	24
*1.57	Terephthalic acid	$(C_8H_6O_4)H^+$	1.52, 1 77, 1.91	N_2/N_2	150	19
1 57	Terephthalic acid	+	1.52, 1 76, 1 91, 2.14	N_2/N_2	150	24
1 58	1-Bromo-2-chlorobenzene	+		N_2/N_2 (PI)	110	26
1 58	Diethyl cyanomethyl phosphonate	MH^+	1.13, 1.39, 1 48, 1 82	N_2/N_2	150	11
1.58	Fluoranthene	+		N_2/N_2 (PI)	110	26
*1 58	Isophthalic acid	$(C_8H_6O_4)^-$	1 15	N_2/N_2	150	19
1 58	Isophthalic acid	–		N_2/N_2	150	24
1 58	*n*-Hexyl acetate	MH^+	1 08	N_2/N_2	136	10
1 59	1-Bromo-2-chlorobenzene	+		N_2/N_2 (PI)	85	26
1 59	2,4,6-Trinitrotoluene	–	1 49, 1 54	Air/N_2	200	29
1 59	2,4,6-Trinitrotoluene	–	1 49, 1 54	N_2/N_2	166	30

(Continued on p. 150)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
1 59	2,4,6-Trinitrotoluene	−	1 49, 1 54	Air/N_2	166	29
1 59	*m*-Acetotoluidide	−		Air/N_2	230	28
1 59	*n*-Heptylamine	+		N_2/N_2	146	9
1 59	Pentobarbital	−	1 31, 1 46, 1.53	Air/N_2	230	13
1 60	1-Butanol	+	1.63, 1.77, 1 92, 2 02	N_2/N_2	100	12
1 60	2,4,6-Trinitrotoluene	$(M-NO_2)^-$	1 50	N_2/N_2	193	27
*1 60	Fluoranthene	$(C_{16}H_{10})H^+$		N_2/N_2	140	14
1 60	*m*-Acetotoluidide	+		Air/N_2	230	28
1 60	*p*-Acetotoluidide	−		Air/N_2	230	28
1 61	1-Butanol	+	1 37, 1 76, 1.87, 1 97	N_2/N_2	22	12
1.61	1-Butanol	+	1.57, 1.73, 1.84, 1 96	N_2/N_2	55	12
1 61	2,4-Dinitrotoluene	−	1 67	Air/N_2	200	29
1 61	2,4-Dinitrotoluene	M^-	1 67	N_2/N_2	193	27
1 61	2,4-Dinitrotoluene	M^-	1.67	N_2/N_2	166	30
1 61	2,4-Dinitrotoluene	M^-	1 67	Air/N_2	166	30
1.61	Aprobarbital	−	1 39	Air/N_2	230	13
1 61	Dichloronitrobenzene	$(C_6H_3Cl_2NO_2)H^+$		N_2/N_2	148	31
1.61	Fluorene	+		N_2/N_2	220	26
1 61	Fluorene	+		N_2/N_2	175	26
*1.61	Hexachlorobenzene	$C_6Cl_5O^-$		N_2/N_2	111	32
1 61	*o*-Acetotoluidide	−		Air/N_2	230	28
1.61	*p*-Acetotoluidide	−		Air/N_2	230	28
1 62	1-Hexanol	+	1 32, 1 76, 2 10	N_2/N_2	100	12
1.62	2,4-Dinitrotoluene	MH^+	1.55	N_2/N_2	193	27
1 62	Iodonitrobenzene	$(C_6H_4INO_2)H^+$		N_2/N_2	148	32
1 62	*n*-Decane	$C_{10}H_{21}^+$	1 71, 1.92, 2 04	N_2/N_2	135	23
1 62	*n*-Dodecane	$C_{10}H_{21}^+$	1 46, 1.54, 1 72, 1 83, 1.92, 2 04	N_2/N_2	135	23
1.62	*n*-Pentadecane	$C_{10}H_{21}^+$	1 28, 1.34, 1.40, 1.47, 1.54, 1.72, 1 86, 1 93, 2 04	N_2/N_2	135	23
1 62	*n*-Tetradecane	$C_{10}H_{21}^+$	1 34, 1 46, 1.54, 1.72, 1.85, 1 92, 2.04	N_2/N_2	135	23

1 62	*n*-Tridecane	$C_{10}H_{21}^+$	1.40, 1 46, 1 54, 1 72, 1.82, 1 92, 2 04	N_2/N_2	135	23
1 62	*n*-Undecane	$C_{10}H_{21}^+$	1 54, 1 72, 1 84, 1 92, 2.04	N_2/N_2	135	23
1 62	*o*-Acetotoluidide	+		Air/N_2	230	28
1 63	"Tabun"	$M(H_2O)H^+$	1 73, 1 82	N_2/N_2	150	11
1 63	1-Butanol	+	1 60, 1 77, 1 92, 2 02	N_2/N_2	100	12
1 63	1-Chlorooctane	+	1.71, 1.82, 1.97, 2.09	N_2/N_2	135	20
1 63	1-Hexanol	+	1 32, 1 72	N_2/N_2	55	12
*1.63	Benzoic acid	$(C_7H_6O_2H_2O)NO^+$	1.74, 1.82	N_2/N_2	150	19
1.63	Benzoic acid	+	1 74, 1 82, 2 05	N_2/N_2	150	24
1.63	Fluorene	+		N_2/N_2	140	26
*1 63	Hexahydrophthalic anhydride	$(M+1)^+$		N_2/N_2	210	22
1 63	Mephobarbital	+	1 44, 1.81	Air/N_2	230	13
1 63	*n*-Hexyl acetate	+		N_2/N_2	140	2
1.63	Phenobarbital	−	1.43	Air/N_2	230	13
1 64	Amobarbital	−	1.30	Air/N_2	230	13
1 64	Aprobarbital	+	1 39, 1.56, 1 75	Air/N_2	230	13
*1 64	Phthalic acid	$(C_8H_4O_3)NO^+$	1 52, 1 77	N_2/N_2	150	19
1 64	Phthalic acid	+	1 52, 1 77, 2 15	N_2/N_2	150	24
1 64	Phthalic anhydride	+	1 52, 1.77, 2 15	N_2/N_2	150	24
1 65	"Soman"	MH^+	1 76, 1 92, 2 06	N_2/N_2	150	11
1 65	1-Hexanol	+	1 18, 1 81	N_2/N_2	140	2
1 65	Diphenyloxide	+		Air/Air	206	18
1 65	Isobutyrophenone	+		N_2/N_2		25
1 65	*m*-Toluic acid methyl ester	+		Air/N_2	230	28
1 66	1-Butanol	+	1 78	N_2/N_2	140	2
1 66	1-Hexanol	+	1 13, 1 36, 1 74	N_2/N_2	22	12
1 66	1-Iodoheptane	+	1.83, 1.95, 2.15	N_2/N_2	135	20
1 66	1-Iodopentane	+	1 86, 2 01, 2 20	N_2/N_2	135	20
1 66	Bromonitrobenzene	$(C_6H_4BrNO_2)H^+$		N_2/N_2	148	31
1 66	Di-*n*-butylamine	+		N_2/N_2	148	9
1 66	Dibromonitrobenzene	$(C_6H_3BrNO_2)^-$		N_2/N_2	148	31
1 66	*m*-Toluic acid methyl ester	−		Air/N_2	230	28
1 66	Mephobarbital	−	1.42	Air/N_2	230	13
*1 66	*trans*-Stilbene	$(C_{14}H_{12})^+$		N_2/N_2	140	14
1 66	Tri-*n*-propylamine	+		N_2/N_2	149	9
*1 67	"Tolan"	$(C_{14}H_{10})H^+$	1 12	N_2/N_2	140	14
1.67	1-Iodobutane	+	1 18, 1 37, 1 57, 1 98, 2 20, 2 33	N_2/N_2	135	20

