Effects of morphology and solvent / temperature on THz spectra: take nucleosides as example

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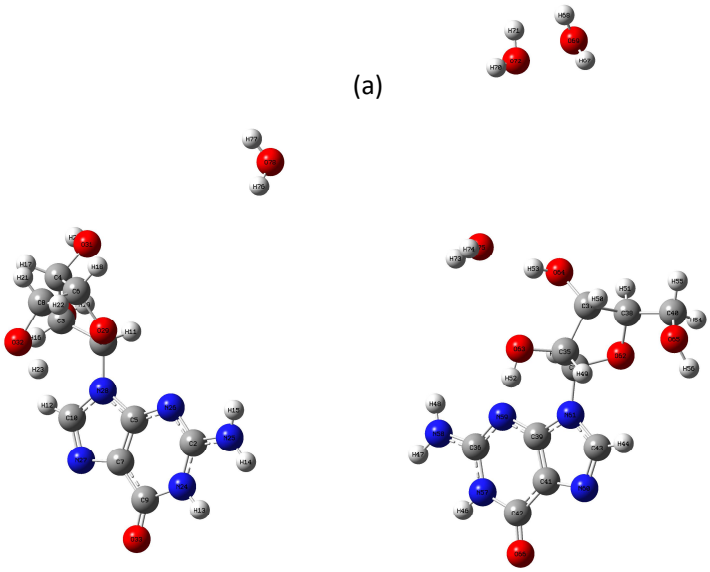
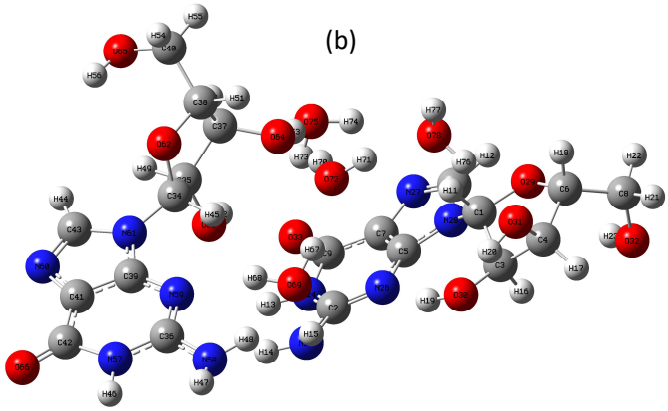
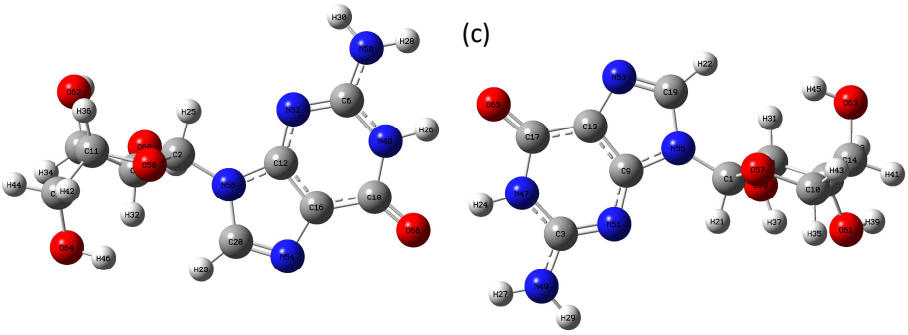
(a)



(b)



(c)



