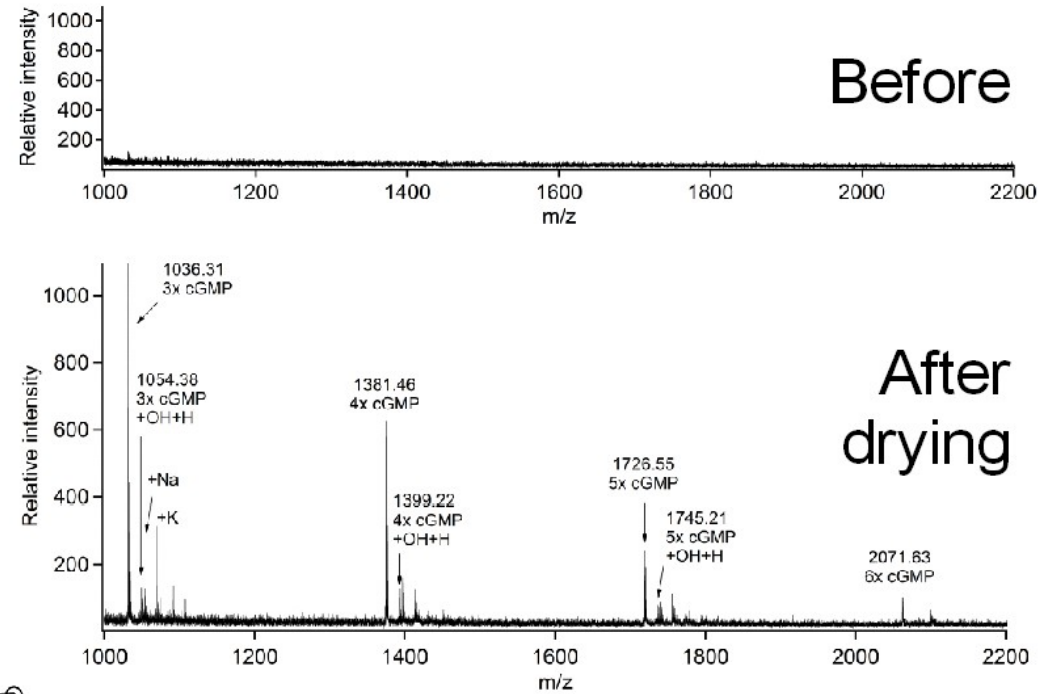
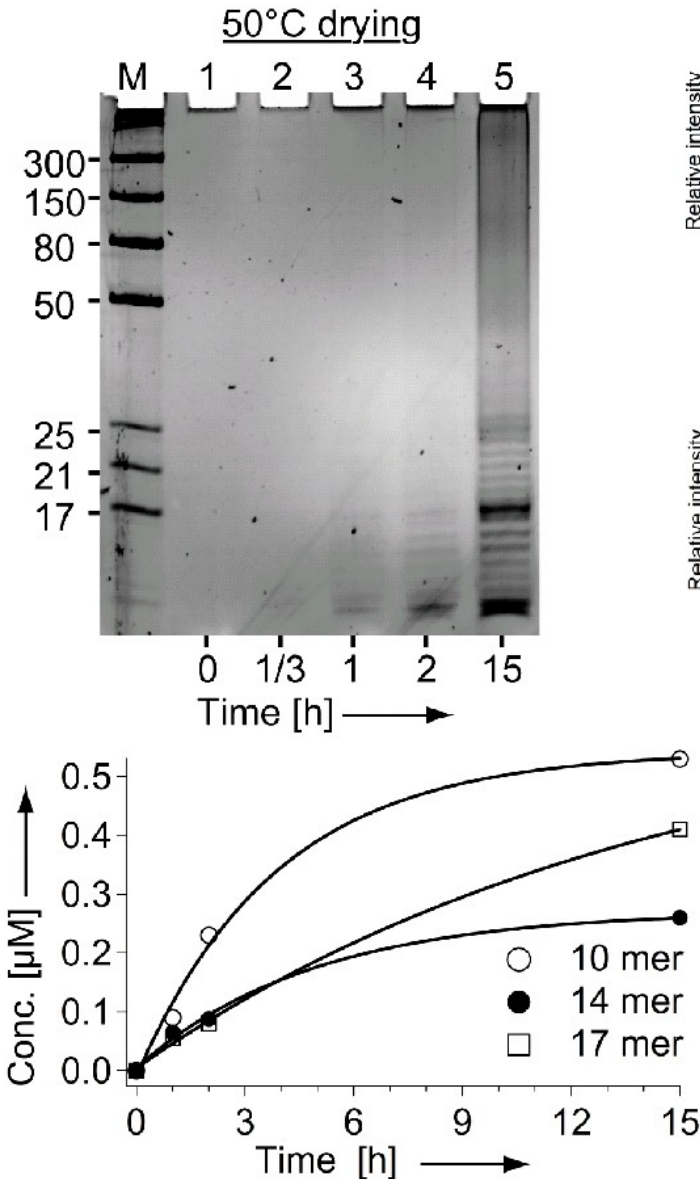


The FORMAMIDE-BASED SCENARIO OF THE ORIGIN OF LIFE THROUGH THE EYES OF A COMPUTATIONAL CHEMIST

Judit E. Šponer

*Institute of Biophysics, Academy of Sciences of the Czech Republic, Královopolská 135,
612 65, Brno, Czech Republic
e-mail: judit@ncbr.chemi.muni.cz*

