Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Material

Spectroscopic evidence for a gas-phase librating G-quartet/Na^+ complex

C. Fraschetti*[a], M. Montagna[a], L. Guarcini[a], L. Guidoni[b], A. Filippi[a]

Figure S1. Calculated structures for the Na^+-**G_2** dimer. In brackets the relative enthalpies in kcal mol^{-1} are reported.

Table S1. Description of calculated frequency of 2 b-d structures.

Figure S2. Calculated structures, energies (in kcal mol^{-1}), and spectra of Watson-Crick type Na^+-**G_4** quartet. The ΔG values are compared with the S_4 global minimum (B3LYP/6-31G(d,p).

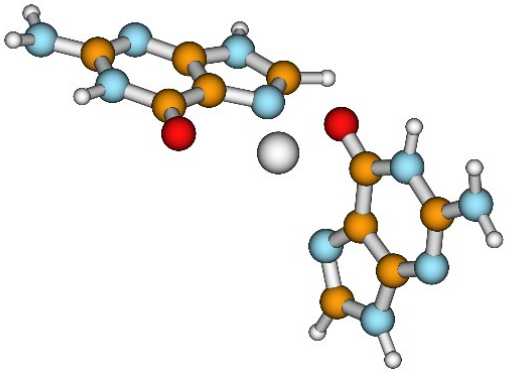
Figure S3. Calculated structures for the Hoogsteen-type Na^+-**G_4** adduct. In the brackets the relative free energies in kcal mol^{-1} are reported ((B3LYP/6-311G(d,p)).

Figure S4. Free energy of Na^+-**G_4** adduct along ϕ dihedral angle during the 17 ps AIMD simulation.

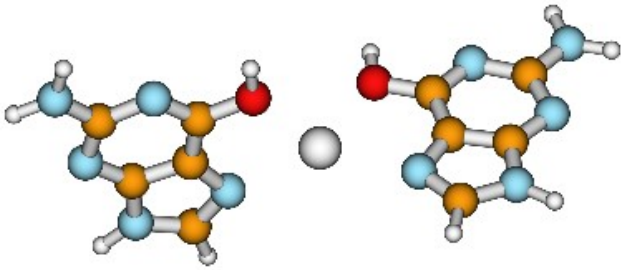
Figure S5. a) Spectrum extracted from the AIMD simulation. b) Calculated spectra of S_4 and c) C_{4h} structures. (B3LYP/6-311G(d,p))

Figure S6. Contributions of the different stretching modes to the calculated IR spectrum.

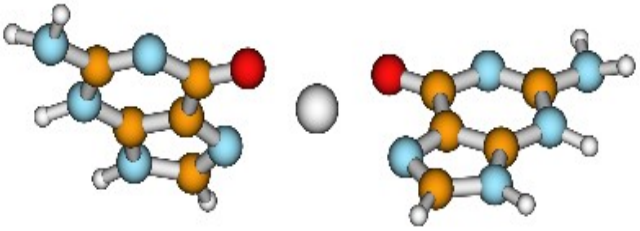
Figure S1



2b (0.0)



2c (19.0)

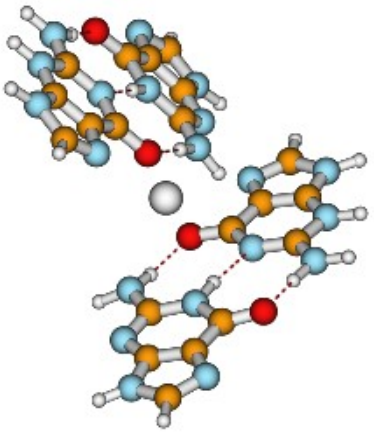


2d (30.3)

