Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Electronic Supplementary Information

Thermal Decomposition Kinetics of Glyphosate (GP) and its Metabolite Aminomethylphosphonic Acid (AMPA)

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List of Figures

List of Tables

Table S1. Energies for GP and *N*-methylene-glycine transition states, relative to their reactants. Energies are 0 K enthalpies in kcal/mol.

Transition State	M06-2X/6-31G(2df,p)	G3X-K/ 6-31G(2df,p)
TS1G	45.4	44.9
TS2aG	65.1	62.3
TS2bG	58.4	55.7
TS3G	59.6	58.3
TS4G	66.4	69.2
TS5G	66.5	66.7
TS1MG	44.7	48.2
TS2aMG	38.9	47.7
TS2bMG	40.8	38.0

Table S2. Calculated rate coefficients (k, s^{-1}) for GP thermal decomposition

Temperature	TS1G	TS2G	TS3G	TS4G	TS5G
300	1.96E-20	9.67E-33	7.59E-39	2.35E-30	2.52E-36
400	4.33E-12	3.67E-21	4.58E-26	1.46E-19	4.19E-24
500	4.62E-07	3.49E-14	2.31E-18	4.66E-13	9.15E-17
600	1.07E-03	1.63E-09	3.28E-13	1.04E-08	7.23E-12
800	1.81E+01	1.17E-03	9.65E-07	2.94E-03	9.77E-06
1000	6.47E+03	3.90E+00	7.66E-03	5.63E+00	4.76E-02
1200	3.34E+05	8.82E+02	3.12E+00	8.77E+02	1.39E+01
1500	1.77E+07	2.01E+05	1.30E+03	1.38E+05	4.13E+03
2000	9.66E+08	4.58E+07	5.59E+05	2.21E+07	1.26E+06

Table S3. Calculated rate coefficients (k, s^{-1}) for *N*-methylene-glycine thermal decomposition and hydrolysis

Temperature	TS1MG	TS2MG
300	6.48E-24	7.21E-31
400	4.09E-15	2.18E-22
500	7.98E-10	2.70E-17
600	2.74E-06	6.93E-14
800	7.48E-02	1.38E-09
1000	3.55E+01	5.74E-07
1200	2.21E+03	3.44E-05
1500	1.41E+05	2.26E-03
2000	9.28E+06	1.73E-01

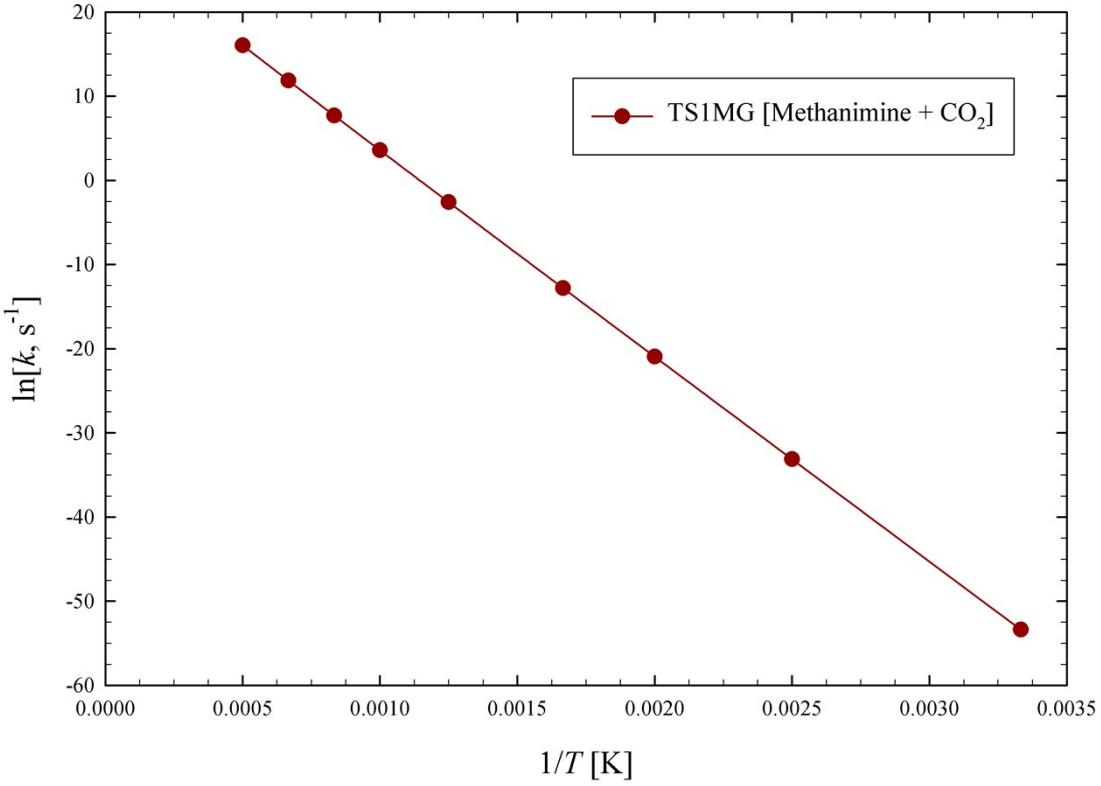

Fig. S1 *N*-methylene-glycine thermal decomposition reaction rate coefficients, k (s^{-1}), in Arrhenius plot.

