Electronic Supplementary Information (ESI) for Physical Chemistry Chemical Physics

Non-thermal Ion Desorption From an Acetonitrile (CH_3CN) Astrophysical Ice Analogue Studied by Electron Stimulated Ion Desorption

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Table S1. Positive ion assignments and their respective time-of-flight (TOF) and full width at half-maximum (FWHM) values (ns) for each ion peak observed in the CH_3CN ESID spectra (Figures 1 and 4) at 120 K due to 2300 eV electron impact. Positive ion yield (Y_i) values (ions/impact) were calculated within a relative error of 5%. Ions with $Y_i \leq 1 \times 10^{-12}$ ions/electron are considered trace.

TOF (ns)	FWHM (ns)	m/z	Assignment	Y_i (10^{-12} ions/electron)
643	17	1	H^+	48208.9
899	17	2	H_2^+	476.0
1098	17	3	H_3^+	12.4
1654	15	7	N^{++}	2.9
1763	17	8	O^{++}	1.4
1921	14	9.5	H_3O^{++}	6.4
2158	15	12	C^+	10.9
2248	14	13	CH^+	9.5
2331	18	14	CH_2^+, N^+	53.1
2413	15	15	CH_3^+, NH^+	149.5
2485	21	16	O^+	16.2
2567	22	17	OH^+	3.8
2644	20	18	H_2O^+	7.9
2708	17	19	H_3O^+	785.9
3043	23	24	C_2^+	trace
3100	18	25	C_2H^+	1.5
3170	17	26	$C_2H_2^+$, CN^+	10.8
3228	17	27	$C_2H_3^+$, HCN^+	46.5
3288	18	28	CH_2N^+	27.2
3345	17	29	CH_3N^+	58.0
3403	19	30	CH_3NH^+	16.1
3457	22	31	$CH_3NH_2^+$	8.4
3510	22	32	$CH_3NH_3^+$	3.0
3823	23	38	C_2N^+	2.1
3874	18	39	$CHCN^+$	16.1
3922	21	40	CH_2CN^+	6.3
3975	19	41	CH_3CN^+	28.4
4021	19	42	CH_3CNH^+	38.4
4067	19	43	$CH_3CNH_2^+$	25.2
4116	19	44	$CH_3CNH_3^+$	11.9
4162	31	45	$CH_3CHNH_3^+$	4.7
4209	20	46	$CH_3CH_2NH_3^+$	2.7
4387	22	50	C_3N^+	1.2
4429	18	51	HC_3N^+	1.9
4473	20	52	$C_2N_2^+$	2.0
4516	17	53	$(CH_3CN)C^+$	4.3
4554	17	54	$(CH_3CN)CH^+$	4.4
4599	19	55	$(CH_3CN)CH_2^+$	7.4
4640	20	56	$(CH_3CN)CH_3^+$	5.9
4682	22	57	$(CH_3CN)O^+$	5.2
4726	23	58	$(CH_3CN)OH^+$	2.6
4764	17	59	$(CH_3CN)H_2O^+$	2.1
4802	17	60	$(CH_3CN)H_3O^+$	2.0
4997	20	65	$(CH_3CN)C_2^+$	1.8
5035	19	66	$(CH_3CN)C_2H^+$	1.3
5073	24	67	$(CH_3CN)C_2H_2^+$	2.7
5111	20	68	$(CH_3CN)C_2H_3^+$	2.4
5148	22	69	$(CH_3CN)CH_2N^+$	3.6
5185	24	70	$(CH_3CN)CH_3N^+$	2.5
5221	24	71	$(CH_3CN)CH_3NH^+$	1.5

Table S1 (Continued). Positive ion assignments and their respective time-of-flight (TOF) and full width at half-maximum (FWHM) values (ns) for each ion peak observed in the CH_3CN ESID spectra (Figures 1 and 4) at 120 K due to 2300 eV electron impact. Positive ion yield (Y_i) values (ions/impact) were calculated within a relative error of 5%. Ions with $Y_i \leq 1 \times 10^{-12}$ ions/electron are considered trace.

TOF (ns)	FWHM (ns)	m/z	Assignment	Y_i (10^{-12} ions/electron)
5257	26	72	$(CH_3CN)CH_3NH_2^+$	1.4
5295	25	73	$(CH_3CN)CH_3NH_3^+$	1.1
5437	19	77	$(CH_3CN)36$	1.5
5472	28	78	$(CH_3CN)37$	1.4
5508	18	79	$(CH_3CN)C_2N^+$	1.3
5541	21	80	$(CH_3CN)CHCN^+$	1.3
5575	25	81	$(CH_3CN)CH_2CN^+$	1.6
5609	16	82	$(CH_3CN)_2^+$	1.1
5643	25	83	$(CH_3CN)_2H^+$	3.1