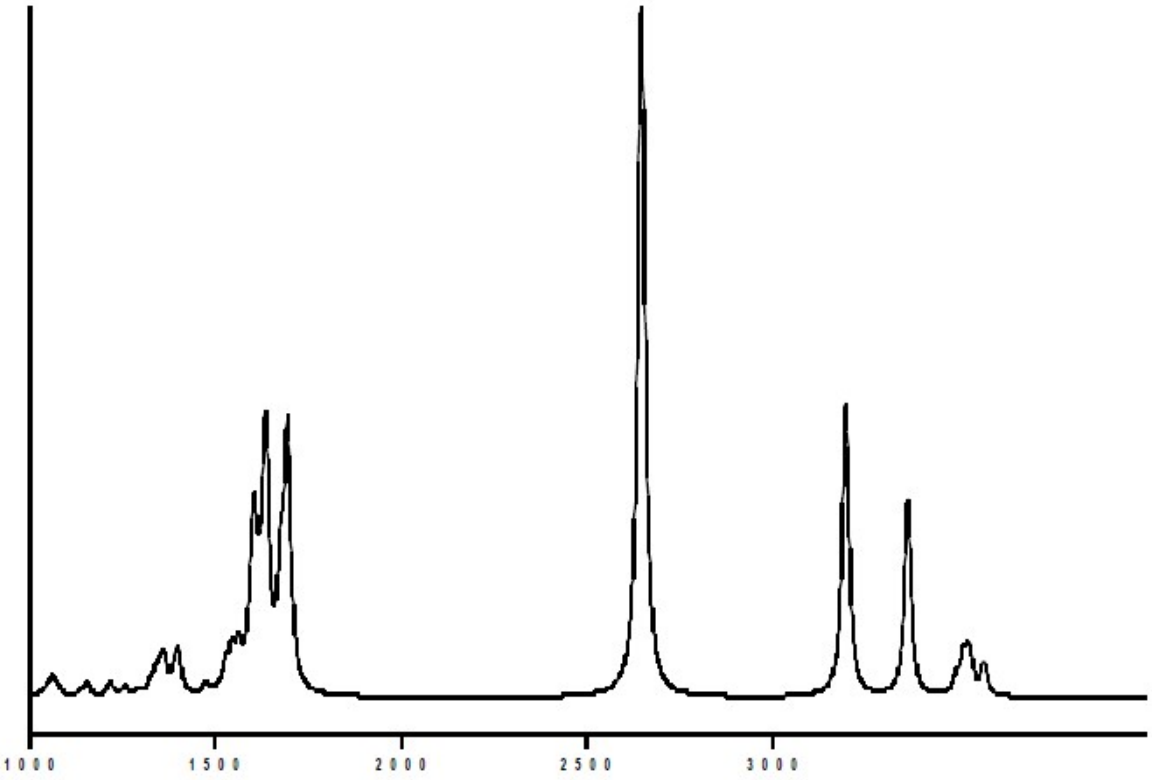
Table S1

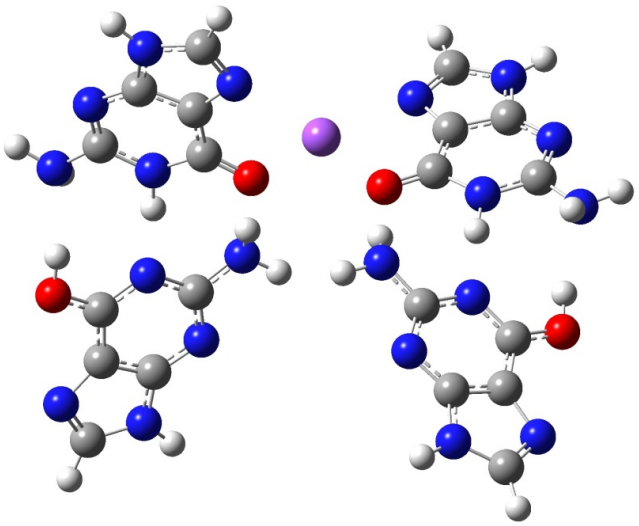
Stretching modes	**2b**	**2c**	**2d**
N1-H	3413		
Symmetric $N2H_2$	3436	3453	3413
N3-H			3444
N9-H	3468	3471	3470
O6-H		3568	
Asymmetric $N2H_2$	3555	3586	3529