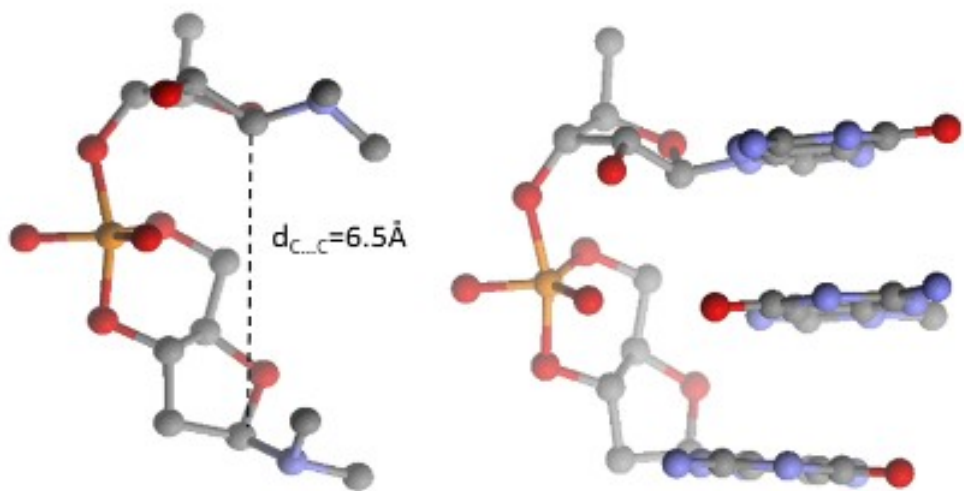
Dry cGMP Polymerization



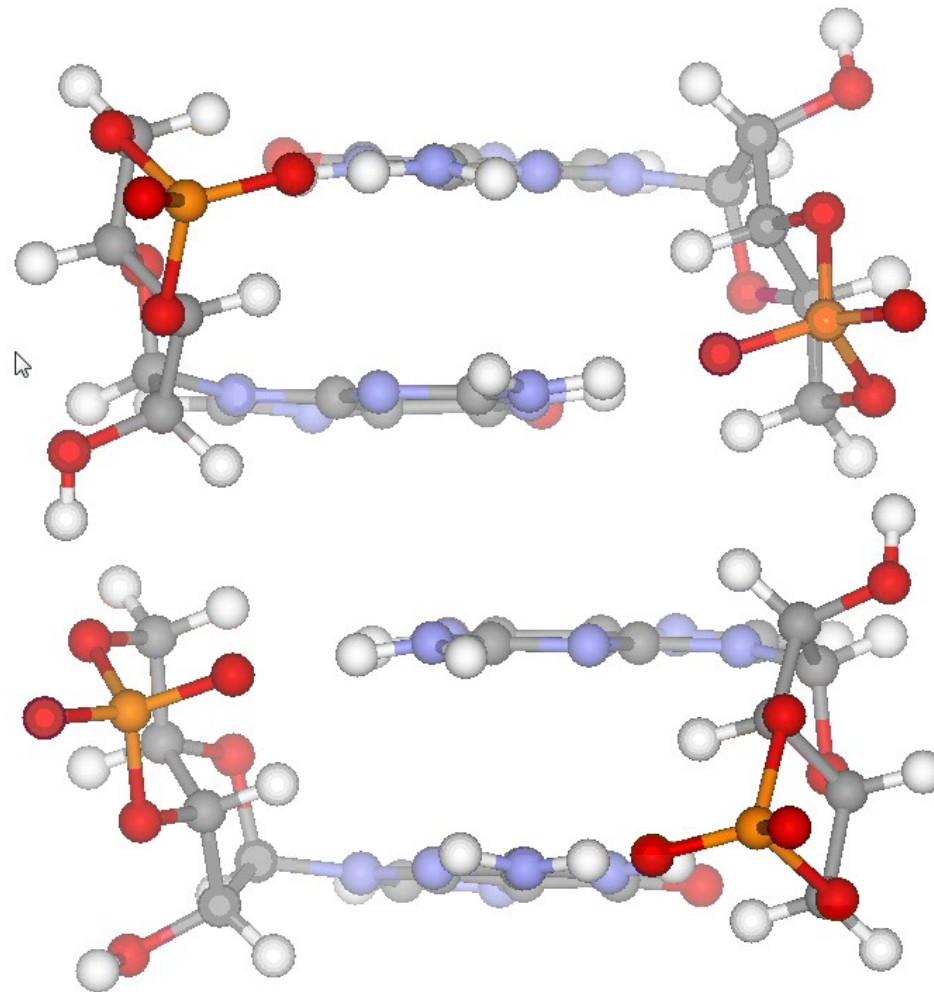
So far no wet polymerization
(Ernesto di Mauro)

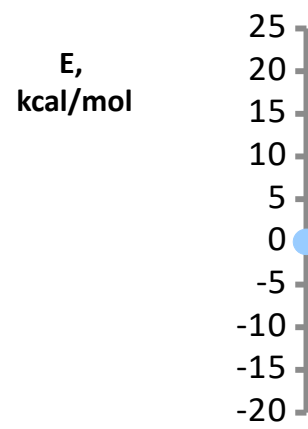
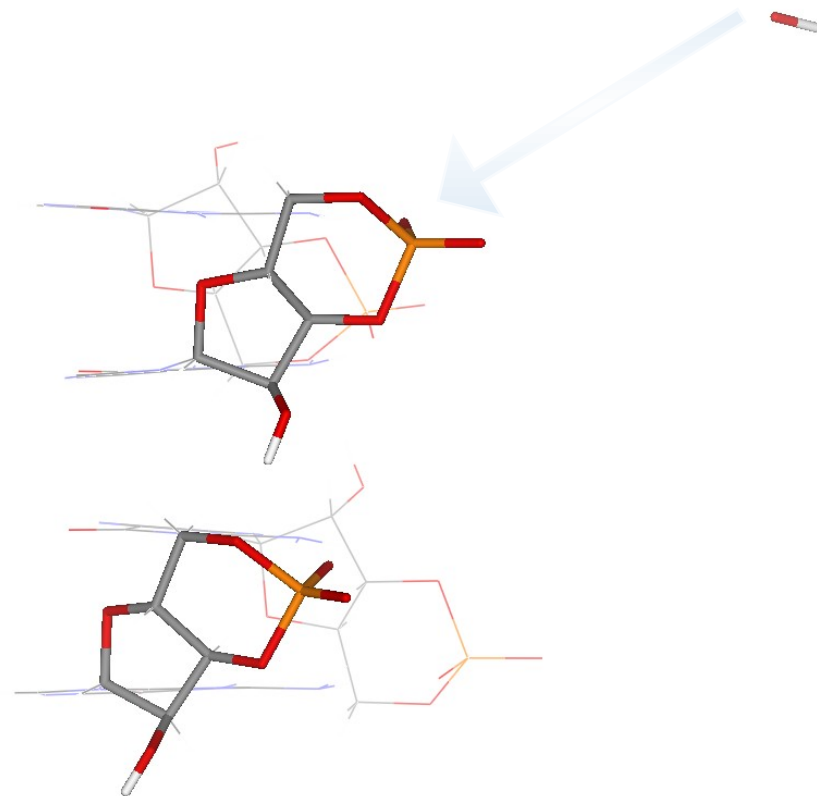
Matthias Morasch, Christof Mast, Johannes Langer,
Pierre Schilcher and Dieter Braun,
ChemBioChem 15, 879-883 (2014), doi:
10.1002/cbic.201300773