(Continued on p 152)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
1.67	2,4,5-Trichlorotoluene	+		N_2/N_2	155	33
*1 67	2,4-Dinitrotoluene	$(M-H)^-$	1 61	N_2/N_2	166	30
*1.67	2,4-Dinitrotoluene	$(M-H)^-$	1.61	Air/N_2	166	30
*1 67	2,4-Dinitrotoluene	$(M-NO_2)^-$	1 61	N_2/N_2	193	27
1.67	2,4-Dinitrotoluene	–	1.61	Air/N_2	200	29
1 67	Bromonitrobenzene	$(C_6H_4BrNO_2)^-$	2.60	N_2/N_2	148	31
1.67	Fluorene	+		N_2/N_2	220	26
1 67	Fluorene	+		N_2/N_2	85	26
1 67	Fluorene	+		N_2/N_2	175	26
1 67	N,N-Diethylaniline	+		N_2/N_2	220	26
*1 67	*p*-Nitrophenol	MNO^+	1.79, 1 91	N_2/N_2	204	34
*1 67	*p*-Nitrophenol	MNO^+	1.80, 1.92	N_2/N_2	204	34
1 67	*p*-Toluic acid methyl ester	+		Air/N_2	230	28
1 67	*p*-Toluic acid methyl ester	–		Air/N_2	230	28
1 68	1-Bromoheptane	+	1 75, 1 83, 1.95, 2.01, 2.13	N_2/N_2	135	20
1.68	2,4-Dinitrotoluene	$(M-NO_2)^-$		Air/N_2	193	27
1 68	2-Methylnaphthalene	+		N_2/N_2 (PI)	175	26
1.68	2-Methylnaphthalene	+		N_2/N_2 (PI)	110	26
1 68	2-Methylnaphthalene	+		N_2/N_2 (PI)	85	26
1.68	Anthracene	+		N_2/N_2 (PI)	110	26
1 68	Diisobutylamine	+		N_2/N_2	148	9
*1 68	Dibenzyl	$(C_{14}H_{14})H^+$		N_2/N_2	140	14
1 68	Fluorene	+		N_2/N_2	220	26
1 68	Fluorene	+		N_2/N_2	140	26
1 68	Fluorene	+		N_2/N_2 (PI)	110	26
1 68	N,N-Diethylaniline	+		N_2/N_2	85	26
1 68	*o*-Toluic acid methyl ester	+		Air/N_2	230	28
1 68	Trimethylphosphonoacetate	MH^+	1 15, 1 26, 1 54, 1 92	N_2/N_2	150	11
1.69	2-Methylnaphthalene	+		N_2/N_2	175	26
1 69	2-Methylnaphthalene	+		N_2/N_2	110	26
1.69	Anthracene	+		N_2/N_2	140	32
1 69	Diethyl-2-bromoethylphosphonate	$(M-Br)H^+$	1 15	N_2/N_2	150	11

1 69	Dimethyl terephthalate	+	1.32, 1 51	N_2/N_2	150	24
1 69	Fluorene	+		N_2/N_2 (PI)	175	26
1.69	N,N-Diethylaniline	+		N_2/N_2	175	26
1 69	*o*-Toluic acid methyl ester	−		Air/N_2	230	28
1.69	Pyridine	+		N_2/N_2 (PI)	85	26
1 69	Pyridine	+		N_2/N_2	85	26
1.69	Quinoline	+		N_2/N_2 (PI)	110	26
1 70	2-Methylnaphthalene	+		N_2/N_2 (PI)	140	26
1.70	2-Methylnaphthalene	+		N_2/N_2	140	26
1 70	2-Methylnaphthalene	+		N_2/N_2	85	26
1.70	4-*tert*-Butylpyridine	+		N_2/N_2	147	9
1 70	Anthracene	+		N_2/N_2	110	26
1 70	*m*-Methyl phenetole	+		Air/N_2	230	28
1 70	N,N-Diethylaniline	+		N_2/N_2 (PI)	220	26
1 70	N,N-Diethylaniline	+		N_2/N_2 (PI)	85	26
1 70	*n*-Hexylamine	+		N_2/N_2	146	9
1 70	*o*-Chloronitrobenzene	$(C_6H_5ClNO_2)H^+$		N_2/N_2	125	17
1 71	"Sarin"	$M(H_2O)_2H^+$	1.84, 1 95	N_2/N_2	150	11
1 71	1-Chlorooctane	+	1 63, 1 82, 1.97, 2 09	N_2/N_2	135	20
1 71	2-Methylnaphthalene	+		N_2/N_2 (PI)	220	26
1 71	Anthracene	+		N_2/N_2 (PI)	85	26
1 71	Anthracene	+		N_2/N_2	85	26
1 71	Dimethylnitrosamine	$[(CH_3)_2N-NO]_2H^+$	2 21	N_2/N_2	136	15
1 71	Fluorene	+		N_2/N_2 (PI)	85	26
1 71	Methyl caproate	+		N_2/N_2	150	7
1 71	*n*-Decane	$C_9H_{19}^+$	1 62, 1 92, 2.04	N_2/N_2	135	23
1 71	*n*-Undecane	$C_9H_{19}^+$	1 54, 1 62, 1.84, 1 92, 2.04	N_2/N_2	135	23
1.71	N,N-Diethylaniline	+		N_2/N_2	140	26
1 71	N,N-Diethylaniline	+		N_2/N_2	140	26
1.71	*o*-Chloronitrobenzene	−	1.86, 2.92	N_2/N_2	125	17
1 71	*o*-Methyl phenetole	+		Air/N_2	230	28
1 71	Quinoline	+		N_2/N_2	85	26
1 72	"Fenitrothion"	$NO_2C_6H_5(CH_3)OH^+$	1 26, 1 31, 1 40, 1.80	N_2/N_2	150	11
1 72	1-Bromooctane	+	1.82, 2 00, 2.20	N_2/N_2	135	20
1 72	1-Chlorohexane	+	1.49, 1.81, 1 90, 2 06	N_2/N_2	135	20
1 72	1-Hexanol	+	1 32, 1.63	N_2/N_2	55	12
1 72	2-Methylnaphthalene	+		N_2/N_2	220	26
1 72	Anthracene	+		N_2/N_2 (PI)	175	26

(Continued on p 154)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
1 72	Anthracene	+		N_2/N_2	175	26
1.72	Chloronitrobenzene	MH^+		N_2/N_2	148	31
1 72	Fluorene	+		N_2/N_2 (PI)	140	26
1.72	Fluorene	+		N_2/N_2	110	26
1 72	N,N-Diethylaniline	+		N_2/N_2 (PI)	175	26
1.72	*n*-Dodecane	$C_9H_{19}^+$	1.46, 1.54, 1 62, 1 83, 1.92, 2 04	N_2/N_2	135	23
1.72	*n*-Nonane	$C_9H_{19}^+$	1.83, 2.06	N_2/N_2	135	23
1 72	*n*-Pentadecane	$C_9H_{19}^+$	1 28, 1 34, 1.40, 1.47, 1.54, 1 62, 1 86, 1 93, 2 04	N_2/N_2	135	23
1 72	*n*-Tetradecane	$C_9H_{19}^+$	1 34, 1 46, 1.54, 1.62, 1 85, 1 92, 2 04	N_2/N_2	135	23
1 72	*n*-Tridecane	$C_9H_{19}^+$	1 40, 1 46, 1.54, 1.62, 1 82, 1 92, 2 04	N_2/N_2	135	23
1 72	*p*-Methyl phenetole	+		Air/N_2	230	28
1 73	"Tabun"	$M(H_2O)^+$	1 63, 1 82	N_2/N_2	150	11
1 73	1-Butanol	+	1.57, 1.61, 1.84, 1.96	N_2/N_2	55	12
1 73	1-Chloroheptane	+	1.81, 1 95, 2 11	N_2/N_2	135	20
1.73	1-Iodohexane	+	1.81, 1.89, 2 06	N_2/N_2	135	20
*1 73	α-Naphthyl iodide	MH^+		N_2/N_2	140	14
1 73	Anthracene	+		N_2/N_2 (PI)	220	26
1 73	Dichloronitrobenzene	$(C_6H_3ClNO_2)^-$		N_2/N_2	148	31
1 73	N,N-Diethylaniline	+		N_2/N_2 (PI)	140	26
1.73	N,N-Diethylaniline	+		N_2/N_2 (PI)	110	26
1 73	*o*-Dimethoxy benzene	+		Air/N_2	230	28
1.74	1-Bromohexane	+	1.85, 1.91, 2.07	N_2/N_2	135	20
1 74	1-Chlorobutane	+	1 83, 1.98, 2 13, 2 38	N_2/N_2	135	20
1.74	1-Hexanol	+	1.13, 1.36, 1 66	N_2/N_2	22	12
1 74	Benzoic acid	+	1 63, 1 82, 2 05	N_2/N_2	150	24
*1 74	Benzoic acid	$(C_7H_6O_2)NO^+$	1 63, 1 82	N_2/N_2	150	19
1 74	Chloronitrobenzene	$(C_6H_4ClNO_2)$	2.91	N_2/N_2	148	31
*1.74	*m*-Mononitrotoluene	M^-	1 81, 2 70	Air/N_2	166	30