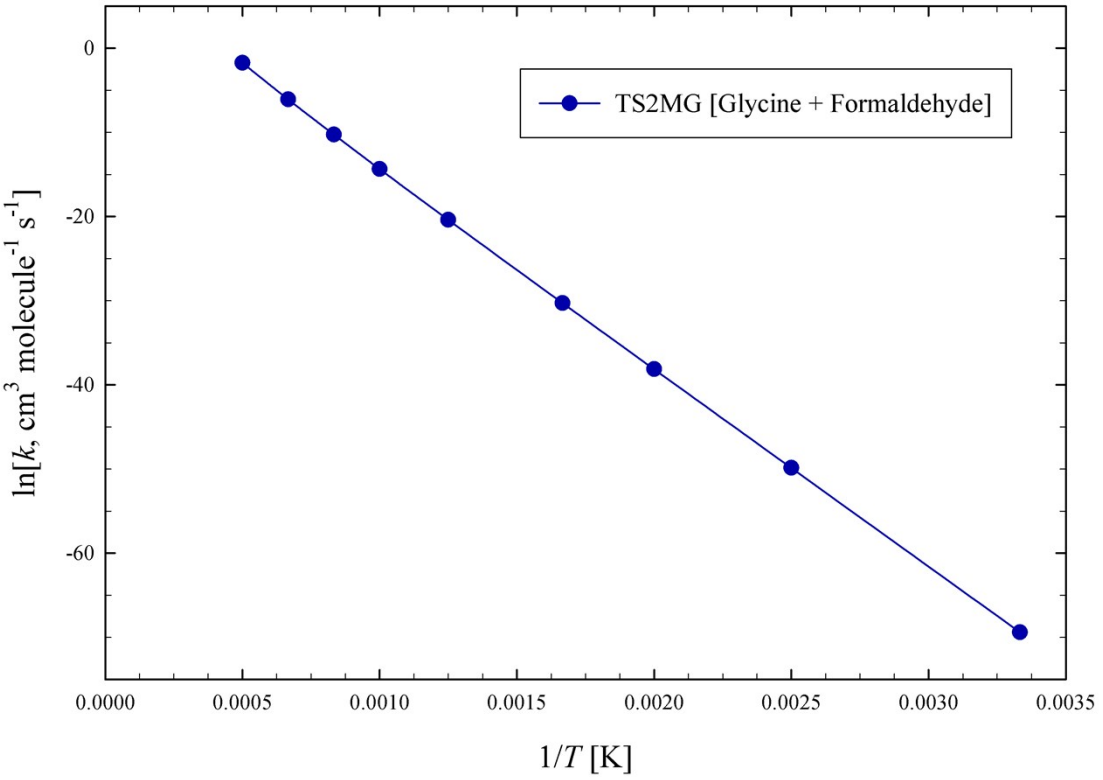

Fig. S2 *N*-methylene-glycine hydrolysis reaction rate coefficients, k (cm^3 $molecule^{-1}$ s^{-1}), in Arrhenius plot.

Table S4. Energies for AMPA and methanimine transition states, relative to their reactants. Energies are 0 K enthalpies in kcal/mol.

Transition State	M06-2X/6-31G(2df,p)	G3X-K
TS1A	45.8	50.1
TS2aA	67.3	65.2
TS2bA	58.4	57.6
TS3A	61.6	64.4
TS4A	62.0	62.5
TSaMA	40.2	47.3
TSbMA	24.7	31.5