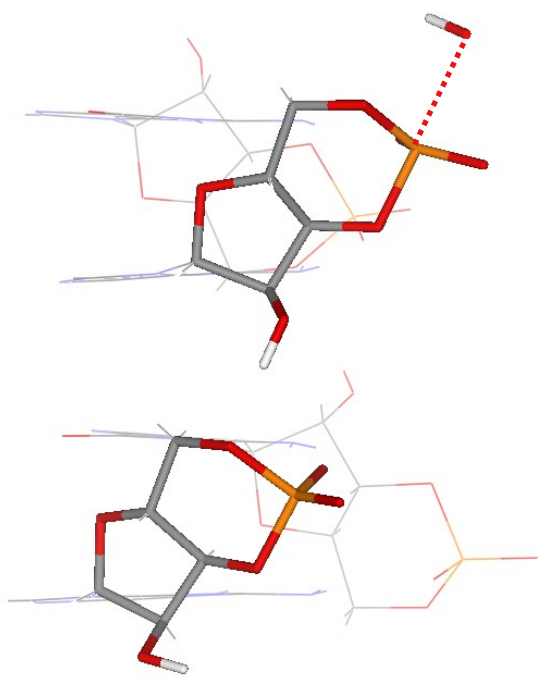
Mechanism of the polymerization of 3',5'-cGMPs from quantum chemical calculations



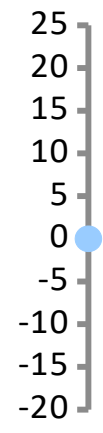
(TPSS-D2/TZVP level of theory)

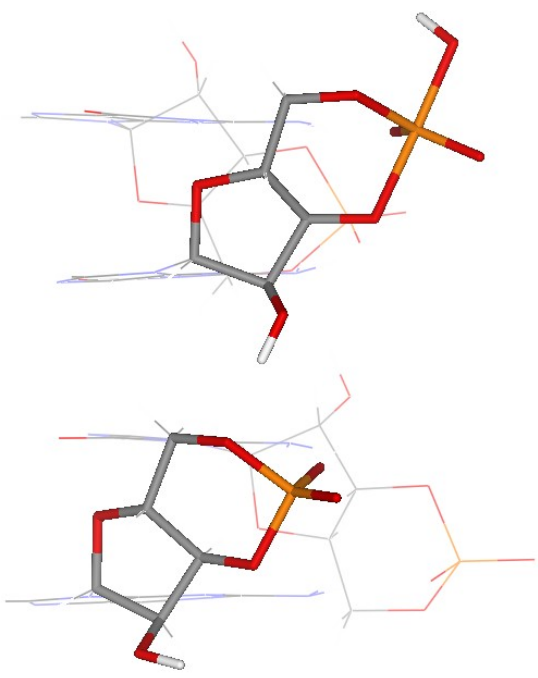




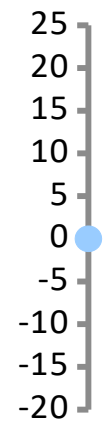


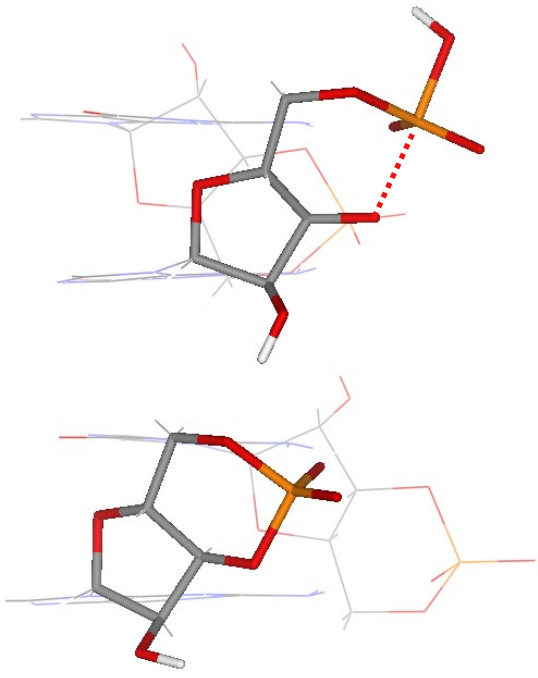
E,
kcal/mol



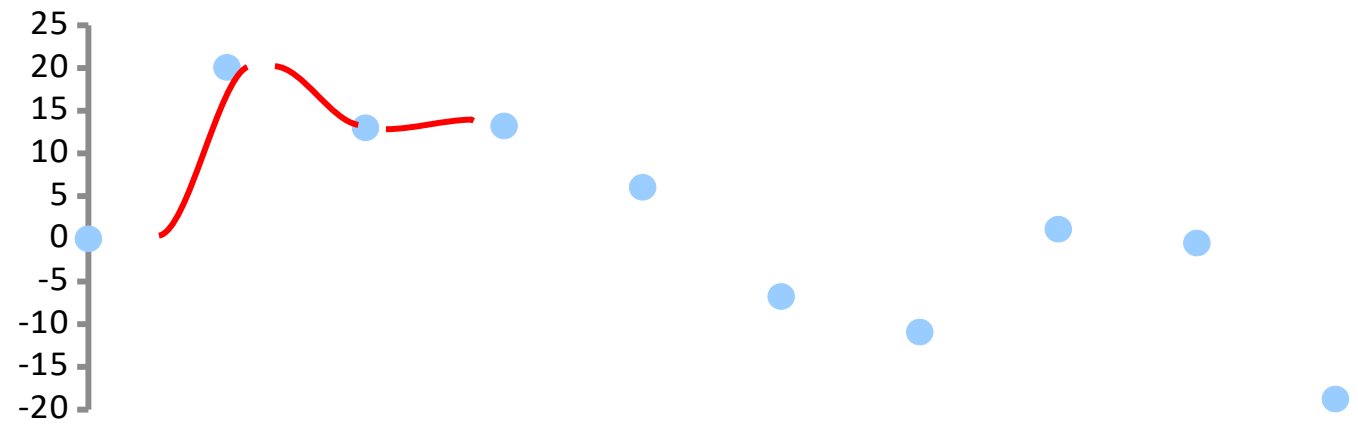
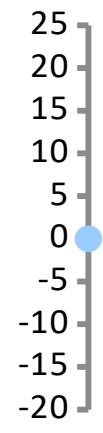


