Electronic Supplementary Material (ESI) for RSC Advances.

Formation and evolution of C–C, C–O, C=O and C–N bonds in chemical reactions of prebiotic interest

Alejandro Arias,[†] Sara Gómez,[‡] Natalia Rojas-Valencia,[†,¶] Francisco Núñez–Zarur,[§] Chiara Cappelli,[‡] Juliana A. Murillo–López,[||] Albeiro Restrepo[†]

[†]*Instituto de Química, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia*

[‡]*Scuola Normale Superiore, Classe di Scienze, Piazza dei Cavalieri 7, 56126, Pisa, Italy*

[¶]*Escuela de Ciencias y Humanidades, Departamento de Ciencias Básicas, Universidad Eafit, AA 3300, Medellín, Colombia*

[§]*Facultad de Ciencias Básicas, Universidad de Medellín, Carrera 87 No. 30-65, 050026, Medellín, Colombia*

[||]*Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, Autopista, Concepción-Talcahuano, 7100 Talcahuano, Chile*

Supplementary Material

Table S1: Intrinsic activation and reaction energies for our 23 elementary steps at 373 K and 1atm, in kcal/mol units. An asterisk attached to a label means that HNC is involved instead of HCN. Notice that reaction **14** leads to different products than those reported by Das and coworkers[1] in gas phase.

Label	Reaction	$\Delta G^{\dagger}_{act}$		ΔG_{rxn}	
		In gas phase	In solution	In gas phase	In solution
1	$HCN + H_2O \rightarrow CH_3NO$	50.5	52.5	13.7	12.1
2	$CH_3NO \rightarrow CH_3NO$	10.8	10.2	-10.9	-13.2
3	$CH_3NO + H_2O \rightarrow NH_3 + CH_2O_2$	47.1	47.5	5.5	10.2
4*	$CH_2O_2 + HCN \rightarrow C_2HNO + H_2O$	59.7	63.8	26.1	25.4
5*	$C_2HNO \rightarrow CO + HCN$	31.1	21.3	-31.7	-31.4
6	$CO + H_2O \rightarrow CH_2O_2$	64.9	64.9	47.7	47.0
7	$HCN \rightarrow HNC$	54.8	43.2	16.2	15.0
8	$CH_2O_2 \rightarrow CO_2 + H_2$	51.3	50.1	-12.7	-6.8
9	$CH_2O_2 + H_2 \rightarrow CH_4O_2$	53.2	56.5	-3.6	5.8
10	$CH_4O_2 \rightarrow CH_2O + H_2O$	31.7	30.0	-0.2	-4.1
11*	$CH_2O + HNC \rightarrow C_2H_3NO$	26.6	22.9	-24.0	-24.6
12	$CH_2O + NH_3 \rightarrow CH_5NO$	39.2	31.7	-1.0	-0,8
13	$CH_5NO \rightarrow CH_3N + H_2O$	36.4	34.4	0.1	-0.6
14*	$CH_3N + HCN \rightarrow C_2H_4N_2$	NA	5.5	NA	-29.6
14	$CH_3N + HCN \rightarrow C_2H_4N_2$	36.6	NA	8.9	NA
15	$C_2H_4N_2 + H_2O \rightarrow C_2H_6N_2O$	50.3	50.5	13.6	12.6
16	$C_2H_6N_2O \rightarrow C_2H_6N_2O$	9.8	8.9	-11.3	-13.7
17	$C_2H_6N_2O + H_2O \rightarrow C_2H_5NO_2$	47.3	46.1	1.9	6.0
18	$C_2H_3NO + CH_2O \rightarrow C_3H_5NO_2$	50.0	43.7	-12.9	-14.3
19*	$C_3H_5NO_2 \rightarrow C_2H_4O_2 + HCN$	37.8	29.2	21.6	17.3
20	$C_2H_3NO + CH_3NO \rightarrow C_3H_6N_2O_2$	35.5	36.4	17.8	19.3
21	$C_3H_6N_2O_2 + HCN \rightarrow C_4H_7N_3O_2$	50.2	56.8	11.5	13.2
22	$C_4H_7N_3O_2 \rightarrow C_4H_7N_3O_2$	48.9	38.7	-7.5	-8.5
23	$C_4H_7N_3O_2 \rightarrow C_4H_5N_3O + H_2O$	31.9	30.4	-6.2	-6.2

