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Supporting Information for:

Gas-Phase Formation of Glycolonitrile in the Interstellar Medium

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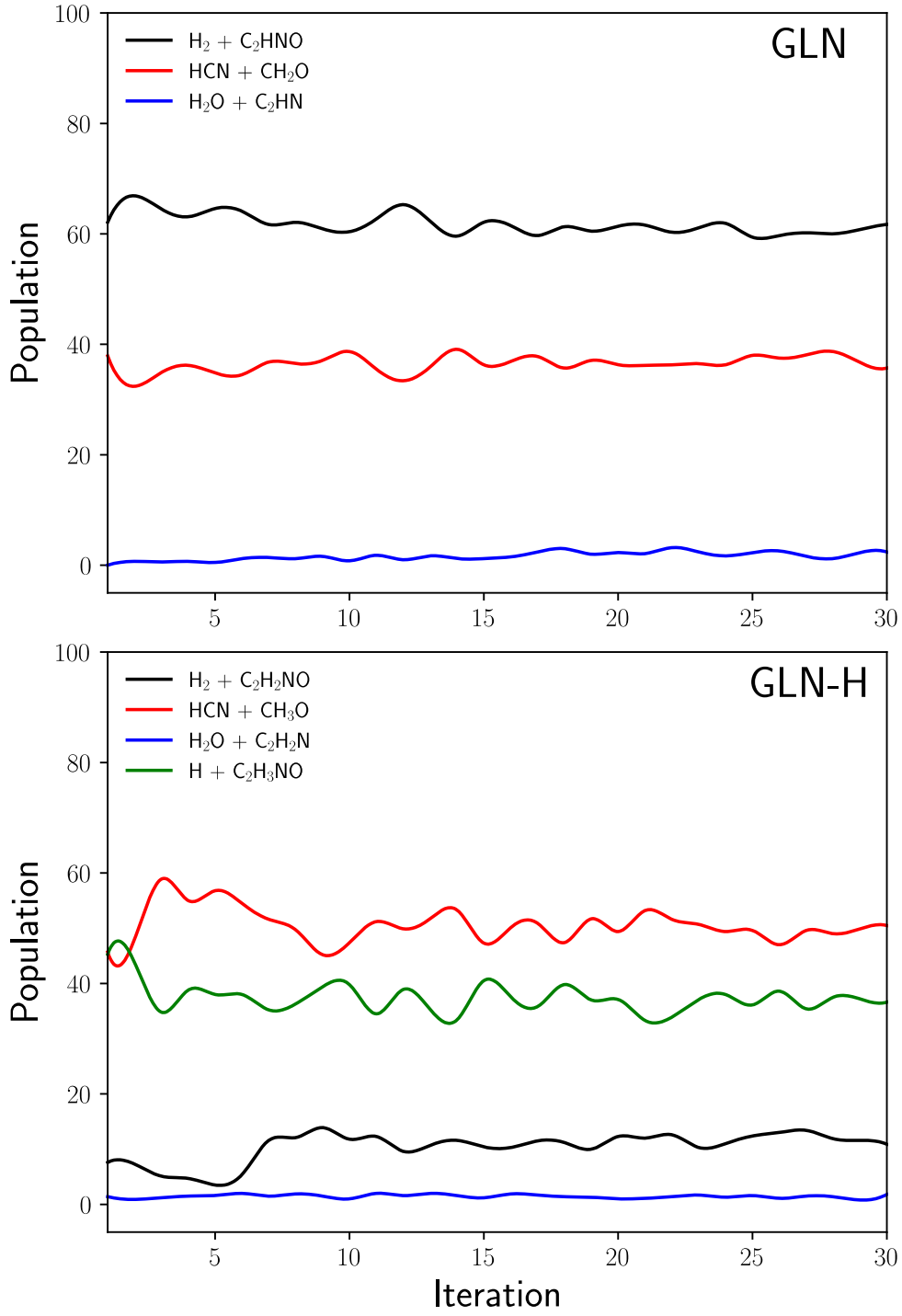

Fig. S1 Product abundances as a function of number of iterations obtained from the KMC simulations for GLN and GLN-H, using an excitation energy of 250 kcal/mol. The Level1-calculated energies and vibrational frequencies are employed in the calculations of the RRKM rate coefficients, and barrierless reactions are not included.