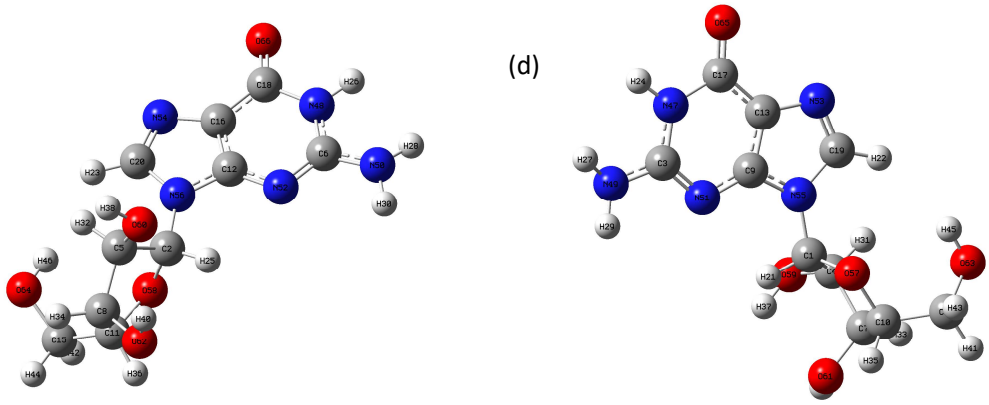
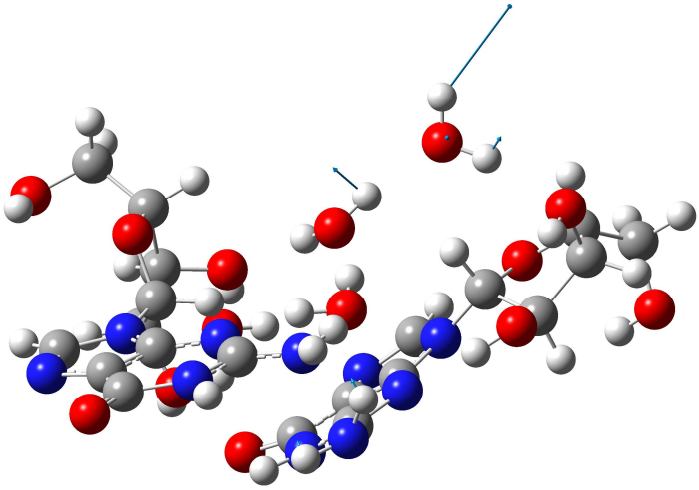
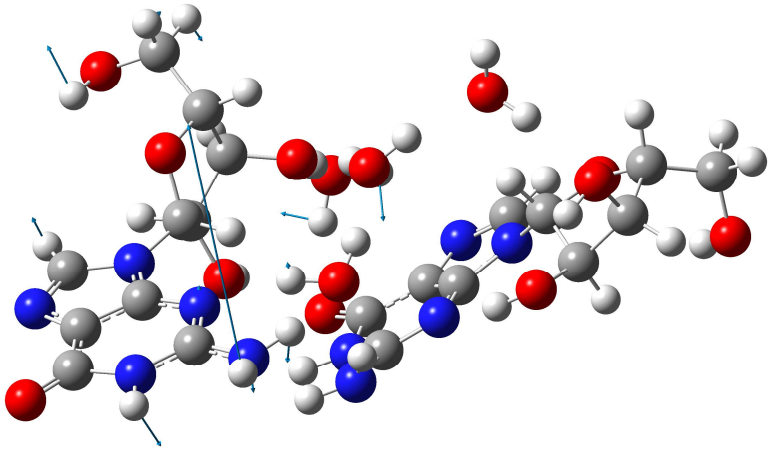


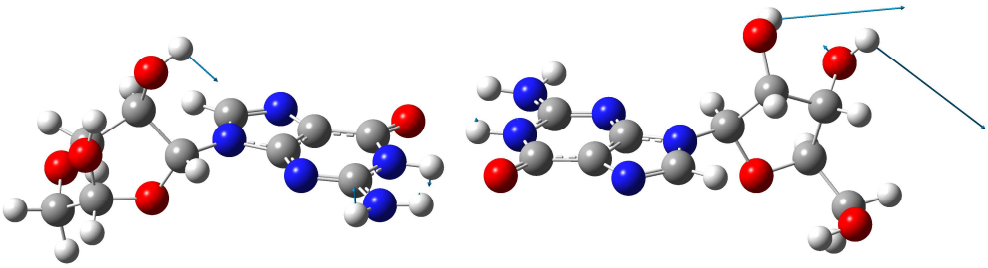
Figure S1. The structure of (a) Guanosine-dimer-2H2O before optimization, (b) and the structure of Guanosine-dimer-2H2O, (c) Guanosine-dimer, (d) Guanosine-dimer-water after optimization.



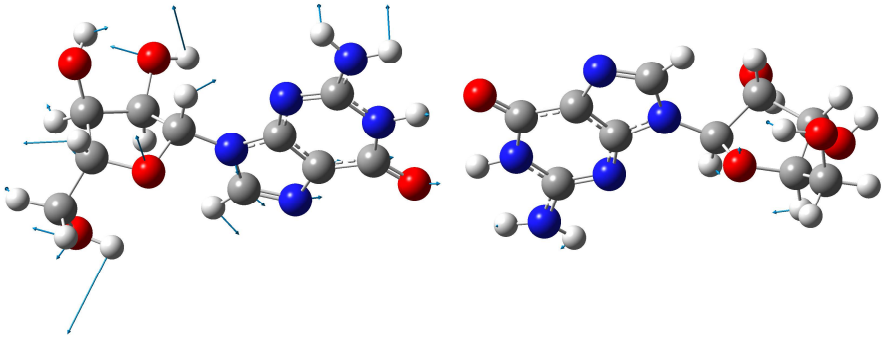
5.7 THz (Guanosine-dimer-2H2O)