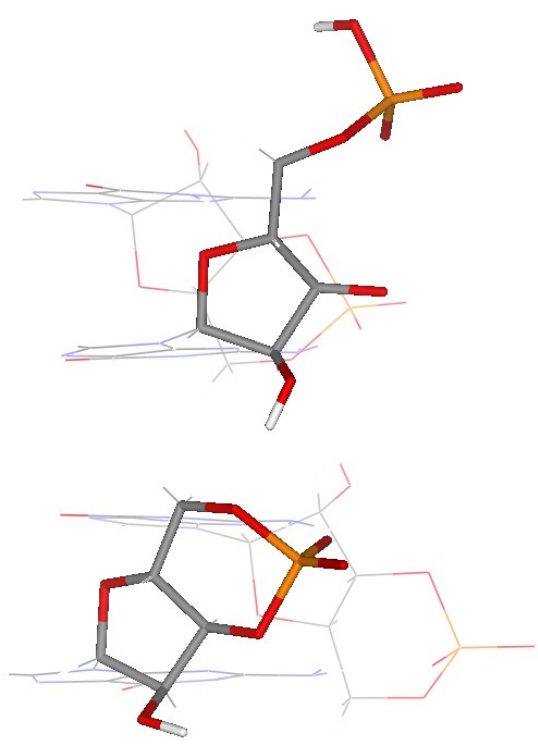
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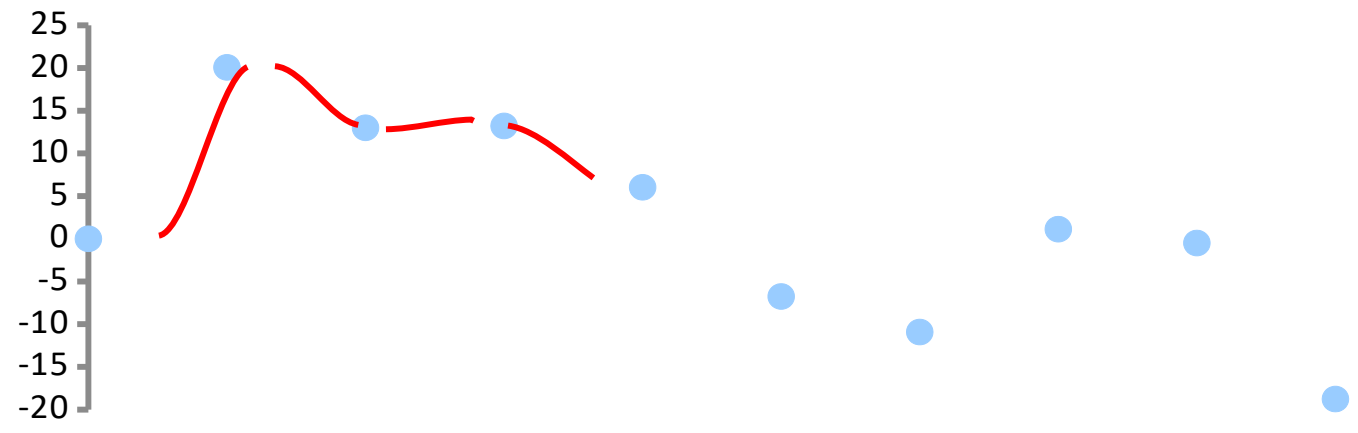
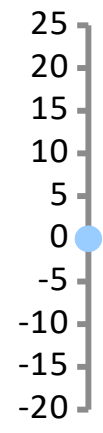


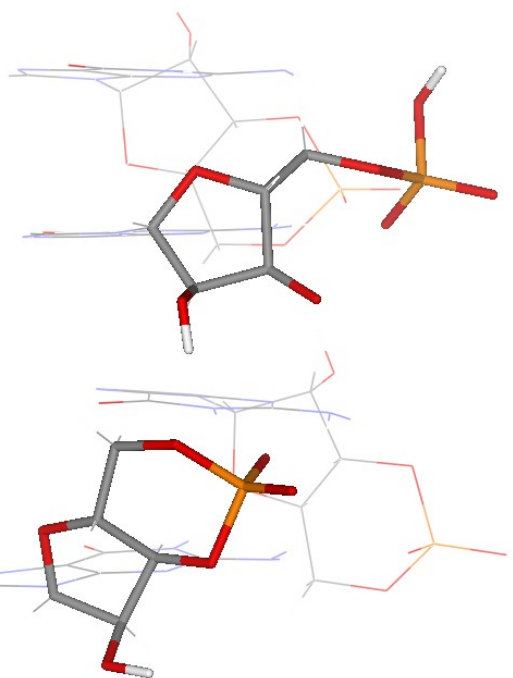
E,
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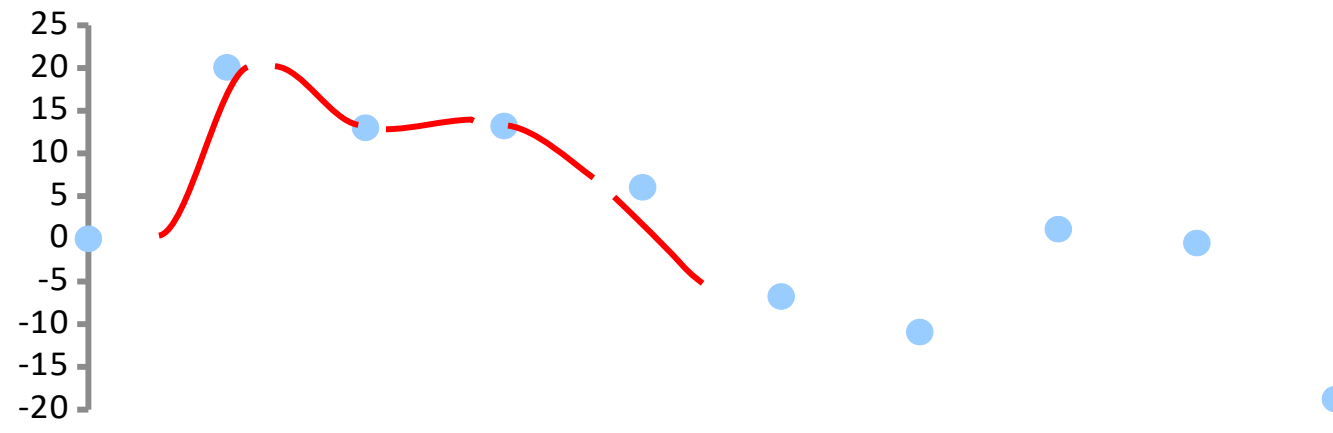
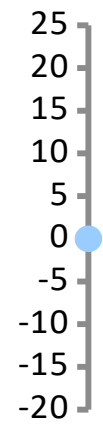