The relative energies depicted in Figures S2-S6 are referenced to the initial geometry utilized for the AutoMeKin calculations of the GLN and GLN-H systems.

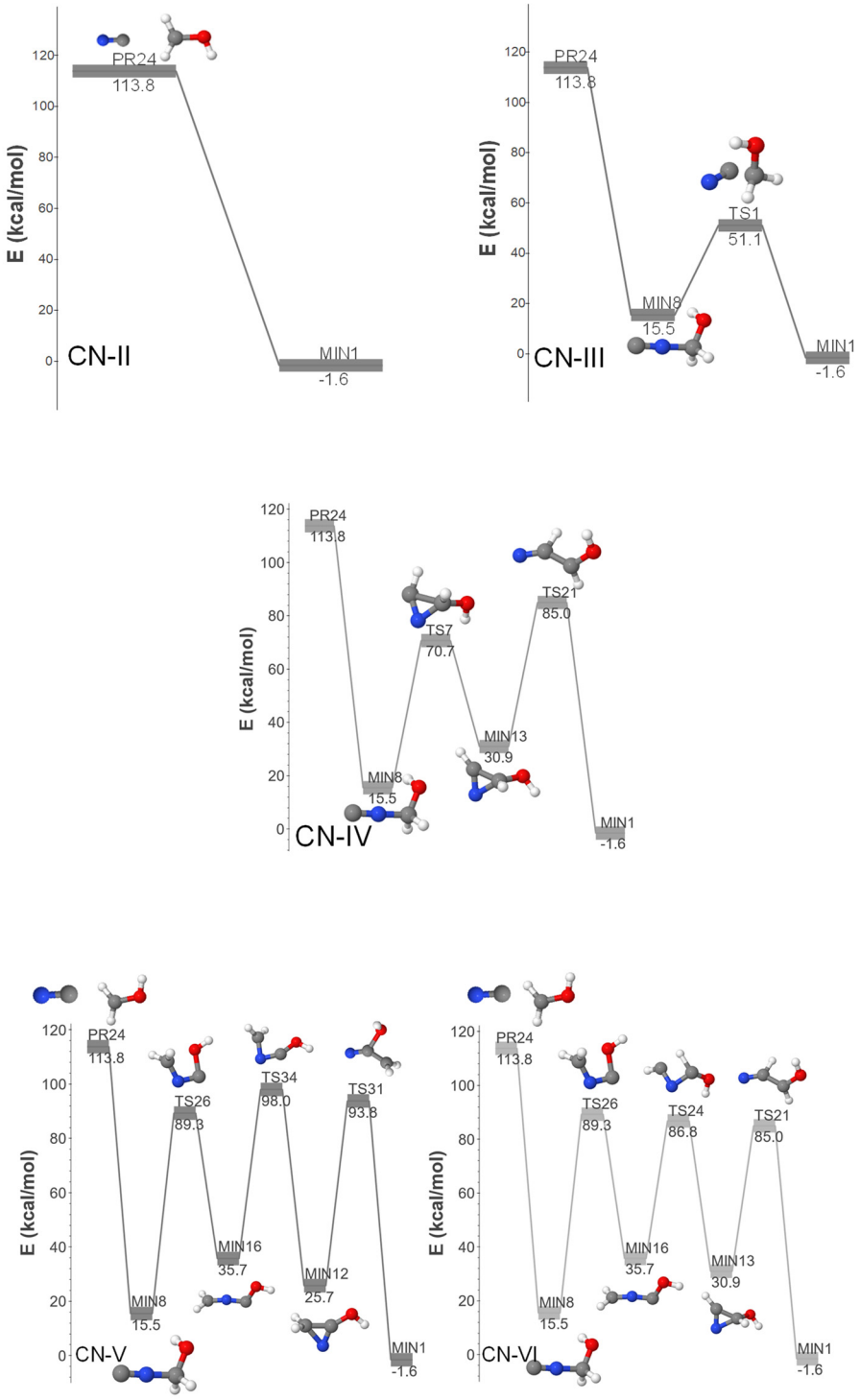

Fig. S2 Additional DFT-computed energy profiles for the barrierless formation of GLN from CN+ CH_2OH.

