

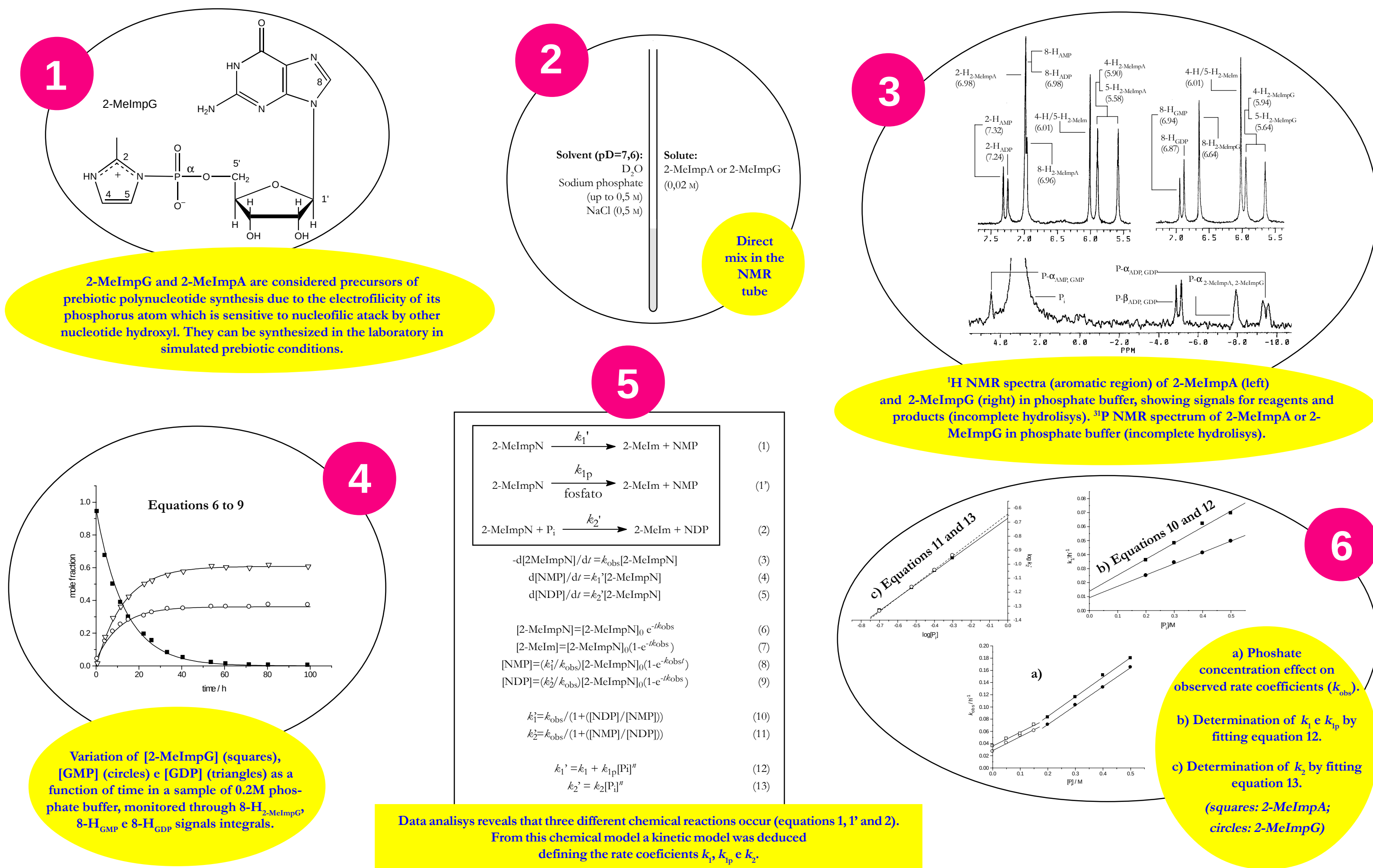


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Possible prebiotic pathway for phosphonucleotide synthesis

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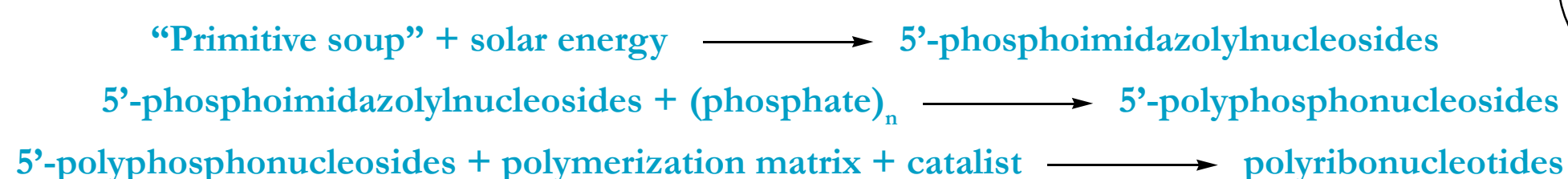


Calculated rate coefficients for reactions 1, 1' e 2

	k ₁ ^b /h ⁻¹	k _{1p} ^b /M ⁻¹ h ⁻¹	k ₂ ^c /M ⁻¹ h ⁻¹	n ^c
2-MeImpA	0,014±0,003	0,11±0,01	0,21±0,01	0,94±0,02
2-MeImpG	0,009±0,001	0,081±0,003	0,23±0,01	0,99±0,02

2-methylimidazole activated nucleotides show high susceptibility to nucleophile substitution and therefore doesn't seem good prebiotic precursors for direct synthesis of primitive polyribonucleotides.

The following alternative is proposed:



PM3 semi-empirical simulation

- 1) Water has an important role in the proposed mechanism for phosphate catalysed hydrolysis because it forms a stable weak complex with the phosphoryl group.
- 2) The phosphoryl group spontaneously accepts 2-methylimidazole S_N2 substitution forming adenosine (or guanosine) 5'-biphosphate.