*1.74	*m*-Mononitrotoluene	M^-	2 70	N_2/N_2	166	30
1 74	Mononitrotoluene	–	1.81	Air/N_2	200	29
1 74	N-Methylaniline	+		N_2/N_2	85	26
*1 74	*o*-Mononitrotoluene	M^-	1 81, 2.70	Air/N_2	166	30
*1.74	*o*-Mononitrotoluene	M^-	2 70	N_2/N_2	166	30
*1 74	*p*-Mononitrotoluene	M^-	1 81, 2.70	Air/N_2	166	30
*1 74	*p*-Mononitrotoluene	M^-	2 70	N_2/N_2	166	30
1 74	Propiophenone	+		N_2/N_2		25
1 74	Pyridine	+		N_2/N_2 (Pl)	110	26
1 74	Pyridine	+		N_2/N_2	110	26
1 74	Quinoline	+		N_2/N_2 (Pl)	220	26
1 74	Quinoline	+		N_2/N_2	110	26
1 74	*tert* -Butylbenzene	+	2,01, 2 18, 2 34	N_2/N_2 (Pl)	150	5
1,75	1-Bromoheptane	+	1 68, 1 83, 1 95, 2.01, 2.13	N_2/N_2	135	20
1 75	Anthracene	+		N_2/N_2 (Pl)	140	26
1 75	Anthracene	+		N_2/N_2	140	26
*1 75	Anthracene	MH^+		N_2/N_2	140	14
1,75	Aprobarbital	+	1 39, 1 56, 1 64	Air/N_2	230	13
1 75	Quinoline	+		N_2/N_2 (Pl)	140	26
1 75	*tert* -Butylbenzene	+	2 03, 2 21	N_2/N_2	150	5
1 76	"Soman"	$(M-CH_3)H^+$	1,65, 1 92, 2 06	N_2/N_2	150	11
1 76	1-Butanol	+	1 37, 1 61, 1.87, 1 97	N_2/N_2	22	12
1 76	1-Hexanol	+	1.32, 1,62, 2.10	N_2/N_2	100	12
*1 76	Ethylcellosolve acetate	$(M+H)^+$	2 11	N_2/N_2	210	22
1 76	Isophthalic acid	+	1 52, 1,57, 1.91, 2.14	N_2/N_2	150	24
1 76	Lutidine	+		N_2/N_2 (Pl)	110	26
1 76	*m*-Dimethoxybenzene	+		Air/N_2	230	28
1 76	*p*-Dimethoxybenzene	+		Air/N_2	230	28
*1,76	Phenanthrene	MH^+		N_2/N_2	140	14
1 76	Quinoline	+		N_2/N_2	220	26
1,76	Terephthalic acid	+	1 52, 1,57, 1 91, 2.14	N_2/N_2	150	24
1 77	1-Butanol	+	1.60, 1 63, 1 92, 2 02	N_2/N_2	100	12
1,77	Anthracene	+		N_2/N_2	220	26
1,77	Dimethyl morpholinophosphoramidate	$(M-CH_3O)H^+$	1.07, 1 14, 1 57	N_2/N_2	150	11
*1 77	Isophthalic acid	$(C_8H_4O_3)H^+$	1 52, 1 57, 1 91	N_2/N_2	150	19
1 77	N-Methylaniline	+		N_2/N_2	140	26
*1 77	Phthalic acid	$(C_8H_4O_3)H^+$	1 52, 1 64	N_2/N_2	150	19
*1 77	Phthalic acid	$(C_8H_6O_4-H_2O)^-$		N_2/N_2	150	19

(Continued on p 156)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
1.77	Phthalic acid	+	1.52, 1.64, 2.15	N_2/N_2	150	24
1.77	Phthalic acid	–	2.15	N_2/N_2	150	24
1.77	Phthalic anhydride	+	1.52, 1.64, 2.15	N_2/N_2	150	24
1.77	Phthalic anhydride	–		N_2/N_2	150	24
1.77	Quinoline	+		N_2/N_2 (PI)	175	26
*1.77	Terephthalic acid	$(C_8H_4O_3)H^+$	1.52, 1.57, 1.91	N_2/N_2	150	19
1.78	"Parathion"	$NO_2C_6H_5OH^+$	1.22, 1.27	N_2/N_2	150	11
1.78	1-Butanol	+	1.66	N_2/N_2	140	2
1.78	Benzylamine	+		N_2/N_2	149	9
1.78	Quinoline	+		N_2/N_2	140	26
1.79	Aniline	+		N_2/N_2	85	26
1.79	N-Methylaniline	+		N_2/N_2	110	26
1.79	*p*-Nitrophenol	MH^+	1.67, 1.91	N_2/N_2	204	34
1.80	"Fenitrothion"	$NO_2C_6H_5OH^+$	1.26, 1.31, 1.40, 1.72	N_2/N_2	150	11
1.80	"Methyl parathion"	$NO_2C_6H_4OH^+$	1.31, 1.36	N_2/N_2	151	11
1.80	Fluoronitrobenzene	$(C_6H_4FNO_2)H^+$		N_2/N_2	148	31
1.80	Naphthalene	+		N_2/N_2	140	26
*1.80	*p*-Nitrophenol	MH^+	1.67, 1.92	N_2/N_2	204	34
1.81	1-Chloroheptane	+	1.73, 1.95, 2.11	N_2/N_2	135	20
1.81	1-Chlorohexane	+	1.49, 1.72, 1.90, 2.06	N_2/N_2	135	20
1.81	1-Hexanol	+	1.18, 1.65	N_2/N_2	140	2
1.81	1-Iodohexane	+	1.73, 1.89, 2.06	N_2/N_2	135	20
1.81	2,4-Dichlorotoluene	+		N_2/N_2	155	33
1.81	Iodobenzene	MH^+		N_2/N_2	125	17
*1.81	*m*-Mononitrotoluene	$(M-H)^-$	1.74, 2.70	Air/N_2	166	30
1.81	Mephobarbital	+	1.44, 1.63	Air/N_2	230	13
1.81	Mononitrotoluene	–	1.74	Air/N_2	200	29
1.81	*n*-Bromooctane	$C_8H_{17}^+$		N_2/N_2	135	23
1.81	Naphthalene	+		N_2/N_2 (PI)	140	26
1.81	Naphthalene	+		N_2/N_2	85	26
*1.81	Nitrobenzene	$(C_5H_6NO_2)^-$		N_2/N_2	210	22
*1.81	*o*-Mononitrotoluene	$(M-H)^-$	1.74, 2.70	Air/N_2	166	30

*1 81	*p*-Mononitrotoluene	$(M-H)^-$	1.74, 2.70	Air/N_2	166	30
1 81	Quinoline	+		N_2/N_2	175	26
1.82	"Tabun"	MH^+	1 63, 1.73	N_2/N_2	150	11
1 82	1-Bromooctane	+	1 72, 2 00, 2 20	N_2/N_2	135	20
1.82	1-Chlorooctane	+	1 63, 1.71, 1 97, 2 09	N_2/N_2	135	20
1 82	Acetophenone	+		N_2/N_2		25
1.82	Azulene	+		N_2/N_2 (PI)	140	26
1 82	Azulene	+		N_2/N_2	140	26
1.82	Azulene	+		N_2/N_2	110	26
1.82	Benzoic acid	+	1.63, 1 74, 2 05	N_2/N_2	150	24
*1 82	Benzoic acid	$(C_7H_6O_2)H^+$	1.63, 1.74	N_2/N_2	150	19
1 82	Diethyl cyanomethyl phosphonate	$(M-CN)H^+$	1.13, 1 39, 1.48, 1.58	N_2/N_2	150	11
1.82	Fluoronitrobenzene	$(C_6H_4FNO_2)^-$		N_2/N_2	148	31
1 82	Indoline	+		N_2/N_2 (PI)	85	26
1.82	Methyl benzoate	+	1.52, 2.05	N_2/N_2	150	24
1 82	Methyl benzoate	−		N_2/N_2	150	24
1.83	*n*-Dodecane	$C_8H_{17}^+$	1 46, 1.54, 1.62, 1 72, 1 92, 2 04	N_2/N_2	135	23
1.83	*n*-Nonane	$C_8H_{17}^+$	1 72, 2 06	N_2/N_2	135	23
1 82	*n*-Pentylamine	+		N_2/N_2	149	9
1.82	*n*-Tridecane	$C_8H_{17}^+$	1 40, 1.46, 1.54, 1.62, 1.72, 1 92, 2.04	N_2/N_2	135	23
1.84	*n*-Undecane	$C_8H_{17}^+$	1.54, 1.62, 1 71, 1 92, 2 04	N_2/N_2	135	23
1 82	Naphthalene	+		N_2/N_2	110	26
1.82	Naphthalene	+		N_2/N_2 (PI)	85	26
1 83	1-Bromoheptane	+	1.68, 1 75, 1 95, 2.01, 2.13	N_2/N_2	135	20
1.83	1-Chlorobutane	+	1 74, 1.98, 2 13, 2 38	N_2/N_2	135	20
1 83	1-Iodoheptane	+	1 66, 1 95, 2 15	N_2/N_2	135	20
*1.83	1-Naphthaldehyde	$C_{11}H_8O^-$		N_2/N_2	111	32
1 83	1-Octanol	+	1 08, 1 14, 1 22, 1.47, 1 53	N_2/N_2	55	12
1.83	Aniline	+		N_2/N_2	140	26
1 83	Aniline	+		N_2/N_2	110	26
1 83	Azulene	+		N_2/N_2 (PI)	110	26
1 83	Azulene	+		N_2/N_2	85	26
1.83	*n*-Amylamine	MH^+		N_2/N_2	200	35
1 83	*n*-Octane	$C_8H_{17}^+$	2.06	N_2/N_2	135	23
1.84	"Sarin"	$M(H_2O)H^+$	1 71, 1.95	N_2/N_2	150	11
1 84	1-Bromobutane	+	1.89, 2 00, 2 15, 2.36	N_2/N_2	135	20

