Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Insights into the molecular structure and infrared spectrum of the prebiotic species aminoacetonitrile
Supporting Information

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Geometry

Table S1: Structural parameters computed using the HF-SCF method in conjunction with different basis sets.

Parameter	cc-pVTZ	cc-pVQZ	cc-pV5Z
r(C≡N)	1.171	1.128	1.126
r(C−C)	1.474	1.484	1.484
r(C−H)	1.088	1.081	1.080
r(C−N)	1.456	1.442	1.441
r(N−H)	1.012	0.997	0.997
∠(C−C≡N)	182.7	181.1	181.0
∠(C−C−N)	114.9	114.9	114.9
∠(C−N−H)	109.7	111.6	111.8
∠(C−C−H)	108.3	107.6	107.6
ϕ(C−C−N−H)	122.2	122.4	122.4
ϕ(N≡C−C−H)	58.20	60.46	60.73
A_e	31287.3	31358.7	31373.8
B_e	4811.99	4813.32	4813.13
C_e	4375.43	4377.86	4378.07

Notes: Bond-lengths are in Å, angles in degrees, rotational constants in MHz.

Harmonic frequencies

Table S2: Harmonic frequencies (in cm^{-1}) computed using the HF-SCF method in conjunction with different basis sets

Mode	cc-pVTZ	cc-pVQZ	cc-pV5Z
ν_1	3735	3738	3740
ν_2	3215	3216	3217
ν_3	2579	2578	2577
ν_4	1804	1804	1804
ν_5	1601	1601	1602
ν_6	1492	1493	1494
ν_7	1189	1189	1188
ν_8	994	990	987
ν_9	885	881	879
ν_{10}	626	626	626
ν_{11}	243	244	244
ν_{12}	3817	3819	3821
ν_{13}	3254	3255	3256
ν_{14}	1500	1500	1500
ν_{15}	1295	1295	1295
ν_{16}	969	968	968
ν_{17}	430	429	429
ν_{18}	290	287	286

Vibration-rotation interaction constants

Table S3: Vibration-rotation interaction constants (in MHz) computed at the MP2/ae-CVTZ level of theory

Mode	α^A	α^B	α^C
ν_1	-104.5	1.3	0.1
ν_2	-1.0	-4.3	-1.8
ν_3	-64.7	-21.6	-19.0
ν_4	-78.9	0.0	1.2
ν_5	0.5	4.1	11.2
ν_6	-101.4	1.4	-13.8
ν_7	-271.7	-0.8	-1.8
ν_8	47.2	-16.7	-16.5
ν_9	60.2	-22.5	-15.9
ν_{10}	385.8	-8.0	-7.5
ν_{11}	-117.5	16.3	6.3
ν_{12}	-105.5	3.4	0.8
ν_{13}	31.6	-4.3	-2.4
ν_{14}	-97.1	-1.2	1.8
ν_{15}	26.6	-0.6	1.2
ν_{16}	7.6	-5.2	-6.4
ν_{17}	-125.5	2.8	4.4
ν_{18}	292.5	7.2	4.6