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C·T DNA base pairs as a possibility in direct 3D self-assembly. Quantum-mechanical approach.

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Molecular self-assembly is one of the keystones of nanoscience [1]. Different approaches and techniques are being developed constantly in order to achieve controlled 1D, 2D and even 3D self-assembly [2]. According to [3] there exists primarily two main approaches in this field: free self-assembly and templated self-assembly. While the latter approach offers a powerful technique it's always a wonder what if the same could be achieved through free self-assembly.

STM studies [4] of free self-assembly of nucleic base pairs on different interfaces show patterns for commonly used nucleic acids in synthetic DNA/RNA construction. Resulting structures are planar and have most energetically favorable geometries.

In our study [5] we show that model heteroassociates of m^1Cyt·m^1Thy are capable of forming up to 10 observable molecular complexes. First 3 of them has population ~90% in vacuum and are highly non-planar structures. The most energetically favorable structure has T-shape and next 2 has L-shape. Unfortunately we were unable to find any experimental data available in literature covering self-assembly of CT base pairs, so we encourage experimental scientists to provide such data. Nevertheless we believe that our theoretical discovery can lead to new potential techniques in free 3D self-assembly of synthetic DNA/RNA.

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