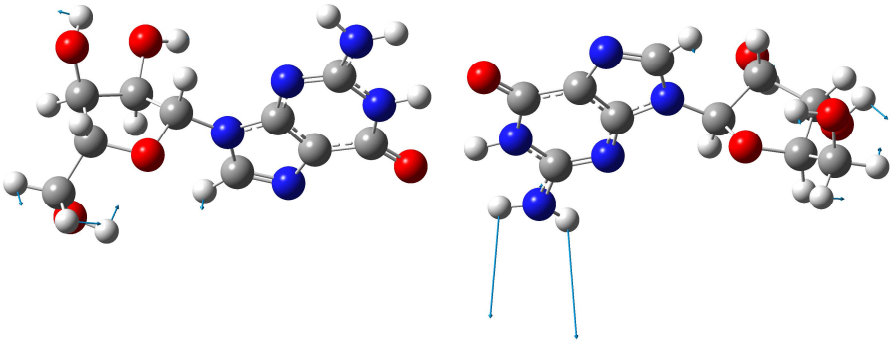
9.7 THz (Guanosine-dimer-2H2O)



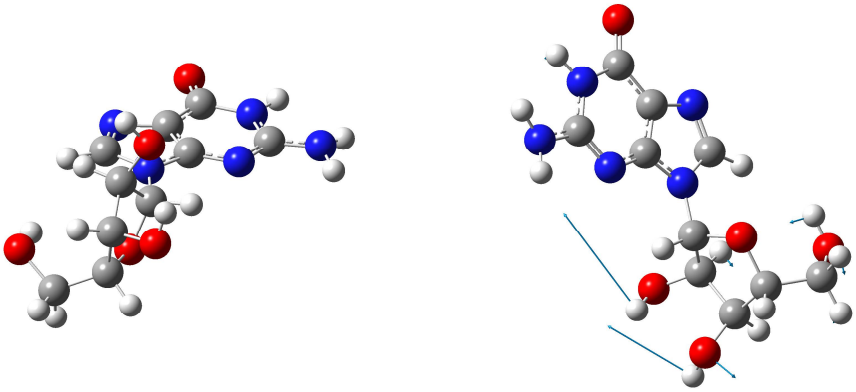
5.5 THz (Guanosine-dimer)



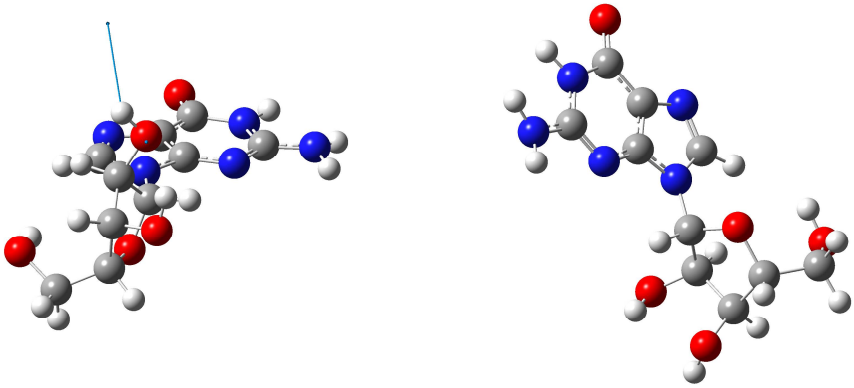
7.1 THz (Guanosine-dimer)



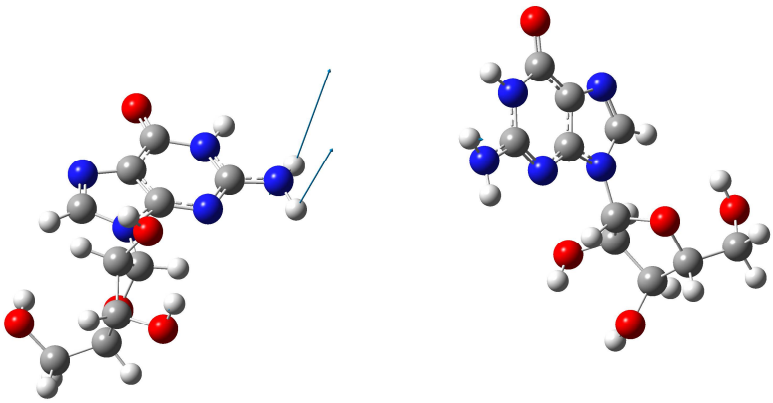
8.7 THz (Guanosine-dimer)



6.2 THz (Guanosine-dimer-water)



7.2 THz (Guanosine-dimer-water)



9.5 THz (Guanosine-dimer-water)

Figure S2. The vibrational modes corresponding to the main characteristic peaks of Guanosine-dimer-2H2O, Guanosine-dimer and Guanosine-dimer-water.