SYNTHESIS AND STRUCTURE OF PURINOPHANES WITH FULLY OVERLAPPED CONFORMATION

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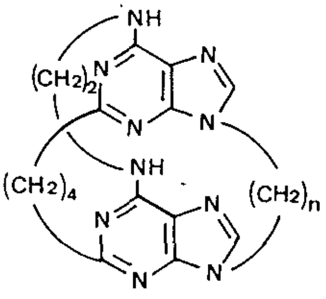
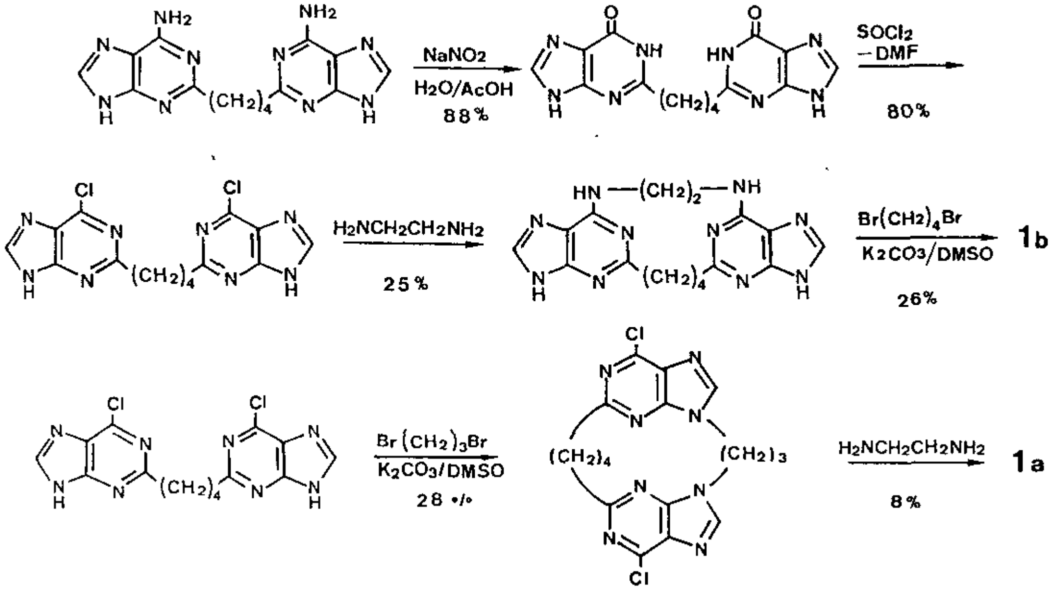


1 a:n=3
b:n=4

As a conformationally frozen model to study the stacking interaction of nucleic acid bases in DNA, we have prepared so far various purinophanes with two bridging chains. However, no purinophanes with fully overlapped conformation could be synthesized owing presumably to the dipole-dipole repulsion of the two heterocyclic rings. We now report on the first member of this series **1**, where two purine rings are forced to take eclipsed conformation by three bridging chains.

The synthesis of **1** was carried out as follows.



The upfield shifts of the aromatic protons in ^1H NMR as well as X-ray crystallographic study on **1b** have shown the fully overlapped structure of **1**. In marked contrast to the small hypochromicity of the reference compounds with one or two bridging chains, large hypochromicity was observed for **1a** (30%) and **1b**(28%) in two different solvents.