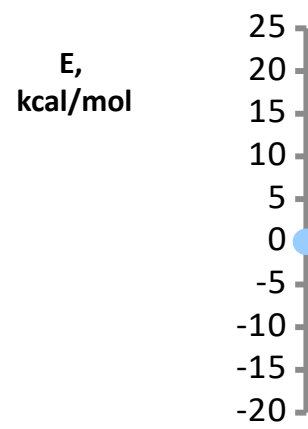
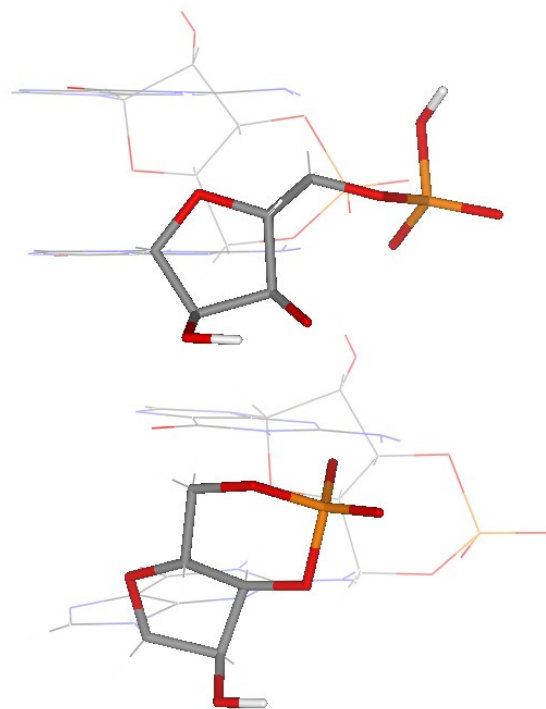
E,
kcal/mol

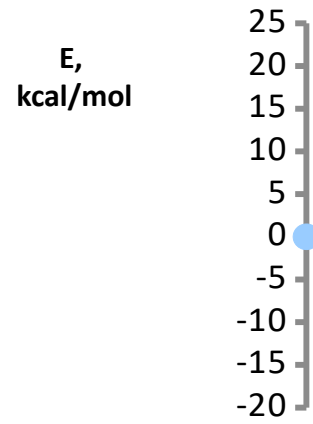
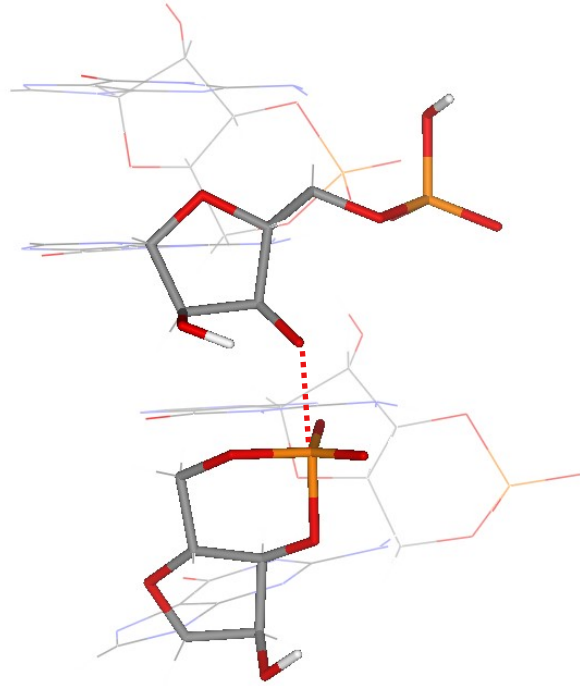