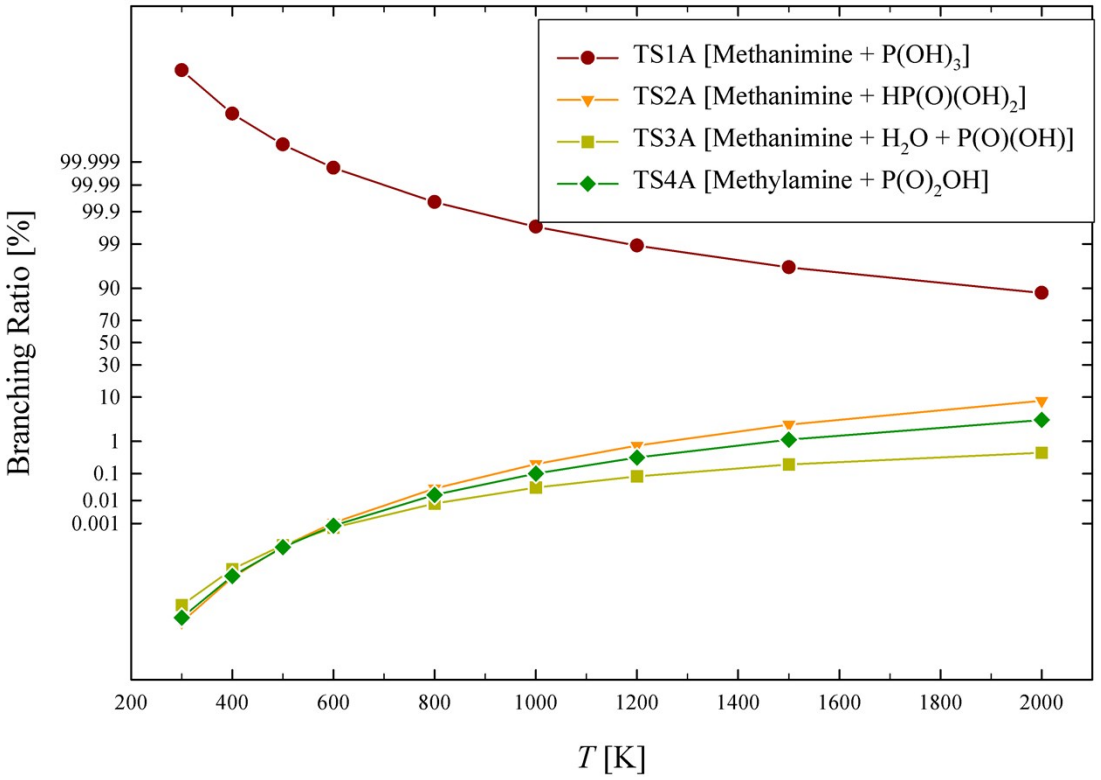

Fig. S3 Branching ratio (%) for each of the reaction channels identified in AMPA decomposition across the temperature range of 300 - 2000 K.

Table S5. Calculated rate coefficients (k, s^{-1}) for AMPA thermal decomposition and Methyleneimine hydrolysis

Temperature	TS1A	TS2A	TS3A	TS4A	TSMA
300	2.05E-24	4.59E-35	9.10E-35	6.24E-34	6.31E-30
400	3.34E-15	5.08E-23	6.23E-23	1.55E-22	1.50E-21
500	1.16E-09	9.04E-16	8.16E-16	1.06E-15	1.63E-16
600	5.83E-06	6.35E-11	4.65E-11	3.84E-11	3.83E-13
800	2.57E-01	7.54E-05	4.25E-05	1.93E-05	6.94E-09
1000	1.62E+02	3.40E-01	1.66E-01	5.14E-02	2.75E-06
1200	1.22E+04	9.34E+01	4.19E+01	1.00E+01	1.60E-04

1500	9.33E+05	2.58E+04	1.08E+04	1.98E+03	1.03E-02
2000	7.38E+07	7.16E+06	2.87E+06	4.01E+05	7.68E-01

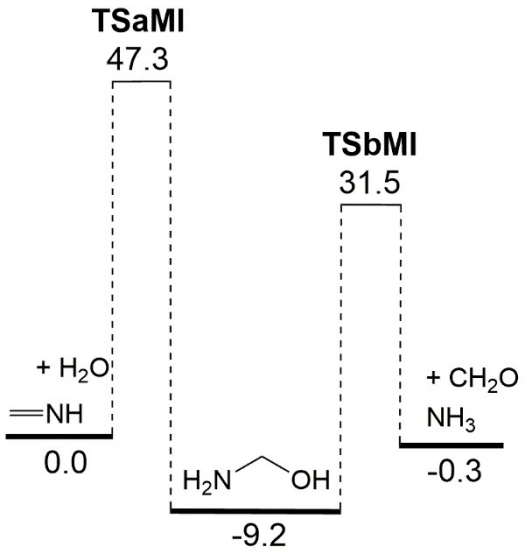

Fig. S4 Potential energy diagram for methyleneimine hydrolysis. Energies (0 K enthalpies) are calculated at the G3X-K level of theory.