Figure S2

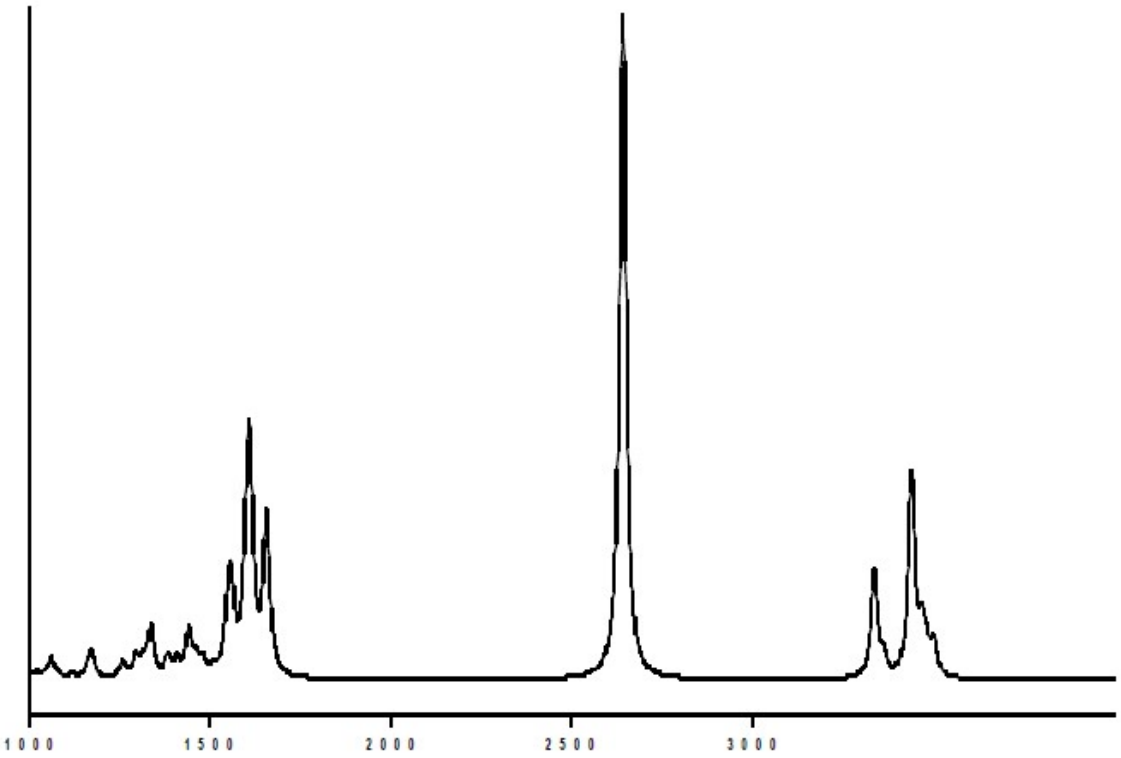


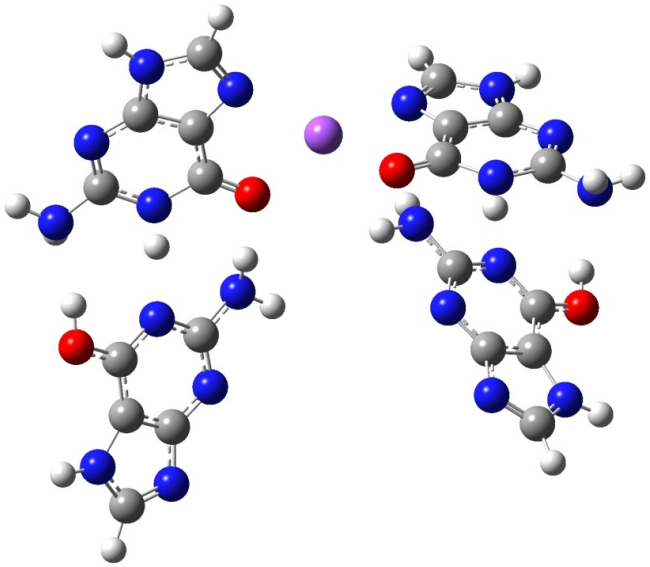
ΔG = 59.4



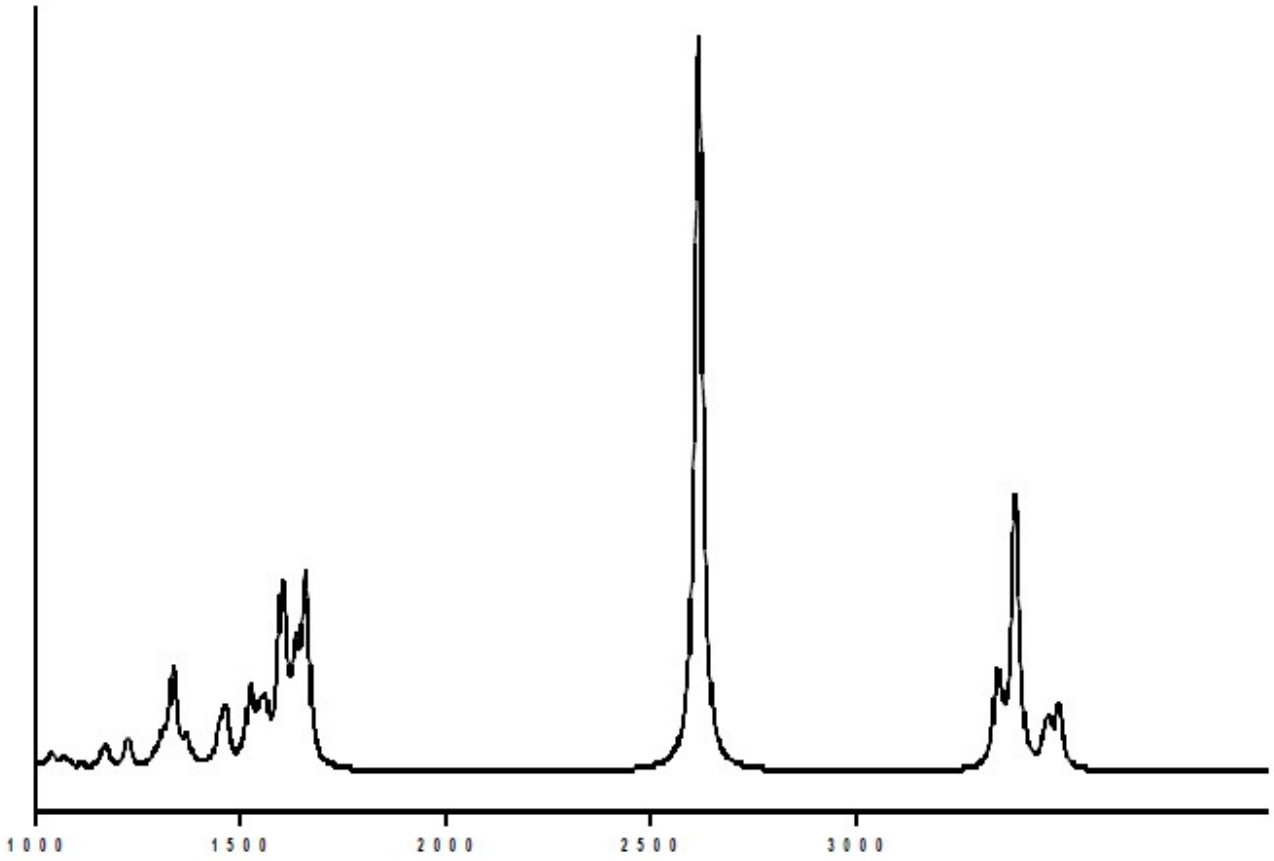