E,
kcal/mol

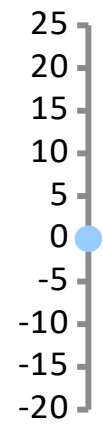


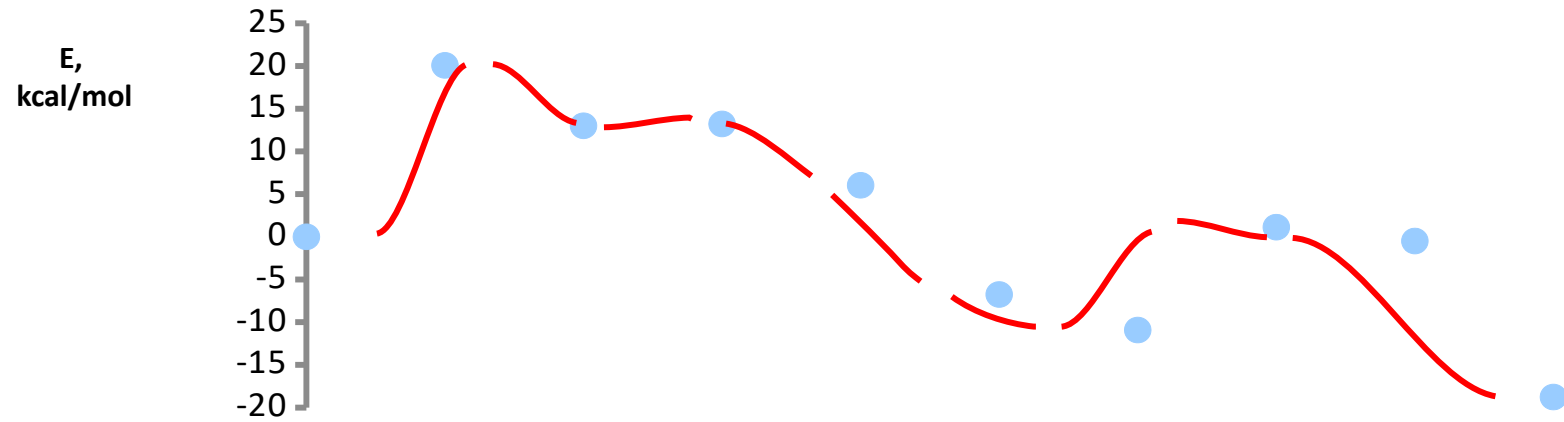




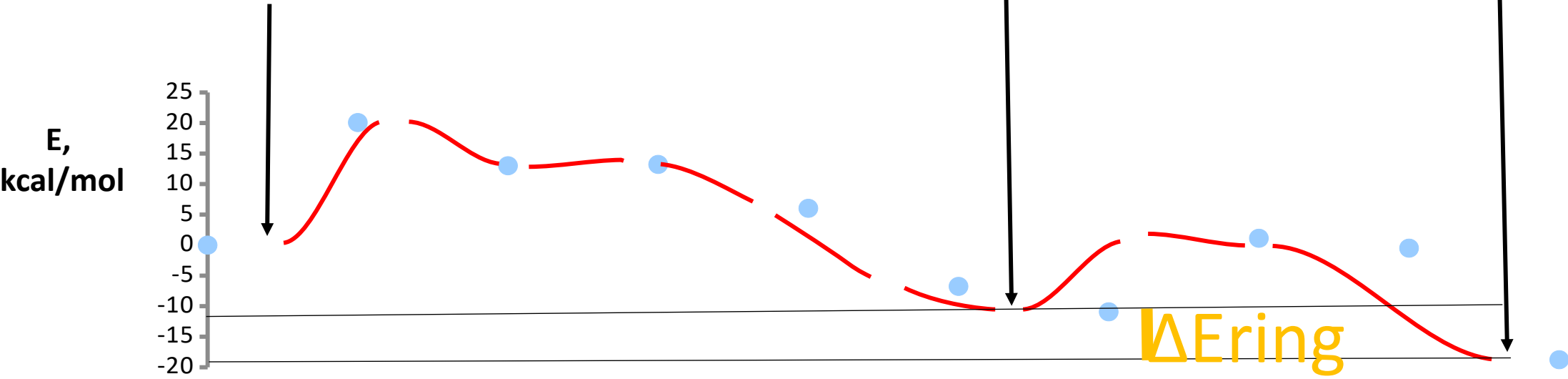
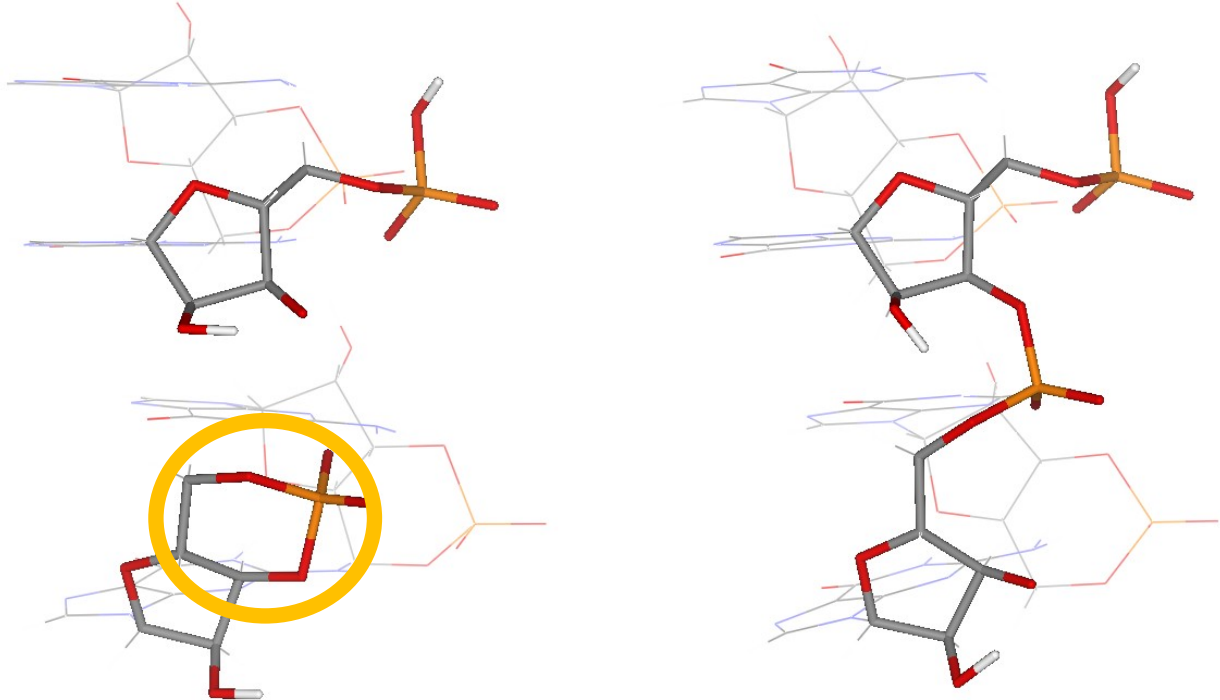