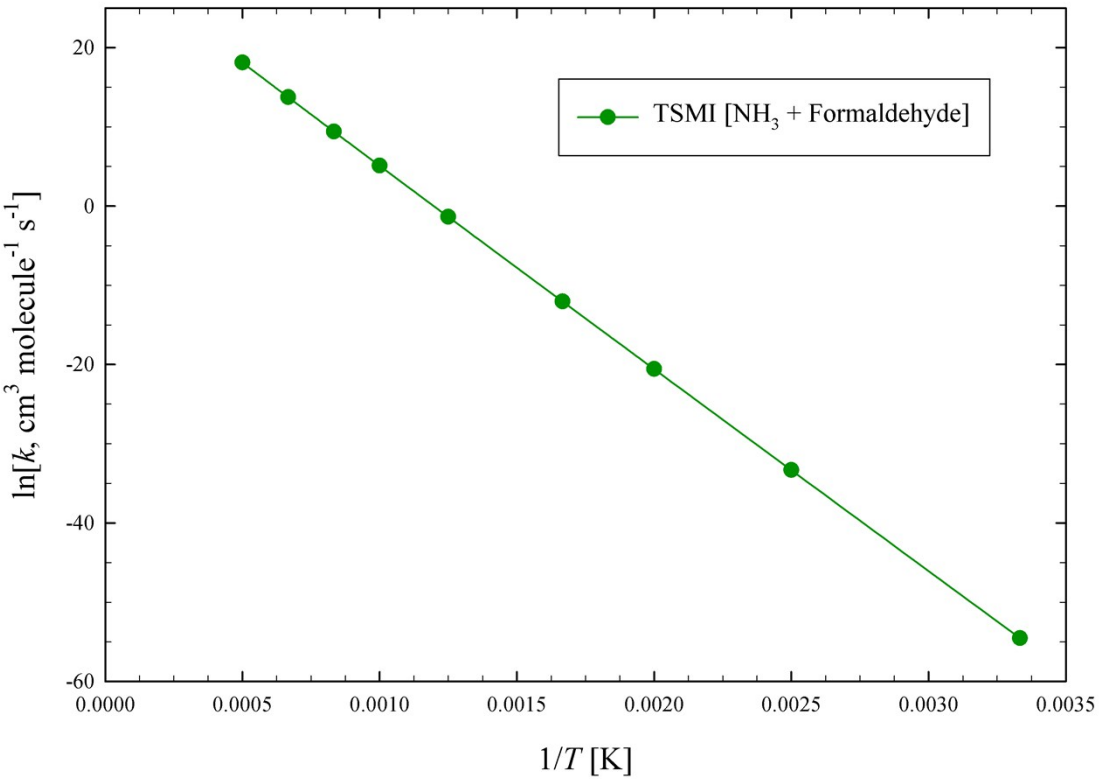

Fig. S5 Methyleneimine hydrolysis reaction rate coefficients, k (cm^3 $molecule^{-1}$ s^{-1}), in Arrhenius plot.

Moments of inertia and vibrational frequencies at M06-2X/6-31G(2df,p) level of the theory

Table S6 to Table S8 represents moments of inertia (Tables S6, S7, and S8) and vibrational frequencies (Tables S9, S10, and S11) at M06-2X/6-31G(2df,p) level of the theory. All input parameters required for the rate coefficient calculations (Arrhenius plot) are provided in these tables.

Table S6. GP moments of inertia (amu Å^2) at M06-2X/6-31G(2df,p) level

Ground State	Transition State				
GP	TS1G	TS2G	TS3G	TS4G	TS5G
184.7314	199.1418	221.7561	212.5116	256.4639	189.6011
939.9731	912.5524	997.7561	963.2152	650.6258	999.6667
993.3875	963.2414	1012.7336	981.2644	721.8309	1071.6352

Table S7. *N*-methylene-glycine moments of inertia (amu Å^2) at M06-2X/6-31G(2df,p) level

Ground State		Transition State	
N-methylene-glycine	Water	TS1MG	TS2MG
56.1729	0.6223	67.3826	101.1638
212.2405	1.1529	175.1296	275.5458
252.0369	1.7751	228.5521	345.7301

Table S8. AMPA moments of inertia (amu Å^2) at M06-2X/6-31G(2df,p) level

Ground State	Transition State				
AMPA	TS1A	TS2A	TS3A	TS4A	TSMI
118.3859	104.9712	87.9207	109.5826	117.8035	16.6618
214.0326	248.0552	283.9618	258.7880	223.4931	48.6544
222.0022	273.1691	329.9302	269.7440	235.5869	58.7426

Table S9. GP vibrational frequencies (cm^{-1}) at M06-2X/6-31G(2df,p) level

Ground State	Transition State				
GP	TS1G	TS2G	TS3G	TS4G	TS5G
26.63	-344.65	-328.95	-270.25	-1587.73	-1420.84
47.35	42.61	39.35	35.78	44.86	23.35
61.32	81.76	41.78	46.77	85.79	42.83
122.24	125.11	66.36	74.64	116.10	58.31
172.43	136.35	69.04	122.99	146.31	114.39
196.99	150.86	133.47	157.69	168.18	156.96
242.77	190.72	155.21	166.79	178.03	193.41
281.49	228.09	166.35	203.27	199.75	230.78
319.61	295.40	207.59	255.52	217.14	286.28
375.90	356.18	270.39	314.42	266.23	378.21
394.17	406.13	285.32	361.84	335.43	394.58
435.93	414.19	357.17	401.61	370.86	434.52
448.46	454.33	391.20	412.61	390.25	465.10
493.76	478.12	435.69	429.99	421.10	467.78
527.79	499.35	475.02	457.56	434.59	529.09
554.53	522.85	495.06	478.40	485.09	541.04
625.21	525.54	547.64	539.93	516.88	615.32
700.76	655.81	567.08	598.56	596.51	659.61
730.25	684.69	648.14	620.53	652.37	693.03
834.25	852.69	714.19	694.81	681.79	716.72
865.97	872.69	787.39	696.56	748.76	758.01
912.29	902.79	812.53	703.98	772.66	908.99
926.78	938.73	866.42	906.38	859.80	916.20
968.66	959.03	888.19	935.28	881.10	982.80
1018.39	1006.42	987.62	999.44	920.55	1024.03
1052.55	1024.50	998.86	1018.79	996.39	1043.36
1056.86	1058.39	1016.34	1042.82	1044.51	1069.03

1113.73	1068.77	1034.90	1053.05	1098.08	1181.02
1166.44	1127.94	1040.12	1075.89	1125.39	1195.96
1199.47	1154.69	1117.28	1189.45	1147.40	1212.85
1252.51	1196.77	1160.95	1230.77	1164.84	1257.99
1255.33	1204.14	1222.98	1252.97	1246.18	1275.63
1323.27	1286.13	1303.52	1285.90	1283.18	1314.91
1346.43	1316.53	1362.23	1350.18	1317.47	1350.54
1363.75	1386.75	1416.45	1415.69	1352.67	1409.47
1418.30	1403.85	1423.41	1452.74	1373.45	1415.32
1461.63	1432.07	1459.27	1467.96	1422.60	1446.13
1483.47	1454.54	1499.96	1510.25	1428.10	1494.53
1507.88	1538.56	1670.98	1766.30	1464.55	1517.95
1919.99	1860.43	1920.23	1926.26	2130.37	1917.79
2986.29	2428.78	2931.57	2675.13	2298.97	1963.26
3027.20	2990.94	3184.95	3041.49	3050.82	2959.43
3131.65	3064.67	3228.30	3165.10	3139.43	3004.25
3141.86	3102.22	3351.84	3181.03	3155.56	3044.76
3589.01	3136.64	3625.95	3310.89	3266.90	3166.07
3777.88	3818.68	3820.71	3811.45	3592.53	3603.50
3827.83	3821.65	3821.20	3821.30	3610.57	3827.68
3890.41	3838.31	3846.88	3841.39	3885.24	3867.28