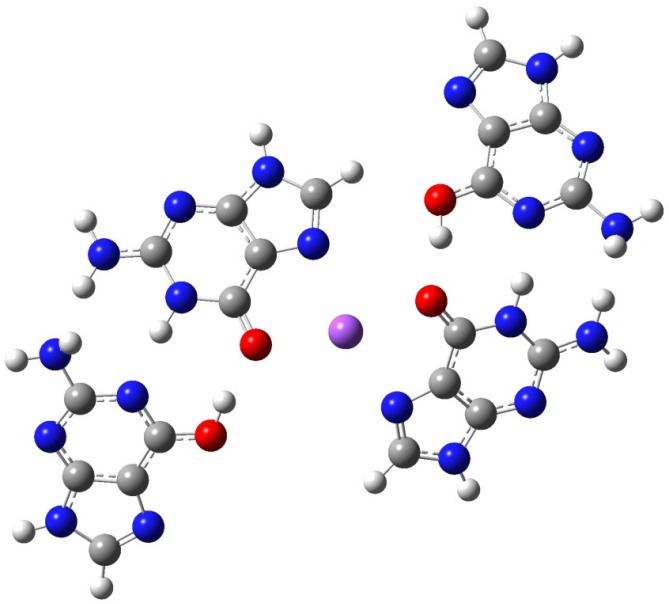
ΔG = 53.8



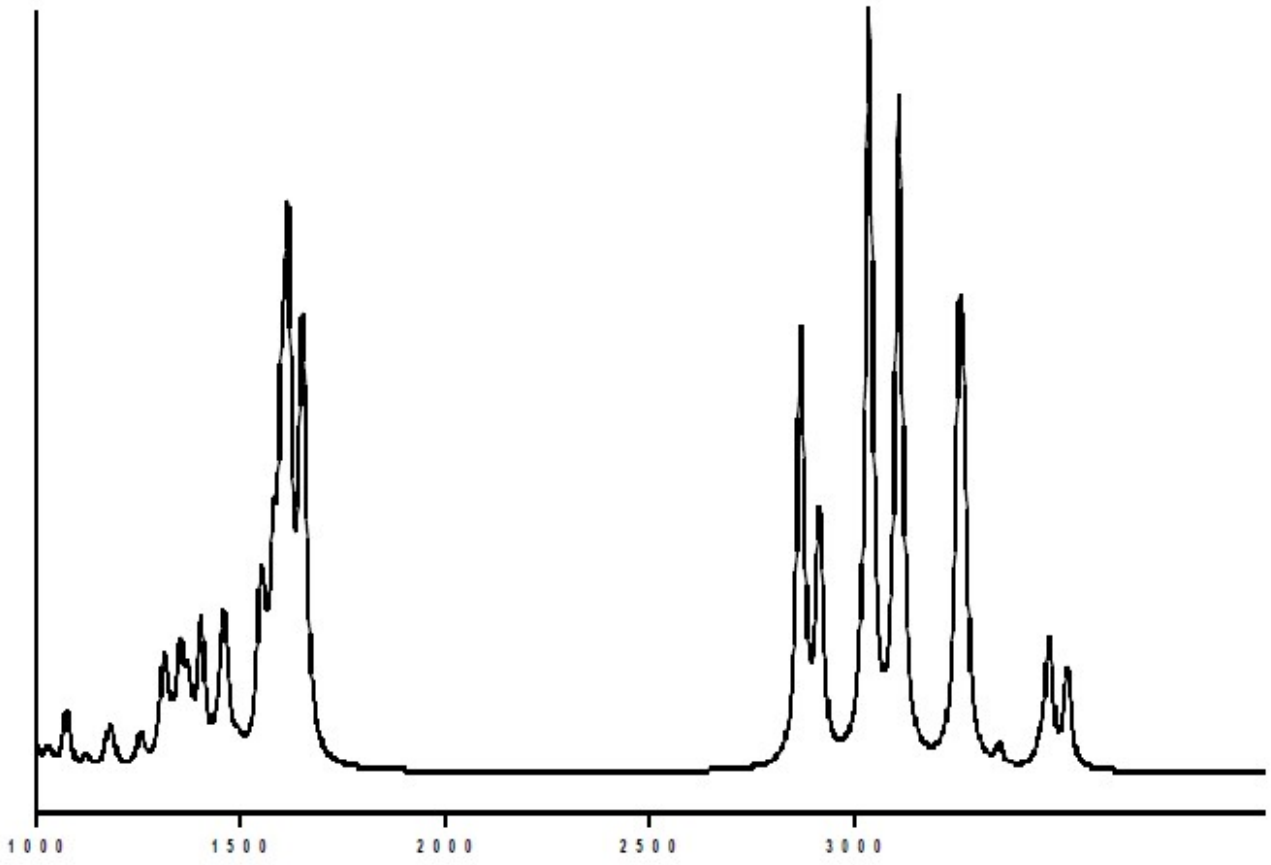


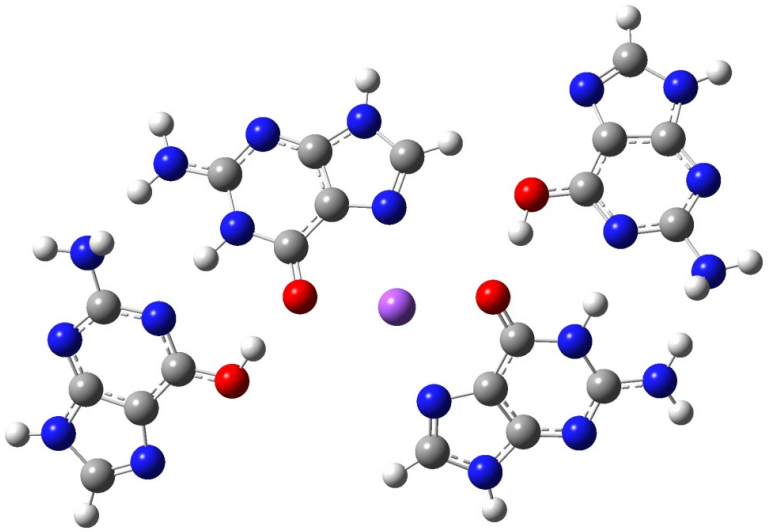
