

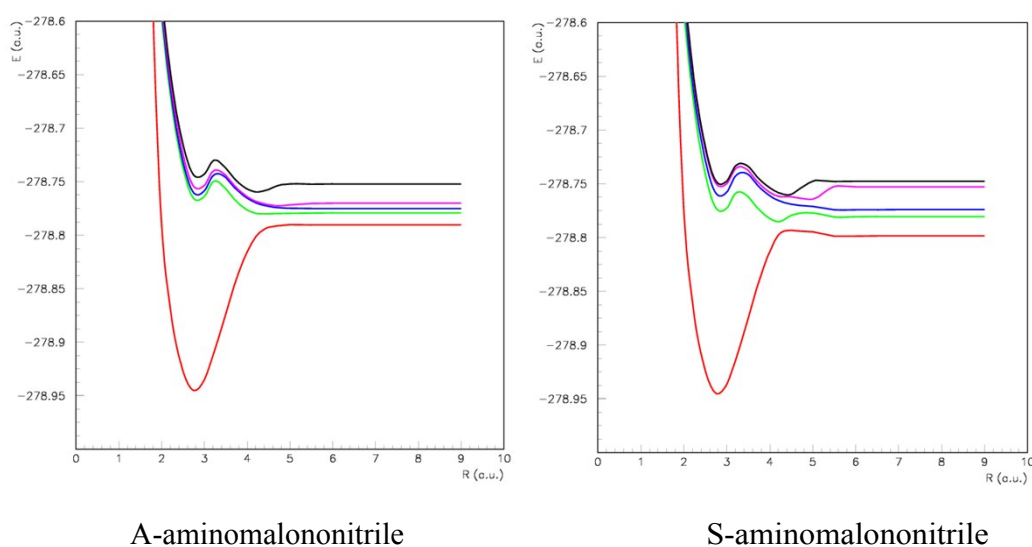
## Theoretical investigation of proton collisions on prebiotic candidates: hydrogen cyanide polymers

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### SUPPLEMENTARY INFORMATION

Fig. S1 Adiabatic potential energy curves of the  $^1A$  states of the proton-aminomalnonitrile charge transfer system in the perpendicular geometry. Black, entrance channel  $\{AMN + H^+\}$ ; color, charge transfer channels  $\{AMN^+ + H\}$ .



**Table S1** Proton-induced charge transfer cross sections in collisions of protons with Z-C-cyanomethanimine (in  $10^{-16} \text{cm}^2$ ).

Velocity (a.u.)	$E_{\text{lab}}$ (eV)	along x	along y	along z	Mean xy value $\sigma_{//}$	Mean xyz value $\sigma^{\text{xyz}}$	Mean
0.015	5.7	0.076	$5.41 \times 10^{-3}$	0.014	0.041	0.032	0.027
0.02	10.0	0.151	0.028	$7.48 \times 10^{-3}$	0.089	0.062	0.048
0.03	22.6	0.144	0.022	0.013	0.083	0.060	0.048
0.04	40.0	0.290	0.021	0.023	0.155	0.111	0.089
0.05	63.0	0.283	0.048	0.027	0.165	0.119	0.096
0.07	123.4	0.637	0.089	0.024	0.363	0.250	0.194
0.08	161.1	0.529	0.076	0.022	0.302	0.209	0.162
0.09	203.9	0.465	0.109	0.019	0.287	0.197	0.153
0.1	251.8	0.498	0.189	0.017	0.343	0.234	0.180
0.15	566.5	0.992	0.576	0.011	0.784	0.526	0.398
0.2	$1.0 \times 10^3$	1.082	0.616	$9.88 \times 10^{-3}$	0.849	0.569	0.429
0.3	$2.3 \times 10^3$	0.801	0.443	$7.47 \times 10^{-3}$	0.622	0.417	0.315
0.4	$4.0 \times 10^3$	0.554	0.356	$5.71 \times 10^{-3}$	0.455	0.305	0.230
0.5	$6.3 \times 10^3$	0.398	0.299	$4.34 \times 10^{-3}$	0.349	0.234	0.176
0.6	$9.1 \times 10^3$	0.297	0.251	$3.33 \times 10^{-3}$	0.274	0.184	0.139
0.7	$12.3 \times 10^3$	0.229	0.210	$2.61 \times 10^{-3}$	0.219	0.147	0.111

**Table S2** Proton-induced charge transfer cross sections in collisions of protons with E-C-cyanomethanimine (in  $10^{-16} \text{cm}^2$ ).