(Continued on p 158)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
1.84	1-Butanol	+	1.57, 1.61, 1.73, 1.96	N_2/N_2	55	12
1.84	2,4,6-Collidine	+		N_2/N_2	147	9
*1.84	Acenaphthalene	$(C_{12}H_8)H^+$	1.01, 1.27	N_2/N_2	140	14
1.84	Azulene	+		N_2/N_2	220	26
1.84	Azulene	+		N_2/N_2	175	26
1.84	Azulene	+		N_2/N_2 (PI)	85	26
1.84	Benzaldehyde	+	1.40, 1.91, 2.03	N_2/N_2	150	24
*1.84	Cocaine	$(M-C_6H_5CO_2-CO_2CH_3)^+$	1.16, 1.50	N_2/N_2	153	16
1.84	Indane	+		N_2/N_2	140	26
1.84	Indane	+		N_2/N_2	110	26
1.84	Indane	+		N_2/N_2	85	26
1.84	N-Methylaniline	+		N_2/N_2	175	26
1.84	Naphthalene	+		N_2/N_2	220	26
1.84	Naphthalene	+		N_2/N_2	175	26
1.84	Naphthalene	+		N_2/N_2 (PI)	110	26
1.84	Nitrobenzene	$(C_6H_4NO_2)^-$		N_2/N_2	148	31
1.85	1-Bromohexane	+	1.74, 1.91, 2.07	N_2/N_2	135	20
1.85	1-Octanol	+	1.06, 1.12, 1.19, 1.45	N_2/N_2	100	12
1.85	Indoline	+		N_2/N_2	85	26
1.85	Indoline	+		N_2/N_2 (PI)	110	26
1.85	Lutidine	+		N_2/N_2	110	26
1.85	*n*-Pentyl acetate	MH^+	1.18	N_2/N_2	136	10
1.85	*n*-Tetradecane	$C_8H_{17}^+$	1.34, 1.46, 1.54, 1.62, 1.72, 1.92, 2.04	N_2/N_2	135	23
1.86	1-Iodopentane	+	1.66, 2.01, 2.20	N_2/N_2	135	20
1.86	Azulene	+		N_2/N_2 (PI)	220	26
1.86	Indane	+		N_2/N_2	175	26
1.86	Indane	+		N_2/N_2 (PI)	85	26
1.86	*m*-Cresol	+		N_2/N_2	85	26
1.86	Mesitylene	+		N_2/N_2	147	9
1.86	*n*-Pentadecane	$C_8H_{17}^+$	1.28, 1.34, 1.40, 1.47, 1.54, 1.62, 1.72, 1.93, 2.04	N_2/N_2	135	23

1.86	Naphthalene	+		N_2/N_2 (PI)	220	26
1 86	Naphthalene	+		N_2/N_2 (PI)	175	26
1 86	*o*-Chloronitrobenzene	$C_6H_4NO_2^-$	1.71, 2 92	N_2/N_2	125	17
*1 86	*p*-Nitrophenol	$(M-H)^-$		N_2/N_2	204	34
1.87	1-Butanol	+	1 37, 1 61, 1 76, 1 97	N_2/N_2	22	12
1 87	Indoline	+		N_2/N_2	175	26
1 87	Indoline	+		N_2/N_2	110	26
1 87	*m*-Cresol	+		N_2/N_2 (PI)	85	26
1 87	*m*-Xylene	+		N_2/N_2 (PI)	85	26
1 87	Naphthalene	+	2 03, 2 14	N_2/N_2	150	5
1 87	Nitrobenzene	M^-		N_2/N_2	125	17
*1.87	*p*-Nitrobenzaldehyde	$C_7H_6NO_2^-$		N_2/N_2	111	32
*1 87	*p*-Nitrophenol	$(M-H)^-$		N_2/N_2	204	34
1 88	1-Chloropentane	+	1 40, 1.99, 2 20, 2.31	N_2/N_2	135	20
1 88	1-Octanol	+	0.98, 1.12, 1.21, 1 46, 1 53	N_2/N_2	22	12
1.88	Azulene	+		N_2/N_2 (PI)	175	26
1 88	Di-*n*-propylamine	+		N_2/N_2	149	9
1.88	Indane	+		N_2/N_2 (PI)	110	26
1.88	Indoline	+		N_2/N_2 (PI)	175	26
1.88	Lutidine	+		N_2/N_2	140	26
1 88	Nitrobenzene	MH^+		N_2/N_2	125	17
1 89	1-Bromobutane	+	1 84, 2 00, 2.15, 2 36	N_2/N_2	135	20
1 89	1-Iodohexane	+	1 73, 1.81, 2.06	N_2/N_2	135	20
1 89	1-Nitropropane	MH^+		N_2/N_2	108	36
1 89	Aniline	+		N_2/N_2	220	26
*1 89	Fumaric acid	M^-	2.15	N_2/N_2	150	37
*1.89	Fumaric acid	MH^+	1.99	N_2/N_2	150	37
1 89	Indane	+		N_2/N_2 (PI)	140	26
1 89	Indene	+		N_2/N_2	85	26
1 89	Indoline	+		N_2/N_2 (PI)	140	26
1.89	*m*-Toluidine	+		N_2/N_2 (PI)	85	26
1 89	*m*-Toluidine	+		N_2/N_2	85	26
1.89	*m*-Xylene	+		N_2/N_2	85	26
*1 89	Maleic acid	MH^+	1 99	N_2/N_2	150	37
1 90	1-Chlorohexane	+	1 49, 1 72, 1 81, 2 06	N_2/N_2	135	20
1 90	Hexanol	M_2H^+		N_2/N_2	100	36
1.90	Indane	+		N_2/N_2 (PI)	175	26
1 90	Indene	+		N_2/N_2	110	26

(Continued on p. 160)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
1 90	Indoline	+		N_2/N_2 (PI)	220	26
1 90	Indoline	+		N_2/N_2	140	26
1 90	Lutidine	+		N_2/N_2 (PI)	140	26
1 90	Lutidine	+		N_2/N_2 (PI)	110	26
1.90	Lutidine	+		N_2/N_2 (PI)	85	26
1 90	*m*-Toluidine	+		N_2/N_2	110	26
1.90	N,N-Diethylaniline	+		N_2/N_2	220	26
1 90	N-Methylaniline	+		N_2/N_2 (PI)	85	26
1.90	Naphthalene	+	2.09, 2.21	N_2/N_2 (PI)	150	5
1 91	1-Bromohexane	+	1.74, 1 85, 2.07	N_2/N_2	135	20
1 91	Aniline	+		N_2/N_2	149	9
1 91	Aniline	+		N_2/N_2	175	26
1.91	Benzaldehyde	+	1 40, 1 84, 2 03	N_2/N_2	150	24
1 91	Bromobenzene	MH^+		N_2/N_2	125	17
1 91	Diisopropylamine	+		N_2/N_2	149	9
1 91	Ethanol	+	2.07	N_2/N_2	55	12
*1 91	Isophthalic acid	$(C_7H_5O)H^+$	1 52, 1 57, 1 77	N_2/N_2	150	19
1 91	Isophthalic acid	+	1.52, 1 57, 1 76, 2 14	N_2/N_2	150	24
1.91	Lutidine	+		N_2/N_2	220	26
1.91	Lutidine	+		N_2/N_2 (PI)	175	26
1 91	Lutidine	+		N_2/N_2	175	26
1.91	*m*-Toluidine	+		N_2/N_2	220	26
1.91	*m*-Toluidine	+		N_2/N_2 (PI)	110	26
1 91	*m*-Xylene	+		N_2/N_2 (PI)	110	26
1 91	N-Methylaniline	+		N_2/N_2	220	26
1 91	N-Methylaniline	+		N_2/N_2 (PI)	140	26
*1.91	*p*-Nitrophenol	$(M-31)^+$	1.67, 1 79	N_2/N_2	204	34
*1 91	Terephthalic acid	$(C_7H_5O)H^+$	1.52, 1.57, 1 77	N_2/N_2	150	19
1 91	Terephthalic acid	+	1 52, 1.57, 1 76, 2.14	N_2/N_2	150	24
1 92	"Soman"	$[M-C(CH_3)_2]H^+$	1 65, 1 76, 2.06	N_2/N_2	150	11
1.92	1-Butanol	+	1.60, 1 63, 1 77, 2.02	N_2/N_2	100	12
1 92	Indane	+		N_2/N_2	220	26