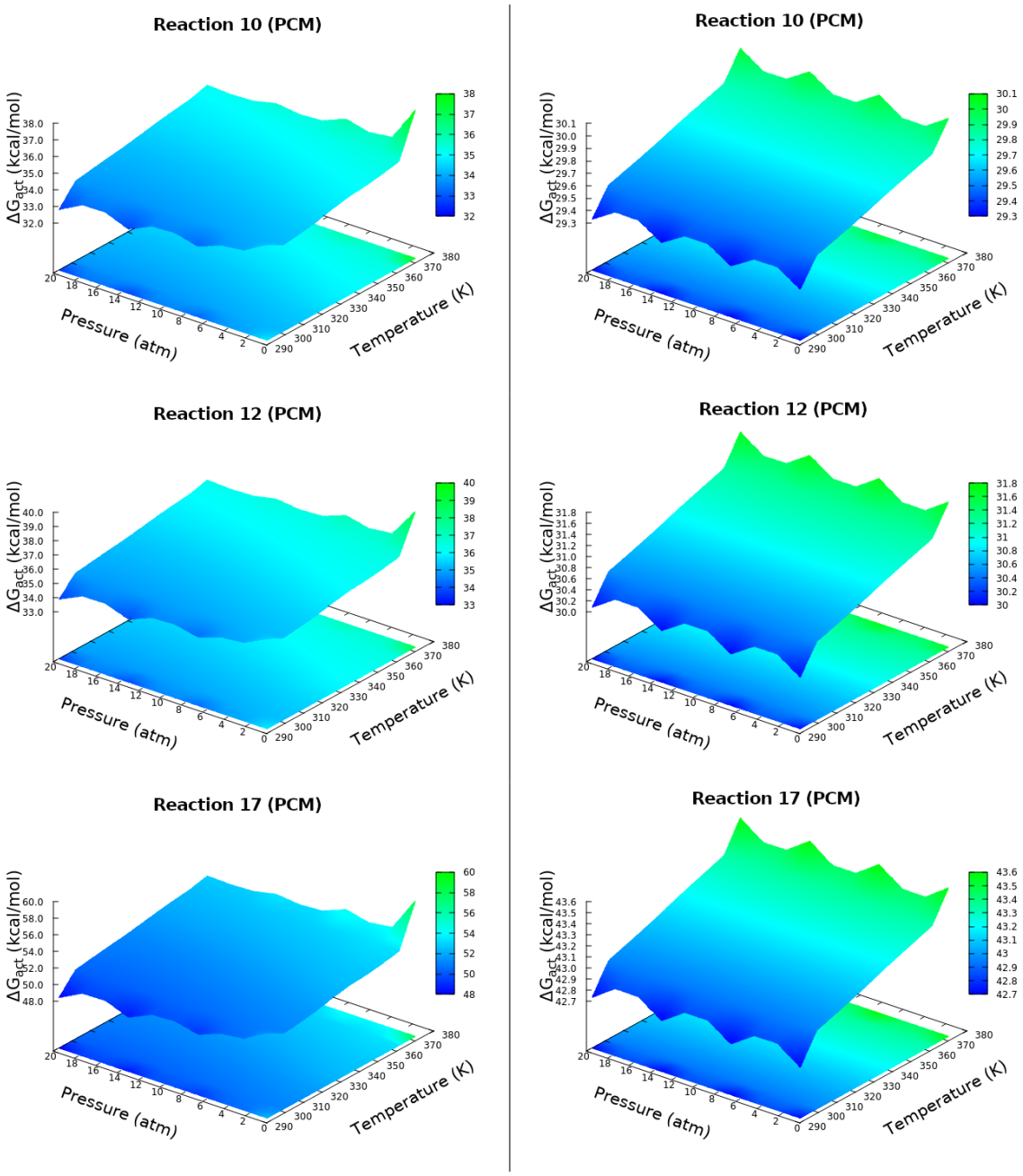

Figure S1: Absolute (left) and intrinsic (right) activation energies for elementary steps **10**, **12** and **17** (Table 1), in *solution*, over a grid of temperatures in [293, 373] K and pressures in [0.5, 20] atm.