Velocity (a.u.)	$E_{\text{lab}}$ (eV)	along x	along y	along z	Mean xy Value $\sigma_{//}$	Mean xyz Value $\sigma^{\text{xyz}}$	Mean
0.015	5.7	$9.2 \times 10^{-3}$	$5.02 \times 10^{-3}$	$3.70 \times 10^{-3}$	0.007	0.006	0.005
0.02	10.0	0.069	$8.64 \times 10^{-3}$	$4.01 \times 10^{-3}$	0.039	0.027	0.021
0.03	22.6	0.206	$8.53 \times 10^{-3}$	$4.91 \times 10^{-3}$	0.107	0.073	0.056
0.04	40.0	0.281	$9.62 \times 10^{-3}$	$4.86 \times 10^{-3}$	0.145	0.098	0.075
0.05	63.0	0.294	0.017	$4.58 \times 10^{-3}$	0.155	0.105	0.080
0.07	123.4	0.254	0.010	$3.45 \times 10^{-3}$	0.132	0.089	0.068
0.08	161.1	0.460	0.016	$2.95 \times 10^{-3}$	0.238	0.160	0.120
0.09	203.9	0.787	0.030	$2.79 \times 10^{-3}$	0.408	0.273	0.206
0.1	251.8	0.943	0.028	$2.91 \times 10^{-3}$	0.486	0.325	0.244
0.15	566.5	0.615	0.107	$3.72 \times 10^{-3}$	0.361	0.242	0.182
0.2	$1.0 \times 10^3$	1.647	0.290	$3.84 \times 10^{-3}$	0.968	0.647	0.486
0.3	$2.3 \times 10^3$	2.342	0.339	$3.81 \times 10^{-3}$	1.340	0.895	0.672
0.4	$4.0 \times 10^3$	2.112	0.319	$3.10 \times 10^{-3}$	1.216	0.811	0.609
0.5	$6.3 \times 10^3$	1.922	0.275	$2.38 \times 10^{-3}$	1.098	0.733	0.551
0.6	$9.1 \times 10^3$	1.748	0.229	$1.83 \times 10^{-3}$	0.989	0.660	0.495
0.7	$12.3 \times 10^3$	1.557	0.191	$1.43 \times 10^{-3}$	0.874	0.583	0.438

**Table S3** Proton-induced charge transfer cross sections in collisions of protons with A aminimalononitrile (in  $10^{-16}\text{cm}^2$ ).

Velocit y (a.u.)	$E_{\text{lab}}$ (eV)	along x	along y	along z	Mean xyz Value $\sigma^{\text{xyz}}$
0.015	5.7	0.264	0.454	5.573	2.097
0.02	10.0	0.325	0.788	5.321	2.145
0.03	22.6	0.564	1.231	5.682	2.493
0.04	40.0	0.817	2.004	7.026	3.282
0.05	63.0	0.720	2.264	7.835	3.606
0.07	123.4	1.198	2.630	7.995	3.941
0.08	161.1	1.104	2.641	7.670	3.805
0.09	203.9	1.119	3.201	7.213	3.844
0.1	251.8	1.301	4.034	6.823	4.053
0.15	566.5	2.529	6.096	4.957	4.527
0.2	$1.0 \times 10^3$	2.622	5.353	4.089	4.022
0.3	$2.3 \times 10^3$	1.833	3.336	2.609	2.593
0.4	$4.0 \times 10^3$	1.232	2.124	2.581	1.979
0.5	$6.3 \times 10^3$	0.863	1.441	2.683	1.662
0.6	$9.1 \times 10^3$	0.632	1.033	2.521	1.395
0.7	$12.3 \times 10^3$	0.480	0.774	2.240	1.165

**Table S4** Proton-induced charge transfer cross sections in collisions of protons with S aminimalononitrile (in  $10^{-16}\text{cm}^2$ ).

Velocit y (a.u.)	$E_{\text{lab}}$ (eV)	along x	along y	along z	Mean xyz Value $\sigma^{\text{xyz}}$
0.015	5.7	0.033	0.820	1.707	0.853
0.02	10.0	0.077	3.857	2.419	2.118
0.03	22.6	0.076	6.997	5.858	4.310
0.04	40.0	0.368	5.927	13.208	6.501
0.05	63.0	0.699	6.353	17.056	8.036
0.07	123.4	0.943	8.597	15.990	8.510
0.08	161.1	0.922	10.709	15.641	9.091
0.09	203.9	0.866	11.893	15.389	9.383
0.1	251.8	0.797	12.426	14.881	9.368
0.15	566.5	0.490	10.790	11.540	7.607
0.2	$1.0 \times 10^3$	0.325	8.087	8.305	5.572
0.3	$2.3 \times 10^3$	0.174	4.656	4.886	3.239
0.4	$4.0 \times 10^3$	0.107	2.918	3.141	2.056
0.5	$6.3 \times 10^3$	0.072	1.971	2.575	1.539
0.6	$9.1 \times 10^3$	0.051	1.411	2.265	1.242
0.7	$12.3 \times 10^3$	0.038	1.056	1.989	1.028