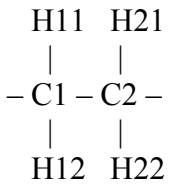
Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Force-field parameter modifications, based on the GAFF force field[1], for an ethyl cross-link between mispair-aligned thymine residues:



Atom number	Atom type	Charge
C1, C2	CT	0.1710
H11, H12, H21, H22	HC	0.0855

Added bond terms:
CT-NA: K=418.0 kcal/mol/Å^2, r_0=1.388 Å
Added angle terms:
C-NA-CT: K=70.0 kcal/mol/rad^2, θ_0=125.20°
NA-CT-CT: K=70.0 kcal/mol/rad^2, θ_0=120.00°
NA-CT-HC: K=50.0 kcal/mol/rad^2, θ_0=109.50°
Added dihedral terms:
-CT-NA-: K=1.35 kcal/mol, n=2, δ=180.0

(1) Wang, J. M.; Wolf, R. M.; Caldwell, J. W.; Kollman, P. A.; Case, D. A. *Journal of Computational Chemistry* **2004**, *25*, 1157-1174.