Table S10. *N*-methylene-glycine vibrational frequencies (cm^{-1}) at M06-2X/6-31G(2df,p) level

Ground State		Transition State		
GP	Water	TS1MG	TS2aMG	TS2bMG
46.48	1658.61	-1695.33	-1534.80	-1319.06
81.82	3884.23	126.16	33.03	60.18
267.02	3990.61	340.55	98.20	63.45

423.75	398.44	213.97	122.62
466.67	427.54	262.77	180.34
565.22	505.06	377.99	330.94
599.85	579.68	448.95	442.35
698.63	665.15	518.31	531.78
749.33	731.12	576.42	637.60
918.30	794.97	604.21	672.49
1020.93	933.68	644.91	708.37
1047.67	1041.95	698.93	819.11
1091.32	1083.91	711.97	881.78
1198.39	1130.19	844.38	903.40
1226.47	1170.41	904.59	1027.18
1274.57	1220.38	993.53	1067.04
1346.21	1282.26	1051.59	1170.42
1414.45	1363.81	1133.71	1196.93
1470.39	1467.33	1173.89	1216.54
1507.40	1546.95	1199.52	1223.48
1798.05	1603.85	1284.06	1294.18
1909.31	1638.35	1308.43	1315.06
2998.64	2095.59	1332.91	1347.75
3041.97	3036.95	1364.88	1398.95
3144.68	3046.22	1399.08	1455.59
3181.60	3214.32	1460.39	1473.23
3827.39	3234.80	1533.58	1489.57
		1552.95	1570.60
		1907.96	1906.41
		1958.35	2250.61
		3002.19	2913.62
		3062.76	2928.46
		3127.64	3080.79
		3152.25	3140.89

				3796.88	3524.19
				3815.29	3819.28

Table S11. AMPA vibrational frequencies (cm^{-1}) at M06-2X/6-31G(2df,p) level

Ground State	Transition State				
AMPA	TS1A	TS2A	TS3A	TS4A	TSMA
66.08	-1217.35	-450.99	-1094.23	-1444.11	-1847.31
138.03	69.71	64.84	60.40	97.22	477.17
191.14	126.77	104.83	132.11	187.06	511.28
234.52	165.14	167.87	159.57	252.35	685.21
293.63	214.66	185.29	256.64	277.58	736.78
324.16	309.23	211.14	276.04	325.56	781.72
356.82	362.37	312.10	375.01	392.23	1032.78
386.71	422.13	332.28	405.20	432.74	1092.26
431.68	432.06	422.63	442.20	467.34	1262.51
488.71	486.36	446.67	523.10	532.46	1301.95
727.32	624.38	473.19	530.81	643.20	1391.67
813.13	689.99	687.75	620.04	706.59	1518.91
886.16	859.84	777.50	721.80	901.21	1565.91
927.79	890.24	816.37	840.93	930.11	1867.13
945.98	962.18	878.30	877.77	1000.24	3084.00
1030.02	1008.90	961.28	1010.18	1041.82	3178.42
1056.19	1034.15	991.39	1026.15	1084.23	3523.70
1104.25	1060.86	1008.78	1060.29	1158.94	3845.09
1135.19	1131.72	1036.86	1094.02	1196.12	
1287.64	1163.95	1098.63	1285.70	1288.00	
1349.31	1286.06	1331.24	1370.29	1372.79	
1393.98	1404.98	1411.20	1437.09	1404.18	

1475.28	1458.23	1550.16	1562.83	1434.06
1646.11	1590.05	1704.80	1637.89	1669.41
3015.93	1735.74	3231.49	1686.18	1980.37
3121.33	3125.90	3358.26	3152.74	3013.97
3548.62	3210.55	3596.48	3250.41	3118.57
3636.66	3550.77	3717.16	3569.55	3530.70
3886.77	3835.82	3817.76	3821.13	3614.89
3890.17	3864.77	3834.89	3881.97	3869.96

Cartesian Coordinates (Angstrom) at M06-2X/6-31G(2df,p) level of the theory

Table S12 to Table S31 represents Cartesian coordinates of the optimized geometries observed in Figures 3 and 9. All these structures are obtained at M06-2X/6-31G(2df,p) level of the theory.