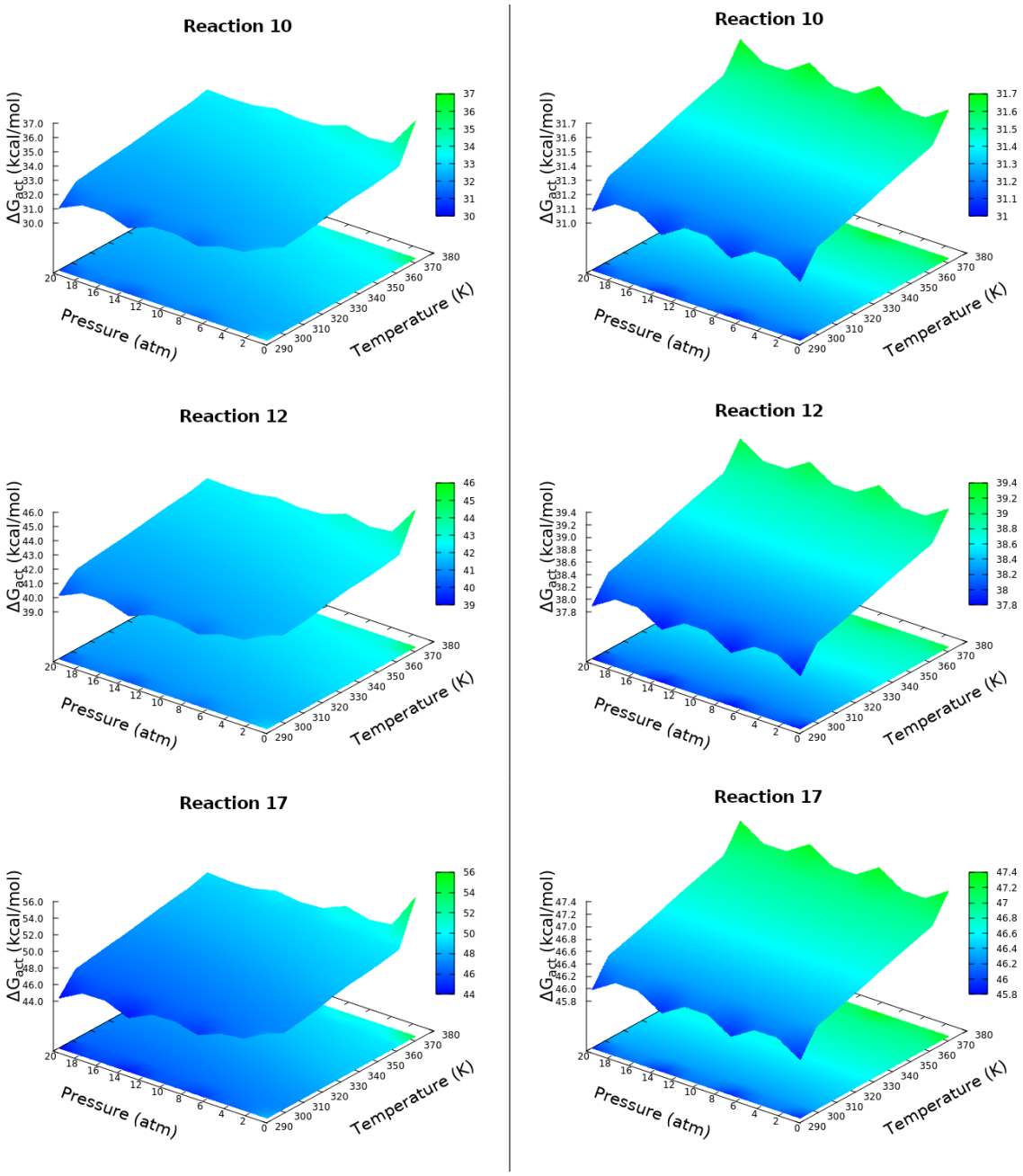

Figure S2: Absolute (left) and intrinsic (right) activation energies for elementary steps **10**, **12** and **17** (Table 1), in *vacuo*, over a grid of temperatures in [293, 373] K and pressures in [0.5, 20] atm.