ΔG = 60.2



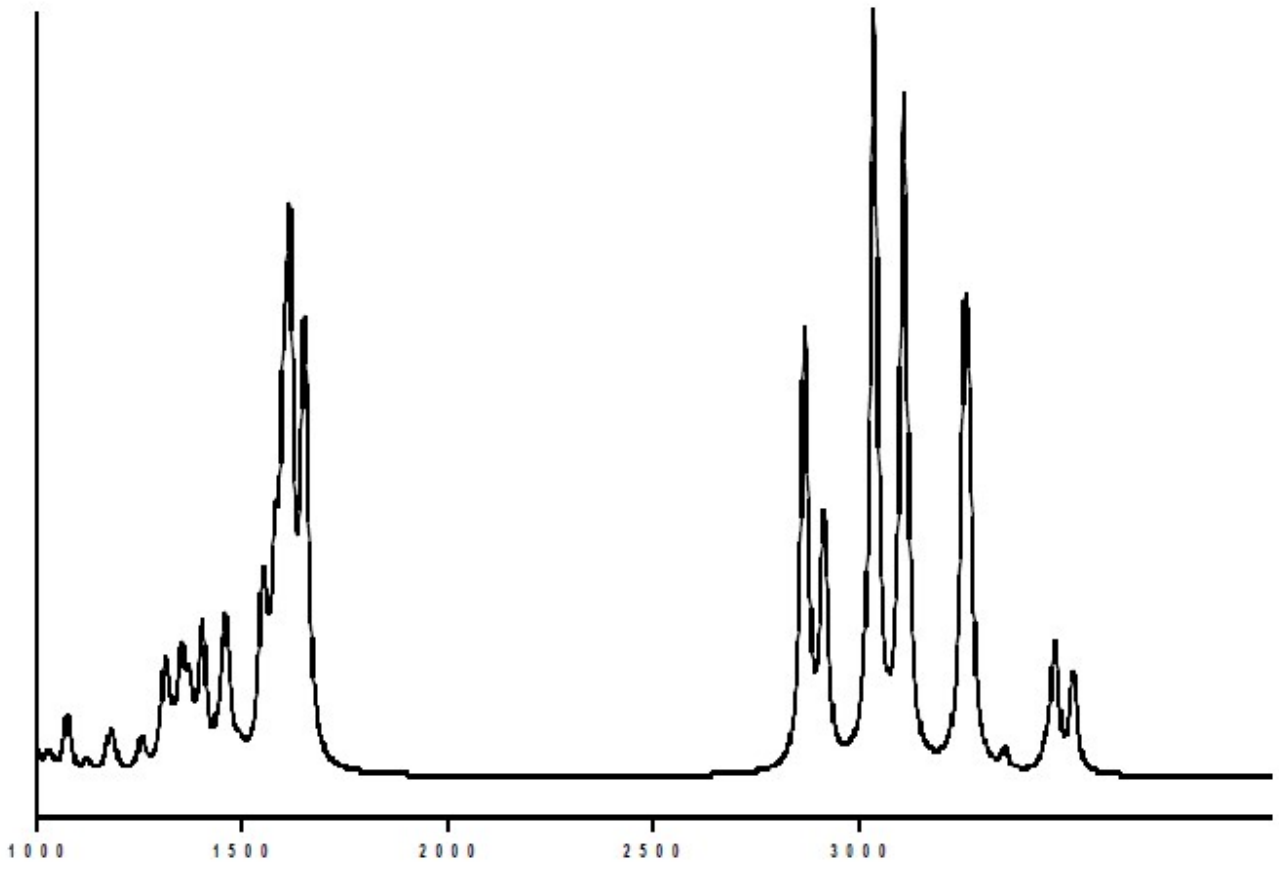


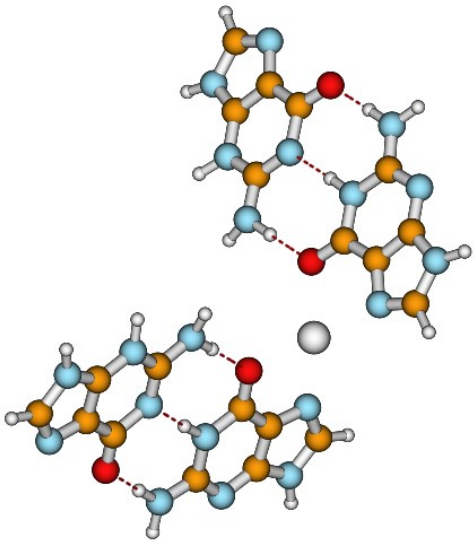
ΔG = 39.8



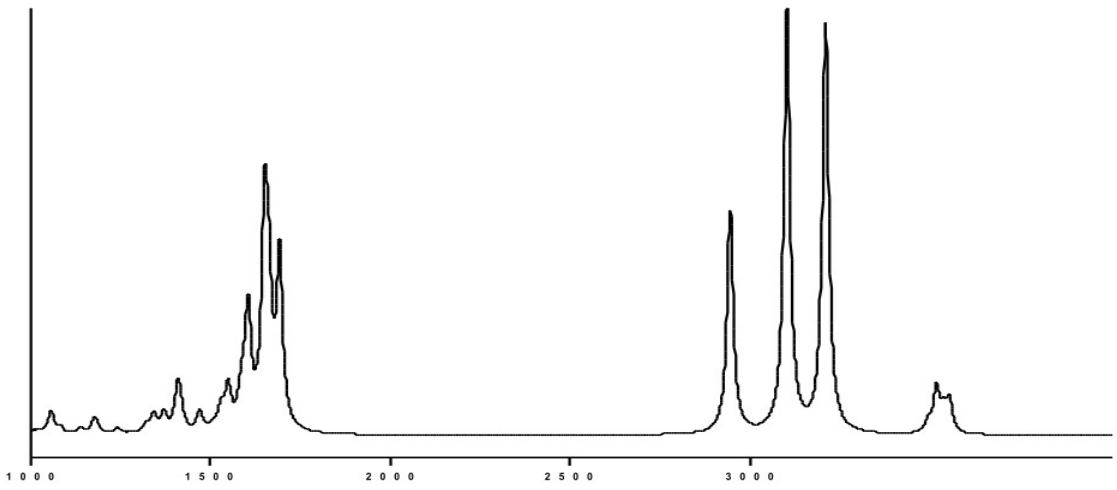


