Supporting Information

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Table S1. Summary of the systems simulated in this work

System	M00	MS01	MS02	MS03	MF01	DHGF	DHGW	Gly
H_2O	32	8	9	—	8	—	10	10
NH_3	8	8	9	9	8	—	—	—
CH_4	8	8	—	—	—	—	—	—
H_2	4	—	—	—	—	10	10	—
N_2	—	5	—	—	—	—	—	—
CO	—	10	—	—	8	—	—	—
Formaldehyde	—	—	9	—	—	—	—	—
HCN	—	—	9	—	—	—	—	—
Formic acid	—	—	—	—	8	10	—	—
Formamide	—	—	—	—	8	—	—	—
Dehydroglycine	—	—	—	—	—	10	10	—
Glycine	—	—	—	9	—	—	—	
C atoms	8	18	18	18	24	30	20	20
H atoms	128	72	72	72	80	70	70	70
O atoms	32	18	18	18	40	40	30	30
N atoms	8	18	18	18	16	10	10	10
Cell side, Å	11.21	11.12	11.12	11.12	12.70	12.62	11.55	11.55
ΔE wrt MS03, kcal/mol	—	40.4	54.3	0.0	—	—	—	—
ΔE wrt Gly, kcal/mol	—	—	—	—	—	—	31.7	0.0
Run time 0.00 V/Å, ps	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
Run time 0.25 V/Å, ps	5.0	5.0	5.0	0.0	0.0	0.0	0.0	0.0
Run time 0.35 V/Å, ps	10.0	10.0	10.0	5.0	5.0	0.0	0.0	0.0
Run time 0.50 V/Å, ps	10.0	20.0	20.0	0.0	20.0	10.0	0.0	0.0

Starting composition of the simulation boxes, labeled as in the main text and/or in *Supporting Information*: Original Miller, M00; Miller–Strecker first step, MS01; Miller–Strecker second step, MS02; Miller–Strecker third step, MS03; Miller–formamide, MF01; dehydroglycine + formic acid and H_2, DHGF; dehydroglycine + water and H_2, DHGW; glycine + water, Gly. For each system we report the initial number of each molecular species, then of each atomic species, the corresponding cubic cell size, chosen as to have, for each system, a density of 1.0 g/mL, the relative average potential energy difference with respect to the reference system (when applicable), and the total simulation time (in picoseconds) for each value of the external electric field.

Table S2. Relative occurrence of potential transition states, as described in text, with respect to all intermediate states observed within the metadynamics trajectories, at zero and finite field

Chemical species	Occurrence at 0.0 V/Å	Occurrence at 0.5 V/Å	Occurrence at 0.5 V/Å, normalized with respect to 0.0 V/Å
TS1: CO + NH_2	0.288	0.228	0.272
TS2: COH + NH_3	0.014	0.505	0.602
TS3: CO – NH_3	0.698	0.267	0.318

In the right column, the values at finite field are normalized with respect to the total occurrence of intermediate states at zero field.

Table S3. Compatibility table of secondary intermediate states (SIS) with respect to the TS states, and relative occurrence in the MetaDynamics formamide trajectories, at zero and finite field

Chemical species	TS1	TS2	TS3	Occurrence at 0.0 V/Å	Occurrence at 0.5 V/Å
SIS1: COH + NH_2	Y	Y	N	0.619	0.358
SIS2: COH – NH_3	N	Y	Y	0.110	0.477
SIS3: CO – NH_2	Y	N	Y	0.271	0.165

Y, yes; N, no.

Table S4. Relative occurrence of "product" chemical species with respect to the full metadynamics trajectories, at zero and finite field

Chemical species	Occurrence at 0.0 V/Å	Occurrence at 0.5 V/Å
Formamide	0.139	0.103
Formimidic acid	0.001	0.039
Hydrogen cyanide	0.086	0.192

Table S5. Chemical species observed along a molecular dynamics run of the MF01 system under a field up to 0.5 V/Å

t, ps	H_2O	NH_3	CO	HCN	Formic acid	Formamide	Dehydroglycine	Glyconitriles	Others
0.0	8	8	8	0	8	8	0	0	0
1.5	9	8	8	0	7	7	0	0	1
2.5	9	8	8	0	7	6	0	0	1
3.6	9	8	7	1	8	5	0	0	1
3.8	8	7	6	1	8	5	0	1	1
4.0	8	7	6	1	7	4	1	1	1
5.0	10	7	6	2	7	4	1	1	1
5.5	12	6	5	3	7	5	1	0	1
7.0	14	5	3	5	4	2	1	2	2