Table S12. Cartesian coordinates (Å) of GP

0	1		
P	-1.81287300	-0.18436200	-0.06138200
O	-3.28794700	0.29883300	0.28461700
H	-3.82074500	-0.44814900	0.57712400
O	-1.63695300	0.34963200	-1.54597000
H	-0.70248400	0.57311300	-1.67758700
O	-1.57097500	-1.60752700	0.18002700
C	-0.71191600	0.93941100	0.84202300
H	-1.11913500	1.94892700	0.74712200
H	-0.68340400	0.67143800	1.90809100
N	0.59036000	0.87686800	0.17819400
H	1.12007400	1.72241500	0.35145800
C	1.37981300	-0.27655600	0.59168600
H	1.51117300	-0.32891500	1.68672900
H	0.88561000	-1.20270700	0.29044800
C	2.76783900	-0.26329700	-0.00451700
O	3.43479000	-1.23365800	-0.21099600
O	3.20511500	0.99075100	-0.23306300
H	4.10283900	0.90963900	-0.58208200

Table S13. Cartesian coordinates (Å) of TS1G

0	1		
P	1.78198800	-0.03692700	0.15512500
O	3.14107100	0.35191500	-0.60268300
H	3.65344200	-0.41578000	-0.88617100
O	2.32777500	-1.15695200	1.19301800
H	1.74387500	-1.92368200	1.18339100
O	0.83039000	-0.81974100	-0.78372100
C	0.38083100	1.73903700	0.00588100
H	0.37963300	2.22691900	0.98162900
H	1.02703300	2.20655800	-0.73703500
N	-0.66982400	1.06159900	-0.43823700
H	-0.03329900	-0.05328700	-0.89508500
C	-1.55402800	0.62015700	0.61801900
H	-1.02036200	-0.05090000	1.32348300
H	-1.95937900	1.44634000	1.20935700
C	-2.72738600	-0.17644700	0.09207100
O	-3.83364700	-0.14613100	0.55134100
O	-2.37325100	-0.97287900	-0.92668600
H	-3.16720700	-1.45963500	-1.18474500

Table S14. Cartesian coordinates (Å) of TS2aG

0	1		
P	1.77810500	0.28088900	-0.23207300
O	2.23618800	-1.03969800	-1.11589700
H	3.17871400	-1.21165800	-0.99595600
O	3.11070500	1.21263600	-0.51445700
H	3.52436400	1.35583600	0.34530400
O	1.85600400	-0.07190900	1.24806400
C	-0.15805000	-1.24609200	0.61039300

N	-0.89785300	-0.38495300	1.23788800
H	-0.66122000	-0.22701900	2.20848300
C	-1.55576500	0.70596500	0.54698000
H	-1.86166400	1.46478900	1.26378700
H	-0.80371500	1.13765300	-0.14317100
C	-2.77626500	0.31346600	-0.26026100
O	-3.66402500	1.07092600	-0.51325000
O	-2.72143600	-0.95325100	-0.69625600
H	-3.50975500	-1.09934600	-1.23739200
H	0.44168400	-1.93901400	1.17960700
H	-0.29401600	-1.38955800	-0.45308400

Table S15. Cartesian coordinates (Å) of TS3G

0	1		
P	-2.27628100	-0.13775500	0.17388500
O	-1.38315300	0.25601700	-1.30209300
O	-1.16249000	0.56512000	1.23935500
O	-3.42246500	0.80921900	0.12916300
N	0.61025300	-0.88875000	-0.31044100
C	-0.01659300	-1.99886000	-0.30089700
H	0.24943900	-2.78065400	0.40446400
H	-0.78573400	-2.15571400	-1.04539400
H	0.10694200	-0.15304400	-0.90092800
H	-1.69768600	1.12666400	-1.57337400
H	-1.49305300	1.45998400	1.39538600
C	1.56558000	-0.46724700	0.68746400
H	1.95413700	-1.32029900	1.24384000
H	1.01253900	0.19492900	1.36985100
C	2.72555700	0.30759600	0.09848400
O	2.39535500	0.89052800	-1.06049700
H	3.16237500	1.40056700	-1.35584300
O	3.78728100	0.41239100	0.63363500

Table S16. Cartesian coordinates (Å) of TS4G

0	1		
P	1.34387900	-0.28458300	-0.16674300
O	2.93133600	-0.27634800	-0.17748600
H	3.27629100	-0.87237600	-0.85127800
O	1.00557500	-1.01360200	1.18528600
H	0.05202900	-1.22596900	1.23967800
O	0.69426500	-0.78797500	-1.37703700
C	1.02611700	1.48137800	0.16222100
H	1.68039200	1.78590400	0.98226000
H	1.29163800	2.04256200	-0.74273500
N	-0.35817100	1.71556900	0.54552100
H	-0.54142000	2.61965400	0.95773900
C	-1.45530500	1.27901500	-0.44591700
H	-2.21986900	2.04162300	-0.54196800
H	-1.01477500	0.93344900	-1.37573200
C	-2.33139000	-0.51593200	0.07806000
O	-3.21068300	-0.59929000	-0.69705600
O	-1.72177400	-0.98974400	1.00912600
H	-1.20155700	0.80381500	0.70566900

Table S17. Cartesian coordinates (Å) of TS5G

0	1		
P	-1.99828500	0.23287900	0.22041300
O	-3.03218300	0.25838000	-0.97858400
H	-2.94729100	1.07119500	-1.49076800
O	-2.44805400	-0.77198700	1.23501400
H	-1.49226400	-1.30119500	0.36620000
O	-1.29494000	1.48933200	0.41314300
C	-0.58005500	-1.11368100	-0.61149900
H	-0.78620200	-2.18947500	-0.73863000