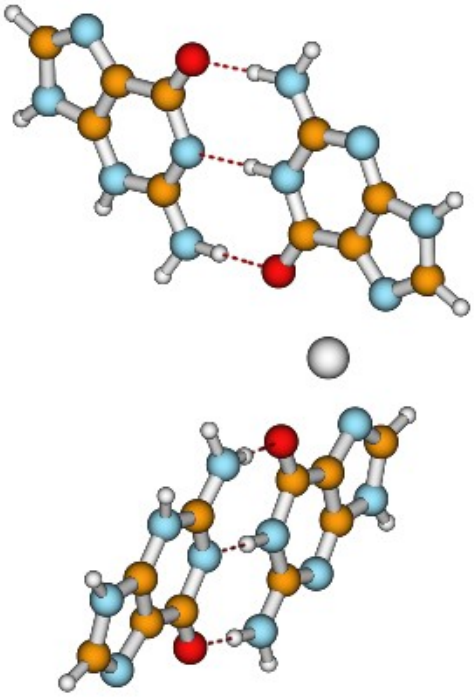
ΔG = 39.8



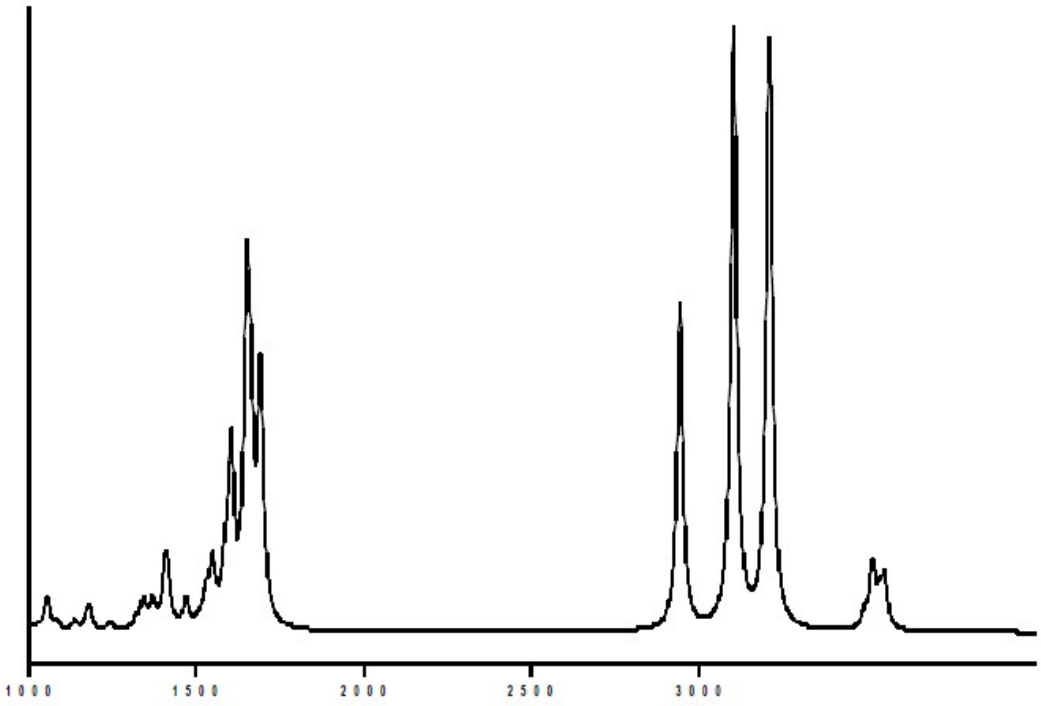


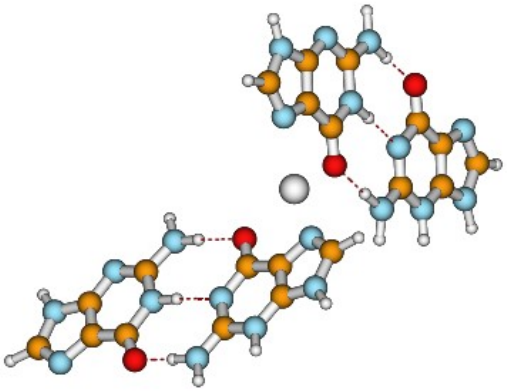
ΔG = 51.6