1 92	Indene	+		N_2/N_2	220	26
1.92	Indene	+		N_2/N_2 (PI)	110	26
1 92	Indene	+		N_2/N_2 (PI)	85	26
1 92	Indoline	+		N_2/N_2	220	26
1 92	Lutidine	+		N_2/N_2 (PI)	220	26
1 92	*m*-Toluidine	+		N_2/N_2	175	26
1.92	*m*-Toluidine	+		N_2/N_2 (PI)	140	26
1 92	*m*-Toluidine	+		N_2/N_2	140	26
1.92	*m*-Xylene	+		N_2/N_2	220	26
1 92	*m*-Xylene	+		N_2/N_2	110	26
1.92	*n*-Bromoheptane	$C_7H_{15}^+$		N_2/N_2	135	23
1 92	*n*-Decane	$C_7H_{15}^+$	1.62, 1.71, 2.04	N_2/N_2	135	23
1.92	*n*-Dodecane	$C_7H_{15}^+$	1 46, 1 54, 1 62, 1.72, 1 83, 2.04	N_2/N_2	135	23
1.92	*n*-Tetradecane	$C_7H_{15}^+$	1 34, 1.46, 1 54, 1 62, 1 72, 1 85, 2.04	N_2/N_2	135	23
1 92	*n*-Tridecane	$C_7H_{15}^+$	1.40, 1.46, 1 54, 1 62, 1.72, 1.87, 2.04	N_2/N_2	135	23
1 92	*n*-Undecane	$C_7H_{15}^+$	1.54, 1.62, 1.71, 1 84, 2.04	N_2/N_2	135	23
1 92	N,N-Diethylaniline	+		N_2/N_2	175	26
1 92	N,N-Diethylaniline	+		N_2/N_2	140	26
1.92	*n*-Heptane	$C_7H_{15}^+$	2 33	N_2/N_2	135	23
*1 92	*p*-Nitrophenol	$(M-31)^+$	1 67, 1.80	N_2/N_2	204	34
1.92	Trimethylphosphonoacetate	$(M-CH_3O)H^+$	1.15, 1 26, 1 54, 1 68	N_2/N_2	150	11
1 93	2-Hexanone	M_2H^+		N_2/N_2	127	36
1.93	Ethanol	+	2.10	N_2/N_2	22	12
1 93	Indane	+		N_2/N_2 (PI)	220	26
1 93	Indene	+		N_2/N_2	140	26
1 93	*m*-Cresol	+		N_2/N_2 (PI)	110	26
1 93	*m*-Cresol	+		N_2/N_2 (PI)	110	26
1 93	*m*-Xylene	+		N_2/N_2	140	26
1 93	Methyl butyrate	+		N_2/N_2	150	7
1 93	*n*-Pentadecane	$C_7H_{15}^+$	1 28, 1 34, 1 40, 1.47, 1.54, 1.62, 1.72, 1 86, 2.04	N_2/N_2	135	23
1.93	N,N-Diethylaniline	+		N_2/N_2	110	26
1 93	N-Methylaniline	+		N_2/N_2 (PI)	110	26
1.94	1-Bromopentane	+	1.99, 2 07, 2 20	N_2/N_2	135	20
*1 94	Azulene	$C_{10}H_6^-$		N_2/N_2	111	32

(Continued on p. 162)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
*1.94	Benżaldehyde	$C_7H_6O^-$		N_2/N_2	111	32
1 94	Indene	+		N_2/N_2	175	26
1 94	*m*-Toluidine	+		N_2/N_2 (PI)	220	26
1 94	*m*-Toluidine	+		N_2/N_2 (PI)	175	26
1 94	*m*-Xylene	+		N_2/N_2	175	26
1 94	*o*-Fluorotoluene	+		Air/N_2	230	28
1 95	"Sarin"	MH^+	1.71, 1.84	N_2/N_2	150	11
1.95	1-Bromoheptane	+	1 68, 1 75, 1 83, 2.01, 2.13	N_2/N_2	135	20
1 95	1-Chloroheptane	+	1 73, 1 81, 2.11	N_2/N_2	135	20
1 95	1-Iodoheptane	+	1 66, 1 83, 2.15	N_2/N_2	135	20
1 95	2,4-Lutidine	+		Air/N_2	147	9
1 95	Anıline	+		N_2/N_2	85	26
1 95	Indene	+		N_2/N_2	220	26
1 95	*m*-Cresol	+		CO_2/CO_2	140	26
1.95	*m*-Fluorotoluene			Air/N_2	230	28
1.95	*m*-Xylene	+		N_2/N_2 (PI)	220	26
1.95	*m*-Xylene	+		N_2/N_2 (PI)	175	26
1 95	*m*-Xylene	+		N_2/N_2 (PI)	140	26
1.95	*p*-Fluorotoluene	+		Air/N_2	230	28
1 95	Phenol	+		N_2/N_2	85	26
1 95	*tert* -Pentylamıne	+		N_2/N_2	149	9
1 95	Trıethylamıne	+		N_2/N_2	146	9
1.96	1-Butanol	+	1.57, 1.61, 1.73, 1.84	N_2/N_2	55	12
1 96	Diethylnitrosamine	$[(C_2H_5)_2N-NO]H^+$	1.40	N_2/N_2	136	15
1 96	Indene	+		N_2/N_2 (PI)	175	26
1.96	Indene	+		N_2/N_2 (PI)	140	26
1 96	*m*-Chlorotoluene	+		N_2/N_2	220	26
1.96	*p*-Chlorotoluene	+		N_2/N_2	155	33
1 96	Phenol	+		N_2/N_2 (PI)	85	26
1.97	1-Butanol	+	1.37, 1.61, 1.76, 1.87	N_2/N_2	22	12
1 97	1-Chlorooctane	+	1.63, 1.71, 1 82, 2 09	N_2/N_2	135	20
1.97	*m*-Chlorotoluene	+		N_2/N_2 (PI)	220	26

1 97	*m*-Cresol	+		N_2/N_2	230	26
1 97	*m*-Cresol	+		N_2/N_2	175	26
1,97	*m*-Cresol	+		N_2/N_2 (PI)	140	26
1 97	*n*-Butylamine	+		N_2/N_2	146	9
1,98	1-Chlorobutane	+	1 74, 1.83, 2 13, 2 38	N_2/N_2	135	20
1 98	1-Iodobutane	+	1.18, 1.37, 1.57, 1.67, 2.20, 2.33	N_2/N_2	135	20
1,98	Ethanol	+	2 10, 2 17	N_2/N_2	100	12
1 98	*m*-Chlorotoluene	+		N_2/N_2 (PI)	175	26
1 98	*m*-Chlorotoluene	+		N_2/N_2	175	26
1 98	*m*-Xylene	+		N_2/N_2	149	9
1 98	*o*-Xylene	+		N_2/N_2	149	9
1 98	*p*-Xylene	+		N_2/N_2	149	9
1 99	1-Bromopentane	+	1 94, 2 07, 2 20	N_2/N_2	135	20
1 99	1-Chloropentane	+	1.40, 1 88, 2 20, 2 31	N_2/N_2	135	20
1 99	Chlorobenzene	MH^+		N_2/N_2	125	17
*1 99	Chloropentafluorobenzene	$(C_6F_5O)^-$		N_2/N_2	111	32
*1 99	Fumaric acid	$(M-18)H^+$	1 89	N_2/N_2	150	37
1 99	*m*-Chlorotoluene	+		N_2/N_2	110	26
1 99	*m*-Chlorotoluene	+		N_2/N_2 (PI)	85	26
1 99	*m*-Chlorotoluene	+		N_2/N_2	85	26
1 99	*m*-Cresol	+		N_2/N_2 (PI)	220	26
*1 99	Maleic acid	$(M-18)H^+$	1 89	N_2/N_2	150	37
2,00	1-Bromobutane	+	1.84, 1 89, 2.15, 2 36	N_2/N_2	135	20
2 00	1-Bromooctane	+	1 72, 1 82, 2.20	N_2/N_2	135	20
2 00	Aniline	+		N_2/N_2	140	26
*2 00	Benzene	$(C_6H_6)NO^+$	2 22	N_2/N_2	50	38
2 00	*m*-Chlorotoluene	+		N_2/N_2 (PI)	110	26
2 00	*m*-Cresol	+		N_2/N_2 (PI)	175	26
2 00	*n*-Butyl acetate	+		N_2/N_2	140	2
2 00	*n*-Butyl acetate	MH^+	1.28	N_2/N_2	136	10
2 00	Phenol	+		N_2/N_2	110	26
2 01	1-Bromoheptane	+	1 68, 1 75, 1 83, 1.95, 2 13	N_2/N_2	135	20
2 01	1-Iodopentane	+	1 66, 1.86, 2.20	N_2/N_2	135	20
2 01	Aniline	+		N_2/N_2	110	26
2 01	Aniline	+		N_2/N_2	85	26
2 01	*m*-Chlorotoluene	+		N_2/N_2 (PI)	140	26
2,01	*m*-Chlorotoluene	+		N_2/N_2	140	26
2 01	Phenol	+		N_2/N_2 (PI)	110	26