E,
kcal/mol

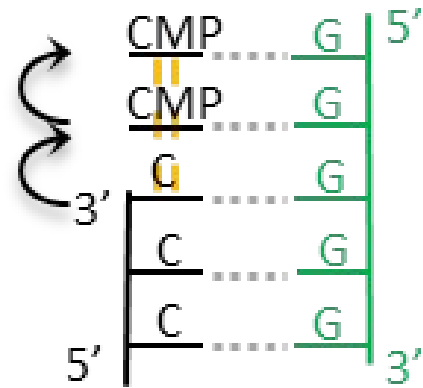




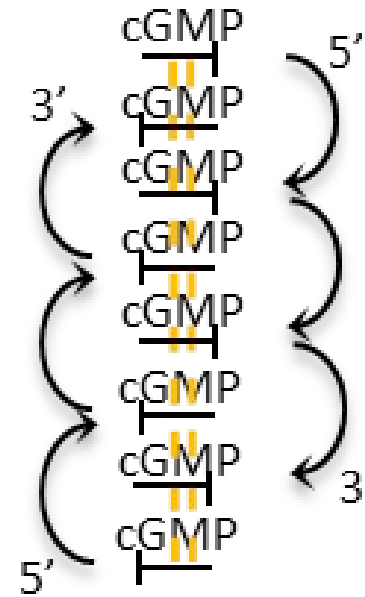
Nucleotide activation



Driving force of the polymerization

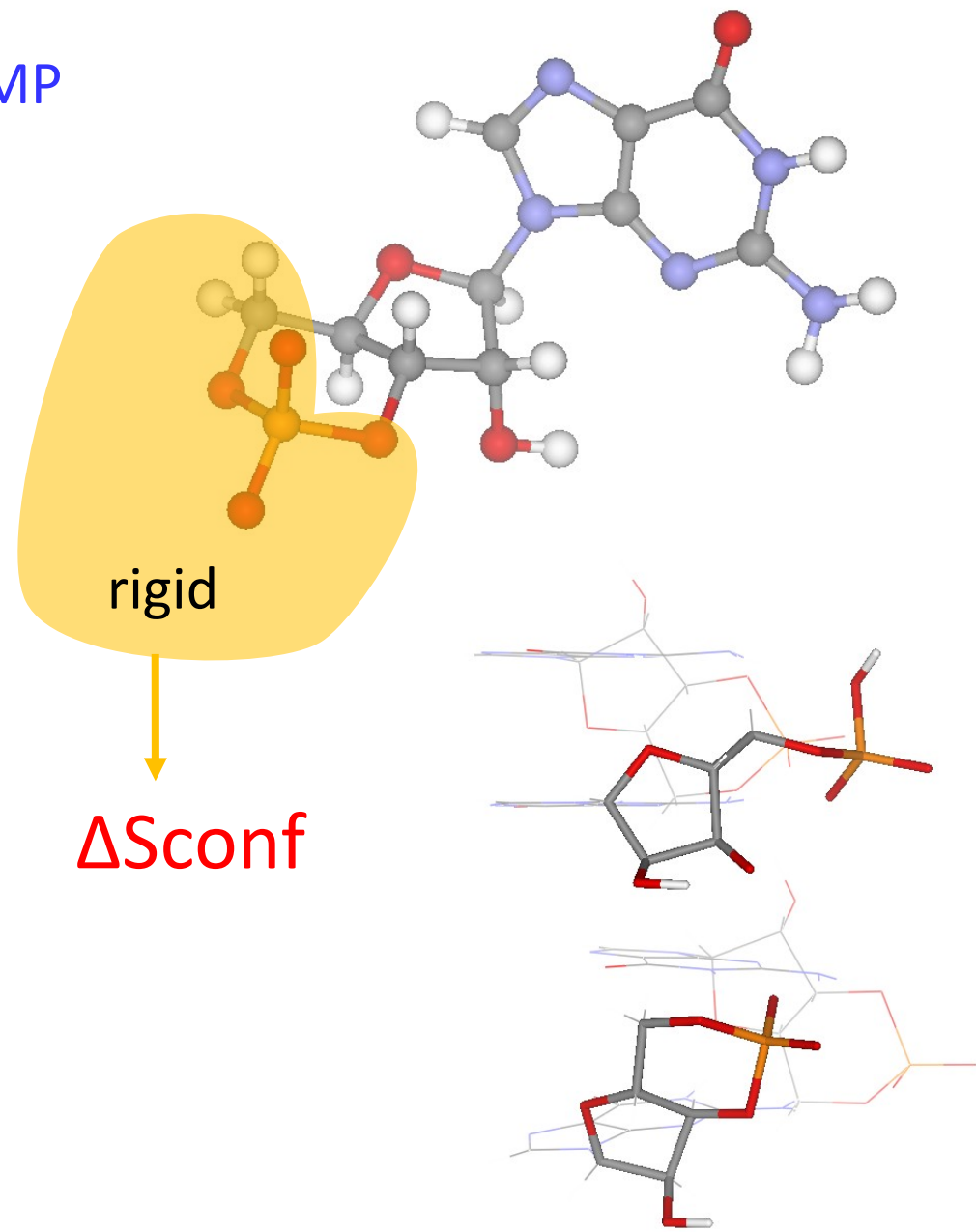
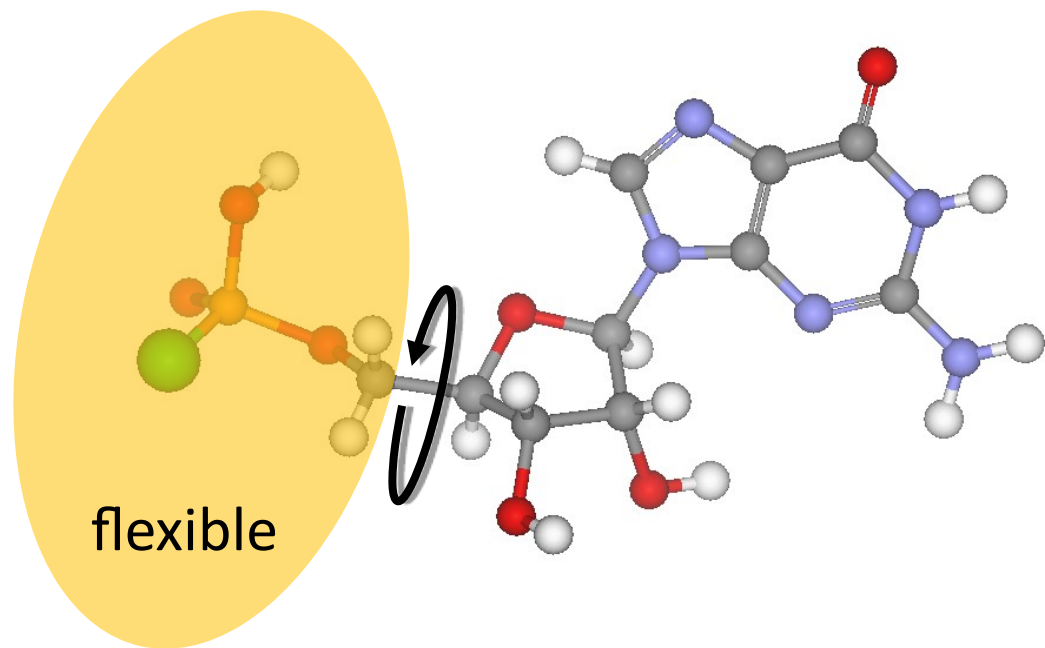