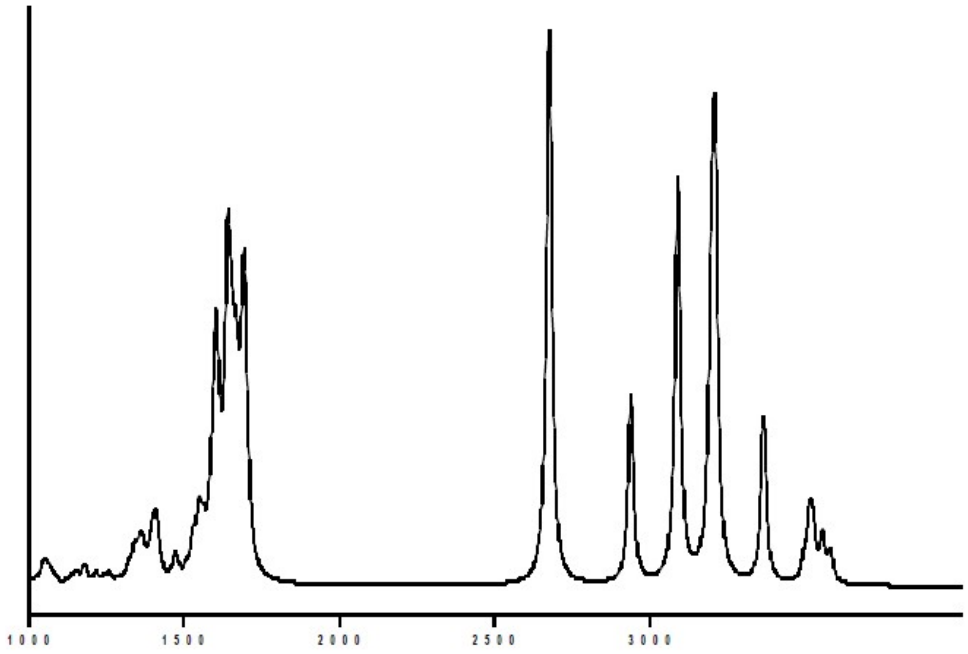


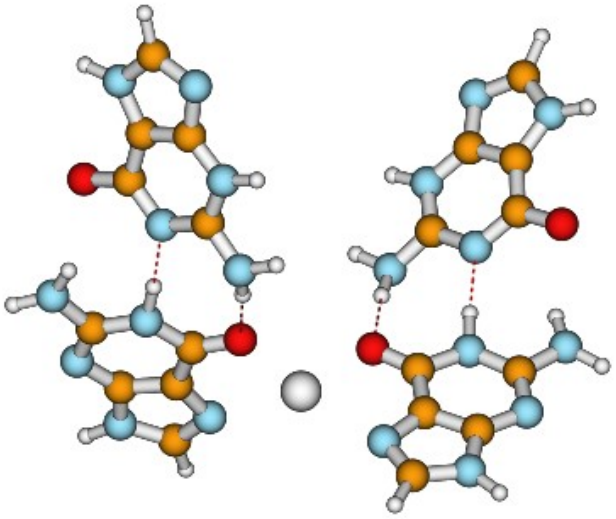
ΔG = 51.8



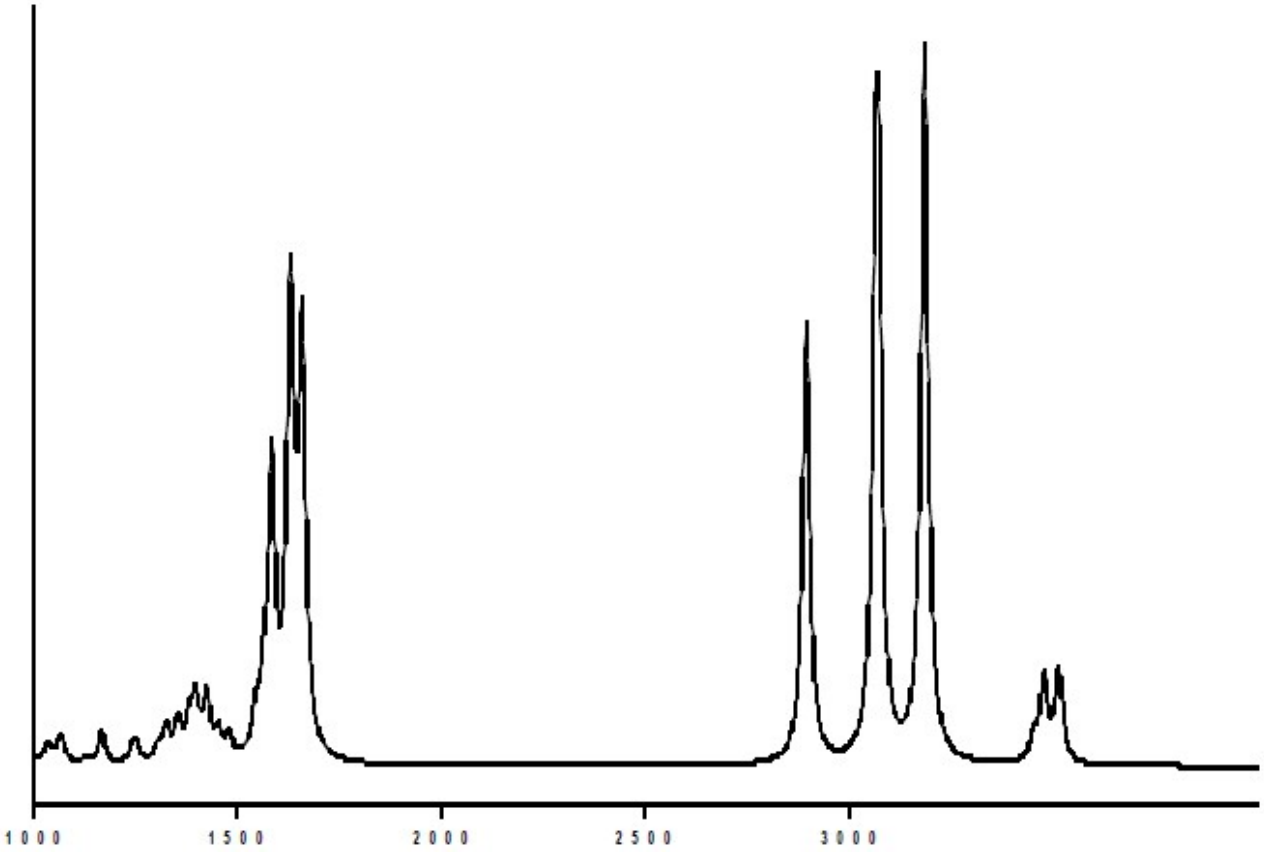


