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Title:	The influence of sugar-phosphate backbone on the stacking interaction in B-DNA helix formation
Authors:	Mittal, Sumit (/jspui/browse?type=author&value=Mittal%2C+Sumit) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
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Abstract:	The influence of sugar-phosphate backbone on the stacking interaction in the adenine...thymine base-pair dimer (A...T) ₂ has been studied using the density functional theoretic method and the dispersion-corrected density functional BLYP-D3 and the triple-zeta quality basis set def2-TZVP. In the absence of the sugar-phosphate backbone, several stacked conform-ers were obtained with a small difference in their stabilization energy values (-20 to -25 kcal/mol). However, the presence of the sugar-phosphate back-bone limits the movement of the two A...T units, and yet the stacking interaction remains significant (-19.4 kcal/mol). Despite the constraints imposed by the backbone, the dimer (A...T) ₂ is found to retain its favourable geometry. The influence of sodium ions on the geometry and the interaction energy is found to be negligible.
Description:	Only IISERM authors are available in the record.
URI:	https://www.semanticscholar.org/paper/The-Influence-of-Sugar-Phosphate-Backbone-on-the-in-Mittal-Mishra/c220f39d9359db03c1eec621c49519541210b4ee (https://www.semanticscholar.org/paper/The-Influence-of-Sugar-Phosphate-Backbone-on-the-in-Mittal-Mishra/c220f39d9359db03c1eec621c49519541210b4ee) http://hdl.handle.net/123456789/3099 (http://hdl.handle.net/123456789/3099)
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