(Continued on p 164)

TABLE I *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
2.01	*tert.*-Butylbenzene	+	1.74, 2.18, 2.34	N_2/N_2 (PI)	150	5
2.02	1-Butanol	+	1.60, 1.63, 1.77, 1.92	N_2/N_2	100	12
2.02	*n*-Propyl acetate	MH^+	1.41	N_2/N_2	136	10
2.02	Pyridine	+		N_2/N_2 (PI)	140	26
2.03	Benzaldehyde	+	1.40, 1.84, 1.91	N_2/N_2	150	24
2.03	Naphthalene	+	1.87, 2.14	N_2/N_2	150	5
2.03	Nitrobenzene	−		N_2/N_2	111	32
2.03	*n*-Bromohexane	$C_6H_{13}^+$		N_2/N_2	135	23
2.03	*tert*-Butylamine	+		N_2/N_2	148	9
2.03	*tert.*-Butylbenzene	+	1.75, 2.21	N_2/N_2	150	5
2.04	Aniline	+		N_2/N_2 (PI)	110	26
*2.04	Benzene	$(C_6H_6)NO^+$	2.20, 2.23, 2.25	N_2/N_2	93	38
2.04	*n*-Decane	$C_6H_{13}^+$	1.62, 1.71, 1.92	N_2/N_2	135	23
2.04	*n*-Dodecane	$C_6H_{13}^+$	1.46, 1.54, 1.62, 1.72, 1.83, 1.92	N_2/N_2	135	23
2.04	*n*-Pentadecane	$C_6H_{13}^+$	1.28, 1.34, 1.40, 1.47, 1.54, 1.62, 1.72, 1.86, 1.93	N_2/N_2	135	23
2.04	*n*-Tetradecane	$C_6H_{13}^+$	1.34, 1.46, 1.54, 1.62, 1.72, 1.85, 1.92	N_2/N_2	135	23
2.04	*n*-Tridecane	$C_6H_{13}^+$	1.40, 1.46, 1.54, 1.62, 1.72, 1.82, 1.92	N_2/N_2	135	23
2.04	*n*-Undecane	$C_6H_{13}^+$	1.54, 1.62, 1.71, 1.84, 1.92	N_2/N_2	135	23
2.04	*o*-Xylene	+		Air/Air	206	18
2.05	Aniline	+		N_2/N_2	220	26
*2.05	Azulene	$(C_{10}H_8)H^+$		N_2/N_2	140	14
2.05	Benzoic acid	+	1.63, 1.74, 1.82	N_2/N_2	150	24
2.05	Methyl benzoate	+	1.52, 1.82	N_2/N_2	150	24
2.05	*n*-Hexane	$C_6H_{13}^+$		N_2/N_2	135	23
2.05	N-Methylaniline	+		N_2/N_2 (PI)	175	26
2.05	Phenol	+		N_2/N_2	140	26
2.05	*sec.*-Butylamine	+		N_2/N_2	148	9
2.06	"Soman"	$[M-C(CH_3)_3]H^+$	1.65, 1.76, 1.92	N_2/N_2	150	11

2 06	1-Bromohexane	$C_6H_{13}^+$		N_2/N_2	136	36
2 06	1-Chlorohexane	+	1.49, 1 72, 1 81, 1.90	N_2/N_2	135	20
2 06	1-Iodohexane	+	1 73, 1.81, 1.89	N_2/N_2	135	20
2 06	Aniline	+		N_2/N_2	175	26
2,06	Aniline	+		N_2/N_2 (PI)	140	26
2 06	Dimethyl methylphosphonate	MH^+	1.40	N_2/N_2	150	11
2,06	Ethyl acetate	MH^+	1 57	N_2/N_2	136	10
2 06	*n*-Hexane	$C_6H_{13}^+$		N_2/N_2	136	36
2 06	*n*-Nonane	$C_6H_{13}^+$	1.72, 1 83	N_2/N_2	135	23
2 06	*n*-Octane	$C_6H_{13}^+$	1 83	N_2/N_2	135	23
*2 06	Naphthalene	MH^+		N_2/N_2	140	14
2,06	Pyridine	+		N_2/N_2	140	26
2 07	1-Bromohexane	+	1.74, 1 85, 1.91	N_2/N_2	135	20
2 07	1-Bromopentane	+	1 94, 1 99, 2.20	N_2/N_2	135	20
*2 07	Benzene	$(C_6H_6)NO^+$	2.27, 2 32	N_2/N_2	207	38
2 07	Ethanol	+	1 91	N_2/N_2	55	12
2 07	N-Methylaniline	+		N_2/N_2 (PI)	220	26
2 07	Phenol	+		N_2/N_2 (PI)	140	26
*2 08	Water	$(H_2O)_5H^+$	2.13, 2 20, 2.34, 2 67	O_2/Air	160	39
2,08	Aniline	+		N_2/N_2 (PI)	175	26
2 08	Benzene	+	2.33, 2.48	N_2/N_2	150	5
*2,08		SF_6^-		Air/SF_6	210	40
2 08	Toluene	+		N_2/N_2	175	26
2,08	Toluene	+		N_2/N_2	110	26
2 08	Toluene	+		N_2/N_2 (PI)	85	26
2,09	"Disyston"	$[S(CH_2)_2SCH_3CH_2]H^+$	1 34	N_2/N_2	150	11
2 09	1-Chlorooctane	+	1 63, 1.71, 1.82, 1 97	N_2/N_2	135	20
2,09	Aniline	+		N_2/N_2 (PI)	220	26
2 09	N,N-Diethylaniline	+		N_2/N_2 (PI)	220	26
2,09	Naphthalene	+	1.90, 2 21	N_2/N_2 (PI)	150	5
2,10	1-Hexanol	+	1 32, 1.62, 1.76	N_2/N_2	100	12
2 10	Benzene	+		N_2/N_2	85	26
2 10	Ethanol	+	1 93	N_2/N_2	22	12
2 10	Ethanol	+	1.98, 2 17	N_2/N_2	100	12
2 10	N,N-Diethylaniline	+		N_2/N_2 (PI)	175	26
2 10	N,N-Diethylaniline	+		N_2/N_2 (PI)	140	26
2 10	N,N-Diethylaniline	+		N_2/N_2 (PI)	140	26
2 10	Toluene	+		N_2/N_2	140	26