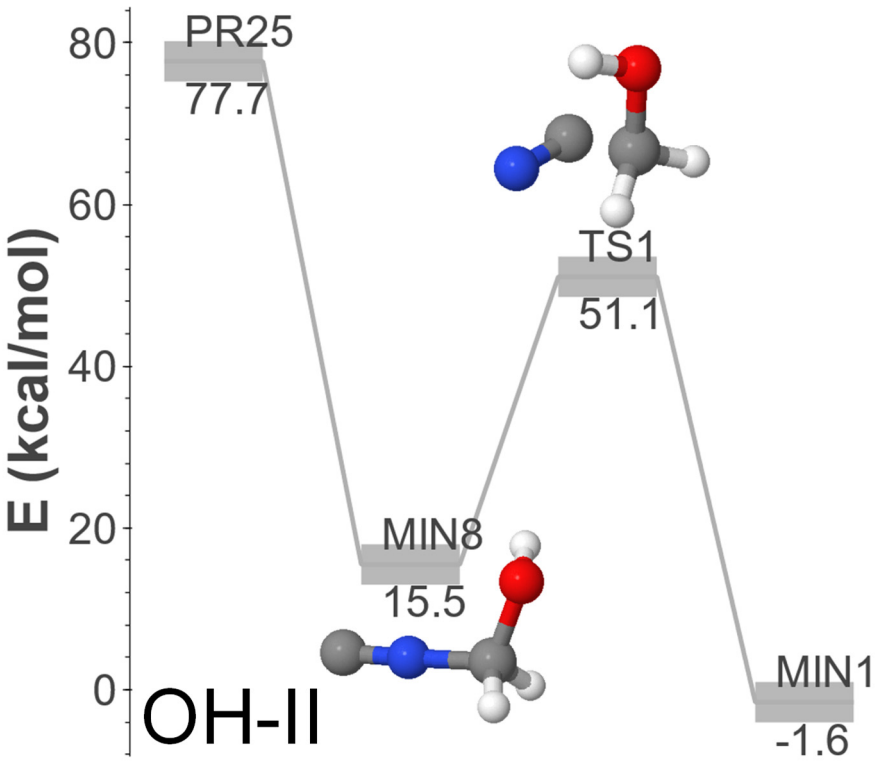

Fig. S3 Additional DFTcomputed energy profile for the barrierless formation of GLN from OH + CH_2NC (OH-II pathway).

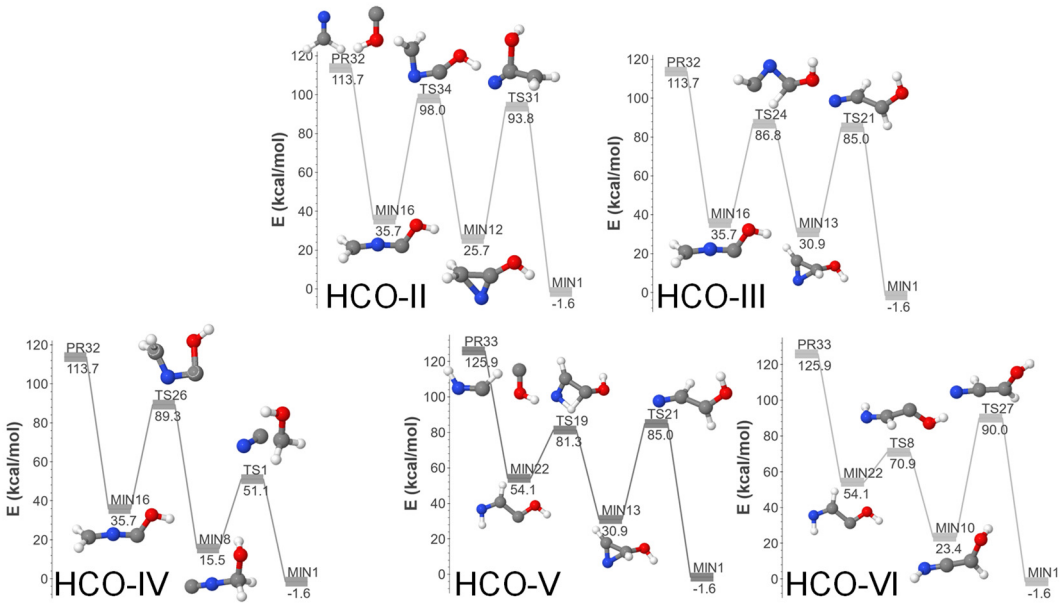

Fig. S4 Additional DFT-computed energy profiles for the barrierless formation of GLN from HCO + CH_2N. Pathways involving 3 elementary steps are displayed.