templated



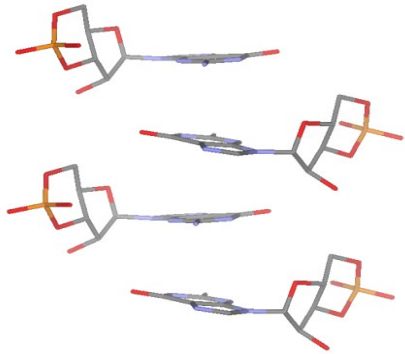
non-templated

GMP vs. cGMP

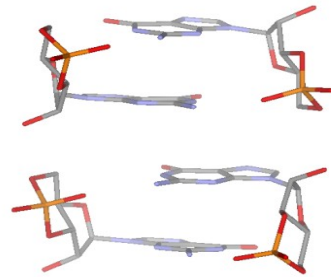


Relevance of the polymerization model

Crystal vs. computed



crystal

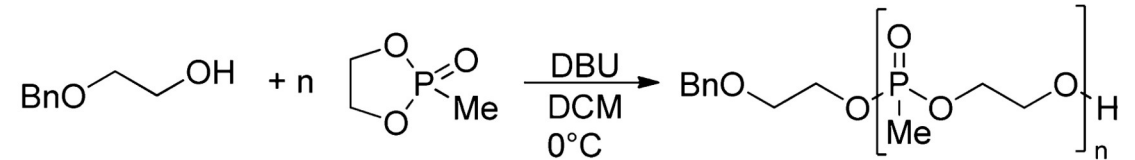


computed

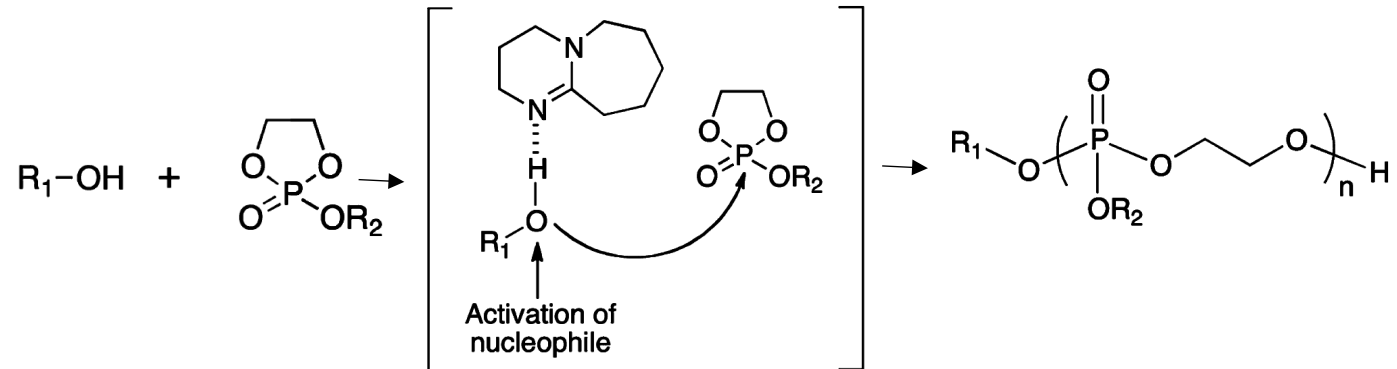
Chwang, A.K.; Sundaralingam, M.
Acta Cryst. B, **1974**, 30, 1233-1240.

Similar ring-opening polymerizations of cyclic phosphate esters

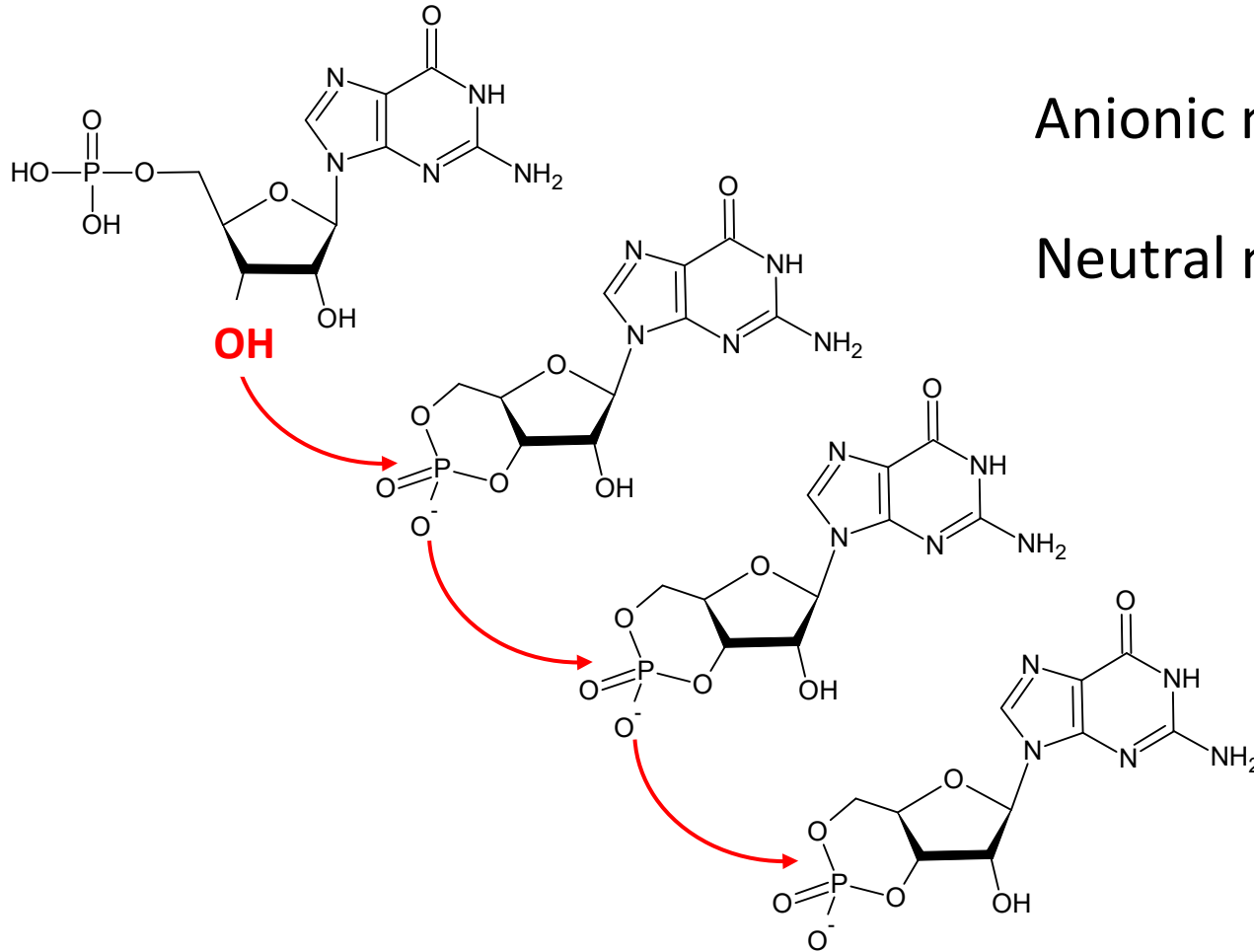
Clément, B. et al. *Macromolecules* **2012**, 45, 4476–4486.



Steinbach, T. et al. *ACS Macro Lett.* **2014**, 3, 244-248.



Sodium-effect



Anionic mechanism –activation energy: 12 kcal/mol

Neutral mechanism –activation energy: 34 kcal/mol

Acknowledgement

Prof. Ernesto Di Mauro, Rome, Italy

Dr. Samanta Pino, Rome, Italy

Dr. Alessandra Giorgi, Rome, Italy

Dr. Giovanna Costanzo, Rome, Italy

Dr. Martin Ferus, Prague, Czech Republic

Prof. Svatopluk Civiš, Prague, Czech Republic

Prof. Jiří Šponer, Brno, Czech Republic

Mr. Petr Stadlbauer, Brno, Czech Republic

GAČR grant No. P208/12/1878