(Continued on p. 166)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
2.10	Toluene	+		N_2/N_2	85	26
2.11	1-Chloroheptane	+	1.73, 1.81, 1.95	N_2/N_2	135	20
2.11	Benzene	+		N_2/N_2 (PI)	85	26
*2.11	Ethylcellosolve acetate	$(C_4H_7O_2)^+$	1.76	N_2/N_2	210	22
2.11	Fluorobenzene	MH^+		N_2/N_2	125	17
*2.11	Mercury	M^+		N_2/N_2	140	14
2.11	Phenol	+		N_2/N_2	175	26
2.11	Toluene	+		N_2/N_2	149	9
2.12	Cyclohexane	+		N_2/N_2	149	9
2.12	Diethylamine	+		N_2/N_2	149	9
2.12	Toluene	+		N_2/N_2 (PI)	110	26
2.13	1-Bromoheptane	+	1.68, 1.75, 1.83, 1.95, 2.01	N_2/N_2	135	20
2.13	1-Chlorobutane	+	1.74, 1.83, 1.98, 2.38	N_2/N_2	135	20
2.13	Water	$(H_2O)_4H^+$	2.08, 2.20, 2.34, 2.67	O_2/Air	160	39
*2.13	*n*-Propylamine	+		N_2/N_2	149	9
2.13	Phenol	+		N_2/N_2	220	26
2.13	Phenol	+		N_2/N_2 (PI)	175	26
2.13	Phenol	+		N_2/N_2	85	26
2.13	Toluene	+		N_2/N_2 (PI)	175	26
2.14	Isophthalic acid	+	1.52, 1.57, 1.76, 1.91	N_2/N_2	150	24
2.14	Naphthalene	+	1.87, 2.03	N_2/N_2	150	5
2.14	Phenol	+		N_2/N_2 (PI)	220	26
2.14	Terephthalic acid	+	1.52, 1.57, 1.76, 1.91	N_2/N_2	150	24
2.15	1-Bromobutane	+	1.84, 1.89, 2.00, 2.36	N_2/N_2	135	20
2.15	1-Iodoheptane	+	1.66, 1.83, 1.95	N_2/N_2	135	20
*2.15	Fumaric acid	$(M-18)^-$	1.89	N_2/N_2	150	37
*2.15	Maleic acid	$(M-18)^-$		N_2/N_2	150	37
2.15	Phthalic acid	+	1.52, 1.64, 1.77	N_2/N_2	150	24
2.15	Phthalic acid	−	1.77	N_2/N_2	150	24
2.15	Phthalic anhydride	+	1.52, 1.64, 1.77	N_2/N_2	150	24
2.15	Toluene	+		N_2/N_2 (PI)	140	26
2.16	*n*-Bromopentane	$C_5H_{11}^+$		N_2/N_2	135	23

2 16	*n*-Propylamine	MH^+		N_2/N_2	200	35
2.16	Pyridine	+		N_2/N_2 (PI)	220	26
2 16	Pyridine	+		N_2/N_2	220	26
2.16	Pyridine	+		N_2/N_2 (PI)	175	26
2 16	Pyridine	+		N_2/N_2	175	26
2.16	Toluene	+		N_2/N_2	220	26
2 17	Ethanol	+	1 98, 2 10	N_2/N_2	100	12
2.17	Toluene	+		N_2/N_2 (PI)	220	26
2 18	Benzene	+		N_2/N_2	110	26
2.18	*n*-Pentane	$C_5H_{11}^+$		N_2/N_2	135	23
2 18	*tert* -Butylbenzene	+	1.74, 2 01, 2 34	N_2/N_2 (PI)	150	5
2 19	Isopropylamine	+		N_2/N_2	149	9
2.19	Pyridine	+		N_2/N_2	145	9
2 20	1-Bromooctane	+	1 72, 1.82, 2.00	N_2/N_2	135	20
2 20	1-Bromopentane	+	1 94, 1.99, 2 07	N_2/N_2	135	20
2 20	1-Chloropentane	+	1 40, 1.88, 1.99, 2.31	N_2/N_2	135	20
2 20	1-Iodobutane	+	1 18, 1 37, 1 57, 1 67, 1.98, 2 33	N_2/N_2	135	20
2.20	1-Iodopentane	+	1 66, 1.86, 2.01	N_2/N_2	135	20
*2 20	Benzene	+	2.04, 2 23, 2 25	N_2/N_2	93	38
2 20	Water	$(H_2O)_3H^+$	2 08, 2 13, 2.34, 2 67	O_2/Air	160	39
2 21	Benzene	+		N_2/N_2 (PI)	110	26
2 21	Dimethylnitrosamine	$[(CH_3)_2N-NO]H^+$	1.71	N_2/N_2	136	15
2.21	Naphthalene	+	1 90, 2 09	N_2/N_2 (PI)	150	5
2.21	*tert* -Butylbenzene	+	1 75, 2 03	N_2/N_2	150	5
*2 22	Benzene	$(C_6H_6)^+$	2.00	N_2/N_2	50	38
*2 22	Benzene	+	2 00	N_2/N_2	50	38
*2 22	Benzene	$[(C_6H_6)(H_2O)(N_2)]H^+$	2.00	N_2/N_2	50	38
*2 22	Benzene	$[(C_6H_6)(N_2)_2]^+$	2 00	N_2/N_2	50	38
*2 22	Benzene	$[(C_6H_6)(N_2)]^+$	2.00	N_2/N_2	50	38
*2.22	Benzene	$[(C_6H_6)(N_2)]H^+$	2 00	N_2/N_2	50	38
*2 22	Benzene	$[(C_6H_6)(N_2)]N^+$	2.00	N_2/N_2	50	38
*2.23	Benzene	$(C_6H_6)H^+$	2.04, 2 20, 2 25	N_2/N_2	93	38
*2 23	Benzene	+	2.04, 2 20, 2 25	N_2/N_2	93	38
*2.23	Benzene	+	2 04, 2 20, 2 25	N_2/N_2	93	38
*2 23	Benzene	$[(C_6H_6)(H_2O)(N_2)]H^+$	2.04, 2.20, 2 25	N_2/N_2	93	38
*2.23	Benzene	$[(C_6H_6)(N_2)]^+$	2 04, 2 20, 2 25	N_2/N_2	93	38
*2 23	Benzene	$[(C_6H_6)(N_2)]H^+$	2.04, 2.20, 2 25	N_2/N_2	93	38
2 24	Benzene	+		N_2/N_2	140	26

(Continued on p. 168)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref*
2 24	Pyrrole	+		N_2/N_2	85	26
*2 25	Benzene	$(C_6H_6)^+$	2 04, 2.20, 2 23	N_2/N_2	93	38
2 25	Pyrrole	+		N_2/N_2	110	26
2 26	Benzene	+		N_2/N_2	220	26
2 26	Benzene	+		N_2/N_2 (PI)	140	26
2 27	Water	$(H_2O)_3H^+$	2 79	N_2/N_2	136	15
*2.27	Benzene	$(C_6H_6)H^+$	2.07, 2.32	N_2/N_2	207	38
2 27	Benzene	+		N_2/N_2	149	9
2 27	Benzene	+		N_2/N_2	175	26
2 27	Benzene	+		N_2/N_2 (PI)	175	26
2 28	CO_2	+		N_2/N_2	150	7
2 28	Pyrrole	+		N_2/N_2 (PI)	85	26
2 29	Benzene	+		N_2/N_2 (PI)	220	26
2 29	Pyrrole	+		N_2/N_2 (PI)	110	26
2 31	1-Chloropentane	+	1 40, 1 88, 1 99, 2.20	N_2/N_2	135	20
2.31	Pyrrole	+		N_2/N_2	175	26
2 31	Pyrrole	+		N_2/N_2 (PI)	140	26
2.31	Pyrrole	+		N_2/N_2	140	26
*2 32	Benzene	$(C_6H_6)^+$	2 07, 2 27	N_2/N_2	207	38
2.32	*n*-Bromobutane	$C_4H_9^+$		N_2/N_2	135	23
*2 32	SF_6	SF_5^-		N_2/N_2	111	32
2.33	1-Iodobutane	+	1 18, 1.37, 1.57, 1.67, 1 98, 2 20	N_2/N_2	135	20
2 33	Benzene	+	2.08, 2 48	N_2/N_2	150	5
2.33	*n*-Heptane	$C_4H_9^+$	1 92	N_2/N_2	135	23
2 34	Water	$(H_2O)_2H^+$	2.08, 2 13,2.20, 2 67	O_2/Air	160	39
2 34	Pyrrole	+		N_2/N_2	220	26
2 34	Pyrrole	+		N_2/N_2 (PI)	175	26
2 34	*tert.*-Butylbenzene	+	1.74, 2 01, 2.18	N_2/N_2 (PI)	150	5
2.34	Trimethylamine	+		N_2/N_2	149	9
2 36	1-Bromobutane	+	1 84, 1 89, 2 00, 2.15	N_2/N_2	135	20
2.38	1-Chlorobutane	+	1.74, 1 83, 1 98, 2 13	N_2/N_2	135	20
2 38	Pyrrole	+		N_2/N_2 (PI)	220	26