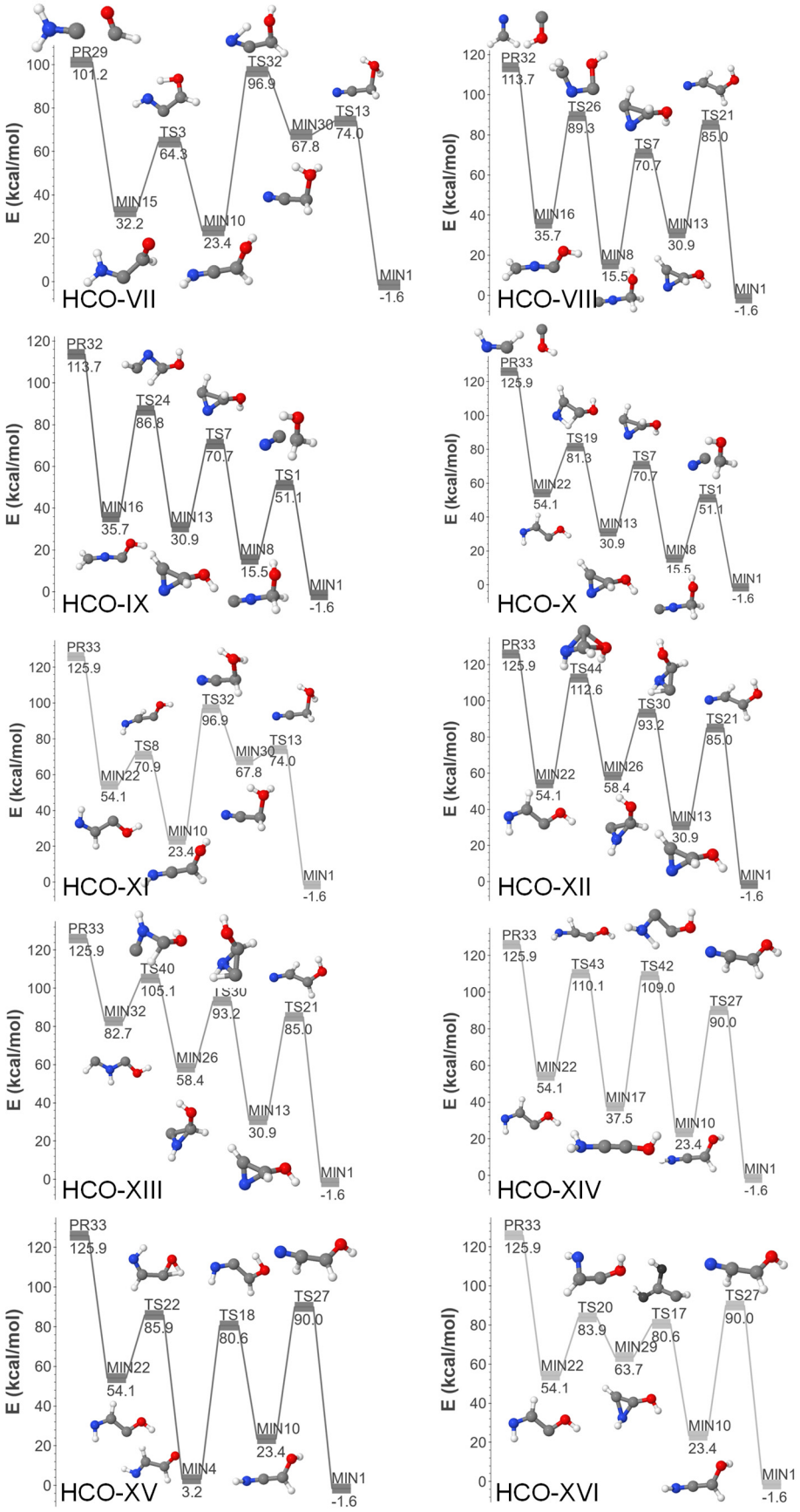

Fig. S5 Additional DFT-computed energy profiles for the barrierless formation of GLN from HCO + CH_2N. Pathways involving 4 elementary steps are displayed.