H	-0.71208300	-0.70355600	-1.62367400
N	0.72059200	-0.93274700	-0.01638100
H	1.31756200	-1.72634200	-0.20697800
C	1.40266500	0.29046300	-0.39782000
H	1.39097900	0.46571000	-1.49023200
H	0.93300900	1.15692100	0.06751000
C	2.85952400	0.28871800	0.00287800
O	3.52630100	1.27188000	0.13922900
O	3.35474400	-0.95674000	0.13970600
H	4.28667800	-0.85713700	0.37561800

Table S18. Cartesian coordinates (Å) of *N*-methylene-glycine

0	1		
C	-2.32181600	0.22209700	-0.12586400
H	-2.37009900	0.18229900	-1.22220300
H	-3.15886800	0.68543900	0.39428500
N	-1.35849900	-0.23667300	0.54269600
C	-0.26860900	-0.83400400	-0.19793100
H	-0.07416300	-1.84089700	0.17448400
H	-0.46394000	-0.89092600	-1.28164700
C	1.02072800	-0.05201200	-0.02439300
O	2.10729200	-0.54447300	0.07587600
O	0.80773100	1.27134800	-0.05260900
H	1.67454900	1.68931600	0.03920600

Table S19. Cartesian coordinates (Å) of Water

0	1		
O	0.00000000	0.00000000	0.11791000
H	0.00000000	0.75623600	-0.47164100
H	0.00000000	-0.75623600	-0.47164100

Table S20. Cartesian coordinates (Å) of TS1MG

0	1		
C	-1.90067700	-0.41415900	0.10006500
H	-1.95523300	-0.50224000	1.19291100
H	-2.72921300	-0.83433500	-0.46126600
N	-1.27590100	0.63805700	-0.44765000
C	-0.25033800	1.14864300	0.22271900
H	0.26085400	1.99511700	-0.22021900
H	-0.22866500	1.08897100	1.31931300
C	1.05361300	-0.22044600	-0.01581200
O	2.12042300	0.29064300	-0.06134300
O	0.49850300	-1.31367700	0.00126300
H	-0.78344100	-1.11387500	-0.05838100

Table S21. Cartesian coordinates (Å) of TS2aMG

0	1		
C	1.75248600	-0.38653100	0.52215400
H	1.37160800	-0.02644000	1.48543400
H	2.80373900	-0.67502200	0.55741700
N	0.94963700	-1.07047000	-0.34165200
C	-0.43988500	-1.19498700	0.03078300
H	-0.93354800	-1.91558100	-0.62494600
H	-0.55427900	-1.59685400	1.05099700
C	-1.34674700	0.02904100	0.01001100

O	-2.52353800	0.01450300	-0.20062300
O	-0.70824000	1.19452900	0.31896500
H	-1.39586400	1.87468900	0.31529600
O	1.94099900	0.97039400	-0.44441200
H	1.36133500	0.14574100	-0.99983200
H	1.23066100	1.56621200	-0.16193200

Table S22. Cartesian coordinates (Å) of TS2bMG

0	1		
C	-2.31666900	0.07541600	-0.43786200
H	-2.23372600	0.97826800	-1.07690000
H	-2.84123500	-0.71432000	-1.01425600
N	-0.84629500	-0.47473100	-0.23987500
C	0.20311500	0.52588500	-0.36583000
H	0.27846100	0.90555200	-1.39024100
H	-0.05007300	1.36560800	0.28681500
C	1.54003000	-0.06631700	0.01500200
O	1.74100300	-1.23945400	0.15124200
O	2.47343900	0.88001500	0.14530100
H	3.30491200	0.43517200	0.36047100
O	-2.61148400	0.23056600	0.84065800
H	-0.58000900	-1.36475600	-0.65853500
H	-1.33678400	-0.46132700	0.80631200

Table S23. Cartesian coordinates (Å) of AMPA

0	1		
P	0.43989400	0.02608800	0.10995300
O	0.25339400	1.16093400	-1.00588100
O	1.40189500	-1.04998100	-0.57043100

O	0.91723800	0.54609100	1.39041500
N	-2.21316000	0.13184500	0.15848400
C	-1.13779000	-0.83894000	0.01465000
H	-1.14179300	-1.43018300	-0.91311000
H	-1.15530700	-1.54054000	0.85331700
H	-3.10769100	-0.33959700	0.21145700
H	-2.23303200	0.73308700	-0.65732700
H	0.48339200	2.02062400	-0.63777900
H	2.29466700	-0.98033400	-0.21596600

Table S24. Cartesian coordinates (Å) of TS1A

0	1		
P	0.47275800	-0.04858000	-0.16582800
O	1.63909900	0.92283700	-0.74357300
O	1.29871600	-1.34374300	0.32200500
O	-0.05481800	0.70801100	1.07872400
N	-2.27984200	0.28641500	0.20355900
C	-1.76061900	-0.61157500	-0.61690100
H	-1.90573700	-0.57950400	-1.69483600
H	-1.53906600	-1.59887400	-0.21335800
H	-1.24068600	0.58485400	0.93241300
H	-2.59774000	1.10824100	-0.30241000
H	1.68657600	1.72174800	-0.20624200
H	1.96390500	-1.14005900	0.99108900