2.39	Ethylamine	+		N_2/N_2	149	9
*2 39	SF_6	SF_6^-		N_2/N_2	111	32
2.40	Dimethylamine	+		N_2/N_2	148	9
2 41	CO_4^-			Air/N_2	166	41
2 45	Benzene	+	2 61	N_2/N_2 (PI)	150	5
2 46	*n*-Ethylamine	MH^+		N_2/N_2	200	35
*2 47	Benzene	MH^+		N_2/N_2	140	14
2 48	Benzene	+	2.08, 2 33	N_2/N_2	150	5
2 50	Iodobenzene	$^{127}I^-$		N_2/N_2	136	42
2.50	All iodinated alkanes	I		N_2/N_2	135	20
2 51	Iodobenzene	I^-		N_2/N_2	125	17
2 51	Iodonitrobenzene	I^-		N_2/N_2	148	31
2 53	Iodobenzene	I^-		N_2/N_2	140	33
*2.53	Methylamine	+		N_2/N_2	149	9
*2 55	Air	CO_3^-		Air/Air	210	40
*2.57	Air	CO_3^-		Air/N_2	220	43
*2 57	Air	CO_3^-		Air/N_2	210	44
*2 58	Air	CO_3^-		Air/SF_6	210	40
2 59	Water	$(H_2O)_2O_2^-$	2.94	Air/N_2	166	41
2 59	Water	$(H_2O)O_2^-$	2 94	Air/N_2	166	41
2 59	All brominated alkanes	Br		N_2/N_2	135	20
2 59	Bromobenzene	Br^-		N_2/N_2	136	42
2.60	Bromonitrobenzene	Br^-	1 67	N_2/N_2	148	31
2 61	Benzene	+	2.45	N_2/N_2 (PI)	150	5
2.61	Bromobenzene	Br^-		N_2/N_2	125	17
2 63	Bromobenzene	Br^-		N_2/N_2	140	33
2.63	*n*-Methylamine	MH^+		N_2/N_2	200	35
*2 64	Iodonaphthalene	I^-		N_2/N_2	111	32
*2 67	Water	$(H_2O)H^+$	2 08, 2 13, 2 20, 2.34	O_2/Air	160	39
2 68	1-Nitropropane	NO_2^-		N_2/N_2	108	36
*2 69	Air	$(H_2O)_2O^-$		Air/N_2	210	44
*2 69	Air	$(H_2O)_2O^-$		Air/N_2	220	43
*2 69	Iodine	I^-		N_2/N_2	140	14
*2 70	Air	$(H_2O)_2O^-$	3 17	Air/SF_6	210	40
*2 70	*m*-Mononitrotoluene	$(NO_2)^-$	1 74	N_2/N_2	166	30
*2.70	*m*-Mononitrotoluene	$(NO_2)^-$	1 74, 1.81	Air/N_2	166	30
*2 70	Air	$(NO_2)^-$		Air/N_2	166	41
*2.70	*o*-Mononitrotoluene	$(NO_2)^-$	1 74	N_2/N_2	166	30

(Continued on p 170)

TABLE 1 *(continued)*

K_0	*Compound*	*Ion*	*Additional product ions*	*Carrier/drift gases*	*Temperature (°C)*	*Ref.*
*2 70	*o*-Mononitrotoluene	(NO_2)	1 74, 1 81	A_ir/N_2	166	30
*2.70	*p*-Mononitrotoluene	$(NO_2)^-$	1 74	N_2/N_2	166	30
*2 70	*p*-Mononitrotoluene	(NO_2)	1.74, 1 81	A_ir/N_2	166	30
*2 75	Air	CNO^-		A_ir/N_2	210	44
*2 75	Air	CNO^-		A_ir/N_2	220	43
*2 76	Air	CNO^-		A_ir/A_ir	210	40
2 76	Nitrobutane	$(NO_2)^-$		N_2/N_2	111	31
*2 76	Air	(NO_2)		A_ir/N_2	210	40
*2.76	Air	(NO_2)		A_ir/A_ir	210	40
*2 77	Air	CNO^-		A_ir/SF_6	210	40
*2 77	Air	(NO_2)		A_ir/SF_6	210	40
*2 78	Bromine	Br^-		N_2/N_2	140	14
2 79	Water	$(H_2O)_2H^+$	2 27	N_2/N_2	136	15
*2 82	Bromobenzene	Br^-		N_2/N_2	111	31
2 90	All 1-chloroalkanes	Cl		N_2/N_2	135	20
2 90	Chlorobenzene	Cl^-		N_2/N_2	136	42
2 91	Chloronitrobenzene	Cl	1 74	N_2/N_2	148	31
2 92	Chlorobenzene	Cl^-		N_2/N_2	140	33
2.92	Chlorobenzene	Cl^-		N_2/N_2	125	17
2 92	Decachlorobiphenyl	Cl^-	1 08, 1 16	N_2/N_2	125	17
2.92	*o*-Chloronitrobenzene	Cl^-	1.71, 1.86	N_2/N_2	125	17
2 92	Octachlorobiphenyl	Cl^-	1 16	N_2/N_2	125	17
2 94	Water	$(H_2O)_2OH^-$	2.59	A_ir/N_2	166	41
2.94	Water	$(H_2O)OH^-$	2 59	A_ir/N_2	166	41
2 94	Chloride	–		A_ir/N_2	166	41
2 95	Dichlorobenzene	Cl^-		A_ir/N_2	166	41
2 97	Ammonia	NH_4^+		N_2/N_2	150	5
*3 01	Chloride	–		A_ir/A_ir	210	40
*3 01	Chloride	–		A_ir/SF_6	210	40
*3.01	Chloride	–		A_ir/N_2	210	44
*3 01	Chloride	–		A_ir/N_2	220	43
3 08	Ammonium	+		N_2/N_2	200	35
*3 13	Chlorine	–		N_2/N_2	140	14
*3 14	Chloroform	Cl^-		N_2/N_2	111	31

*3.17	Air	O_2^-	2.70	Air/SF_6	210	40
*3.17	Air	O_2^-		Air/SF_6	210	40
*3.17	Air	O_4^-		Air/SF_6	210	40
3.28	Oxygen	—		Air/N_2	166	41
*3.31	Air	—		Air/Air	210	40
*3.31	Air	O_4^-		Air/Air	210	40
*3.37	Air	CN^-		Air/Air	210	40
*3.37	Air	CN^-		Air/SF_6	210	40
*3.37	Air	CN^-		Air/N_2	210	44
*3.37	Air	CN^-		Air/N_2	220	43

where t is the ion's drift time in s, d is the drift length in cm, E is the electric field (V/cm) on the ion drift region, P is the gas pressure in the drift region in Torr and T is the temperature of the drift gas in the drift region in K. In theory, these reduced mobility values are independent of instrumental conditions and accurate drift times can be calculated for any set of instrument parameters. In practice it has been found that often K_0 values do change with instrumental conditions if these conditions are varied over wide ranges. For normal analytical ion mobility detection however, the optimal instrumental conditions do not vary greatly and the reduced mobility values can be used as a reasonably reliable method to predict drift times

2 TABLE OF REDUCED MOBILITY VALUES

We here present a comprehensive compilation of reduced mobility constants from 1970 to 1985 (Table 1) Not only will it provide a means to predict interfering product ions for selective ion mobility detection, it also provides a convenient data base for further investigations of reduced ion mobility constants. A more complete understanding of the behavior of these constants with respect to instrumental parameters is needed in order to produce a truly reliable mobility constant.

The table lists compounds in order of their reduced mobility constants. An asterisk preceding a K_0 value indicates that the mass of that particular ion has been identified with a mass spectrometer. Note that only about a quarter of the entries have been mass identified. For compounds which produce multiple product ions, the additional product ions are listed in the third column of the table, followed by the type of carrier and drift gases used and the temperature employed. Pressure is not reported since only reduced mobility data obtained at atmospheric pressure (760 $\pm$ 20 Torr) were considered. The last column provides the reference where more information about the ion mobility spectrum of a particular compound can be found.

While we believe that this table will prove helpful to those who are actively involved in IMS, we would also caution those who use it. Many of the data presented here were obtained in the early days of IMS when the standard practice of sample introduction was to inject vapors or small liquid quantities of the compound directly into the spectrometer If the compound was contaminated or if the spectrometer became saturated, multiple peaks could occur In our work where we only introduce nanogram quantities of a compound after separation by high-resolution capillary gas chromatography or supercritical fluid chromatography we have found very few compounds which exhibit multiple product ions.

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4 SUMMARY

This review presents a list of reduced ion mobilities that have been measured under ambient pressure conditions and reported in the open literature during the 16-year period of 1970–1985. Ions reported are listed in order of increasing reduced

mobility along with the name of the parent compound, the reduced mobility of additional product ions observed in the spectrum, the carrier and drift gases, the temperature of the drift region and the reference where the data were reported. Also, ions that have been identified by mass spectrometry are indicated with an asterisk.

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