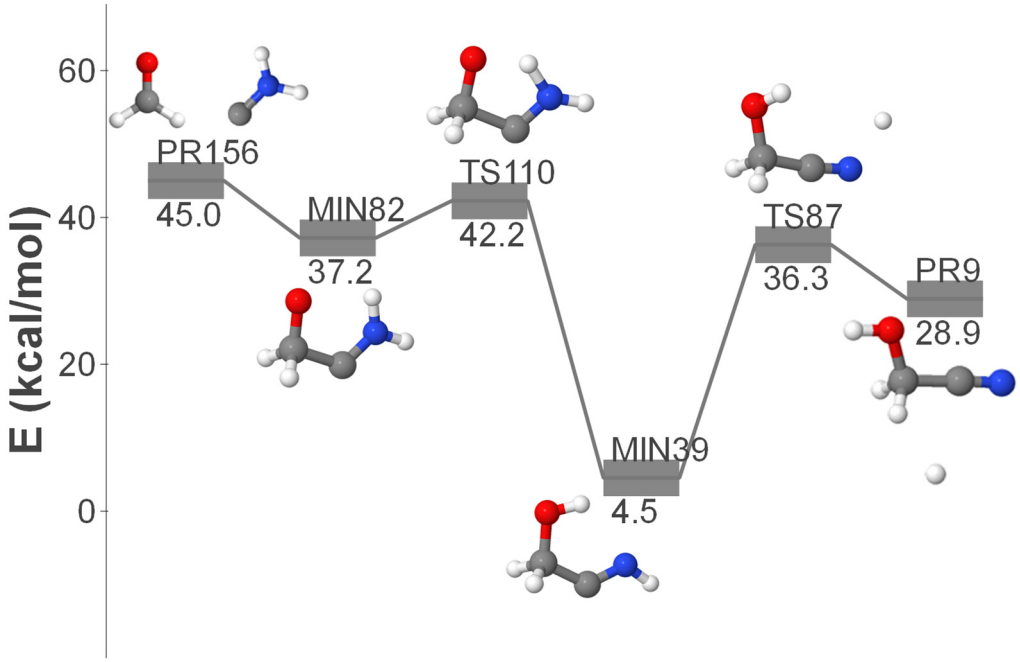

Fig. S6 Additional DFT-computed energy profile for the barrierless (radical-molecule) formation of GLN+H.

Table S1: Rate coefficients (in cm^3 $molecule^{-1}$ s^{-1}) for the $OH+CH_2CN \rightarrow HNC+CH_2O$ reaction

T/K	k_1	k_2	k^{CUS}
10	1.15E-09	2.90E+243	1.15E-09
20	1.02E-09	5.57E+115	1.02E-09
30	9.55E-10	1.15E+73	9.55E-10
40	9.11E-10	4.60E+51	9.11E-10
50	8.78E-10	6.19E+38	8.78E-10
60	8.51E-10	1.56E+30	8.51E-10
70	8.30E-10	1.09E+24	8.30E-10
80	8.11E-10	2.58E+19	8.11E-10
90	7.96E-10	6.45E+15	7.96E-10
100	7.82E-10	8.39E+12	7.82E-10
110	7.69E-10	3.64E+10	7.69E-10
120	7.58E-10	3.89E+08	7.58E-10
130	7.48E-10	8.34E+06	7.48E-10
140	7.39E-10	3.09E+05	7.39E-10
150	7.31E-10	1.77E+04	7.31E-10

Table S2: Rate coefficients (in cm^3 $molecule^{-1}$ s^{-1}) for the $OH+CH_2CNH \rightarrow GLN+H$ reaction

T/K	k_1	k_2	k^{CUS}
10	6.61E-10	5.79E+16	6.61E-10
20	5.89E-10	3.16E+02	5.89E-10
30	5.51E-10	4.29E-03	5.51E-10
40	5.25E-10	1.40E-05	5.25E-10
50	5.06E-10	4.26E-07	5.05E-10
60	4.91E-10	4.01E-08	4.85E-10
70	4.78E-10	7.31E-09	4.49E-10
80	4.68E-10	2.02E-09	3.80E-10
90	4.59E-10	7.41E-10	2.83E-10
100	4.51E-10	3.32E-10	1.91E-10
110	4.43E-10	1.73E-10	1.24E-10
120	4.37E-10	1.00E-10	8.15E-11
130	4.31E-10	6.35E-11	5.53E-11
140	4.26E-10	4.30E-11	3.91E-11
150	4.21E-10	3.09E-11	2.88E-11