Table S25. Cartesian coordinates (Å) of TS2aA

0	1		
P	0.62898300	0.08678700	-0.33685700
O	2.14967700	0.72479900	-0.28482100

O	0.99687300	-1.45756600	0.14506500
O	-0.09306100	0.75865500	0.83326800
N	-2.59338800	0.39522200	-0.19870600
C	-1.81073700	-0.62570700	-0.00130200
H	-1.61928600	-1.30713800	-0.81936300
H	-1.57214400	-0.92789600	1.00511200
H	-2.63989900	1.09373600	0.52991400
H	-2.79353600	0.70543200	-1.13715400
H	2.15083800	1.35011200	0.45065000
H	1.62950300	-1.43545900	0.87435900

Table S26. Cartesian coordinates (Å) of TS2bA

0	1		
P	0.58089900	0.02492300	-0.17755900
O	1.59962800	1.28956100	0.01818100
O	1.60168800	-1.19936400	-0.49404300
O	-0.09925300	-0.19209000	1.15641800
N	-2.12707000	0.32852700	-0.77417800
C	-2.32710300	-0.34426200	0.30495800
H	-1.94215100	-1.35188800	0.37572700
H	-2.95575000	0.03279500	1.10512400
H	-2.45919300	1.28751100	-0.77858800
H	-1.04255000	0.18420300	-1.14774700
H	1.62714500	1.50593400	0.95741400
H	2.09462400	-1.45138200	0.29651600

Table S27. Cartesian coordinates (Å) of TS3A

0	1		
P	0.68574400	0.13192900	-0.36154500
O	-0.04856900	-1.15232300	0.82047400
O	0.68231900	1.27802000	0.79025700
O	2.03340900	-0.41799600	-0.60350700
N	-2.15934500	-0.11822500	0.30372500
C	-1.83226400	0.25494000	-0.89547300
H	-1.97059400	1.27160500	-1.25813000
H	-1.65052300	-0.50658700	-1.64645200
H	-2.35728100	0.65792500	0.92740000
H	-1.20523200	-0.90370300	0.69080000
H	0.23995300	-2.01599700	0.50752500
H	1.42925700	1.15415300	1.39100600

Table S28. Cartesian coordinates (Å) of TS4A

0	1		
P	0.58181800	-0.07138600	0.18182900
O	0.66951700	1.13598300	1.07171700
O	1.58165300	0.10552600	-1.03281800
O	0.33660200	-1.45864400	0.54678600
N	-2.32085200	-0.23084100	-0.08831700
C	-1.23442700	0.52989800	-0.66493900
H	-1.55566500	1.57035100	-0.84404500
H	-0.97085700	0.17808700	-1.66532400
H	-2.63008800	0.20081000	0.77546300
H	-1.97293800	-1.15268800	0.16162600
H	-0.42363600	1.19097000	0.21476000
H	1.77626000	-0.74315200	-1.44754100

Table S29. Cartesian coordinates (Å) of methanimine

0	1		
N	-0.66606900	-0.15444100	0.00000500
C	0.58323100	0.02869800	-0.00000200
H	1.07547200	1.00691200	0.00001600
H	1.24373500	-0.84035500	-0.00001300
H	-1.15610900	0.74234100	-0.00002800

Table S30. Cartesian coordinates (Å) of TSaMI

0	1		
N	-1.08281500	-0.44111800	-0.12268600
C	-0.33042400	0.67156000	0.02280800
H	-0.16526200	1.28113600	-0.86448400
H	-0.27270200	1.23877400	0.95654900
H	-1.38569300	-0.76851100	0.79202700
O	1.20320100	-0.18433700	-0.08729900
H	1.53709300	-0.36627900	0.80022100
H	0.22320700	-0.85195500	-0.26396300

Table S31. Cartesian coordinates (Å) of TSbMI

0	1		
N	1.08535500	-0.19581200	0.00001400
C	-0.30380700	0.60361200	-0.00005700
H	-0.26561800	1.25074800	0.89983300
H	-0.26560600	1.25075800	-0.89992300

H	1.65720700	-0.11782000	-0.83637400
O	-1.10107000	-0.44143300	0.00001800
H	0.25047000	-0.98634000	0.00042300
H	1.65746700	-0.11686100	0.83613800

Table S32. The thermochemical properties of reactant and products

	Entropy (cal/mol/kelvin)	Heat of Formation (kcal/mol)
GP	107.1	-289.9
AMPA	85.9	-202.4
N-methylene-glycine	72.8	-184.6
$P(OH)_3$	79.8	-66.1
$HP(O)(OH)_2$	71.8	-197.3
P(O)OH	62.4	-108.6
$C_2H_8NO_3P$	79.8	-66.1
Sarcosine	81.7	-90.8
$P(O)_2(OH)$	66.6	-166.2
N-methylmethanimine	60.3	20.7
Glycine	74.6	-94.3
Formaldehyde	52.2	-26.5
methanimine	54.2	21.1
Methylamine	57.3	-4.6

Table S33. Bond dissociation energy for different bonds in the GP structure at M06-2X/6-31G(2df,p) level of theory

Bond	Dissociation Energy (kcal/mole)
P—C	121.0
C—N	83.8
N—C	79.8
C—C	88.4
C—O	112.4
P—O	121.6
C—H	87.2
O—H	114.9
N—H	90.4