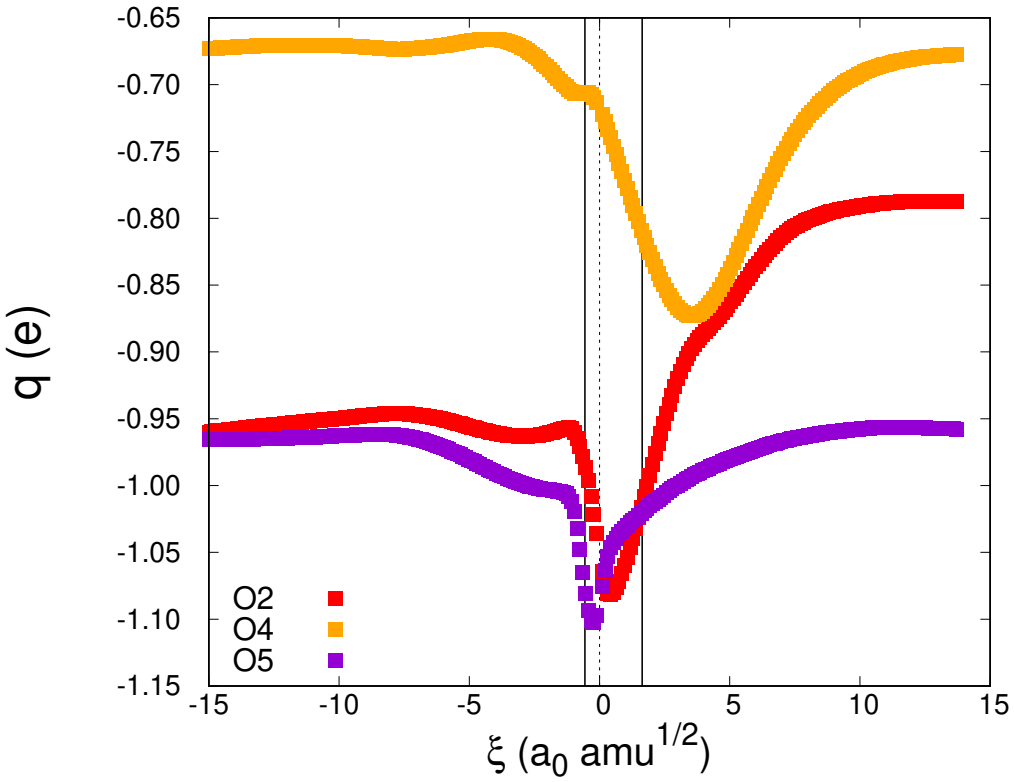

Figure S3: Natural charges at oxygen atoms along the IRC for the reaction **3**.

References

[1] Tamal Das, Siddharth Ghule, and Kumar Vanka. Insights into the origin of life: Did it begin from hcn and h_2o? *ACS central science*, 5(9):1532–1540, 2019.