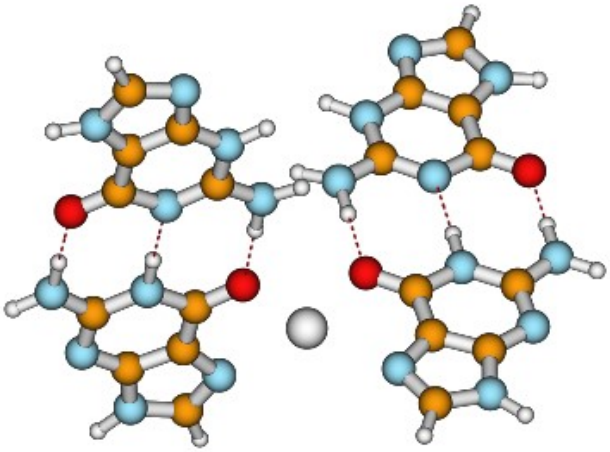
ΔG = 56.1



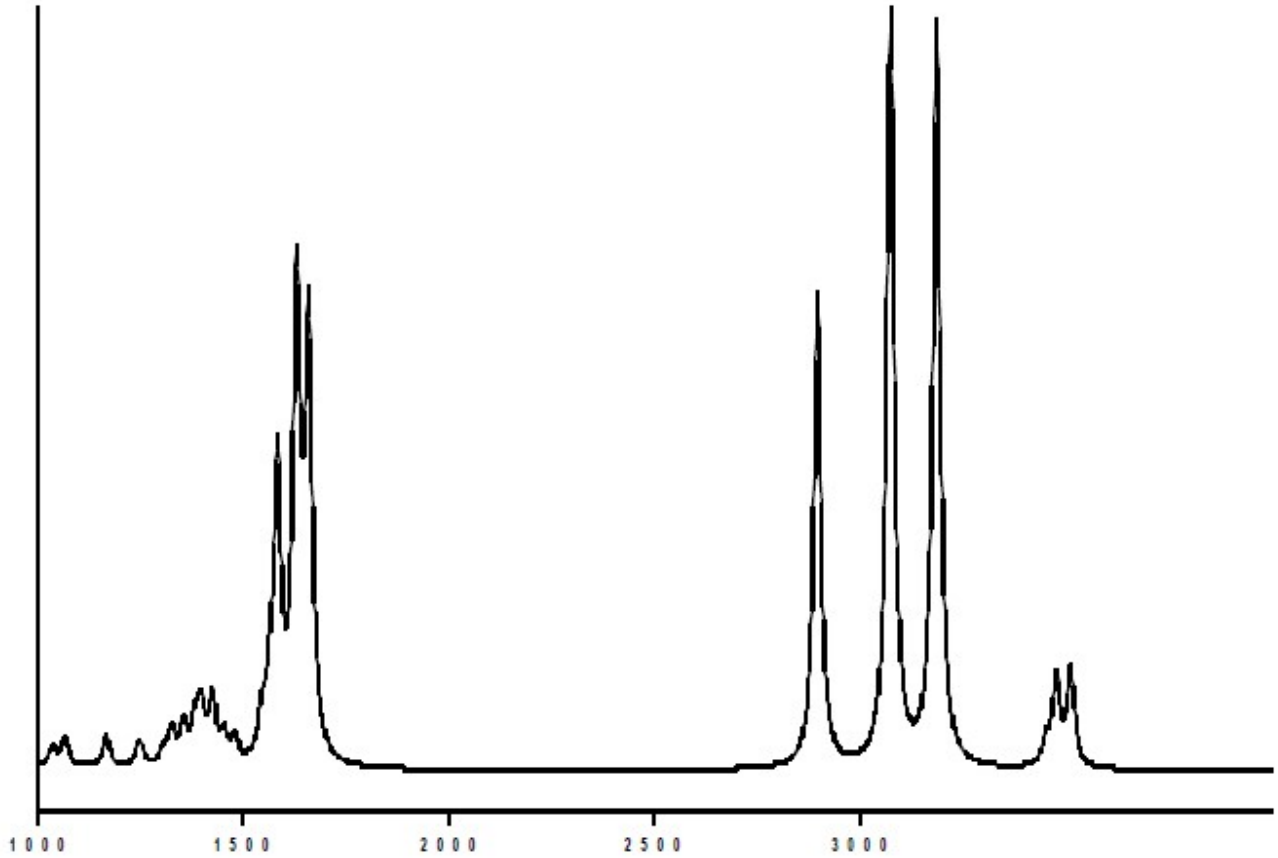


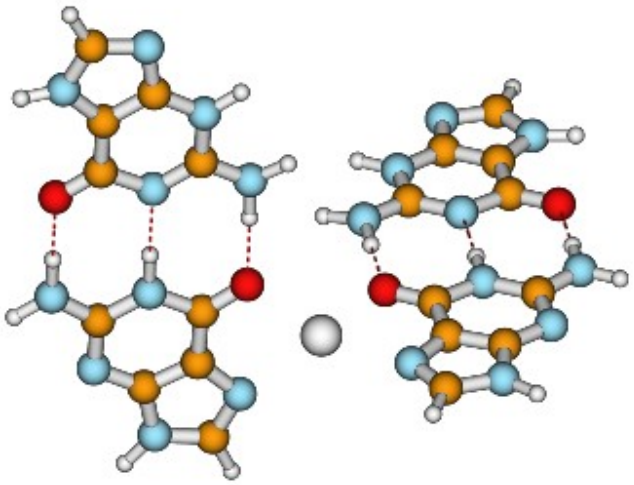
ΔG = 28.0



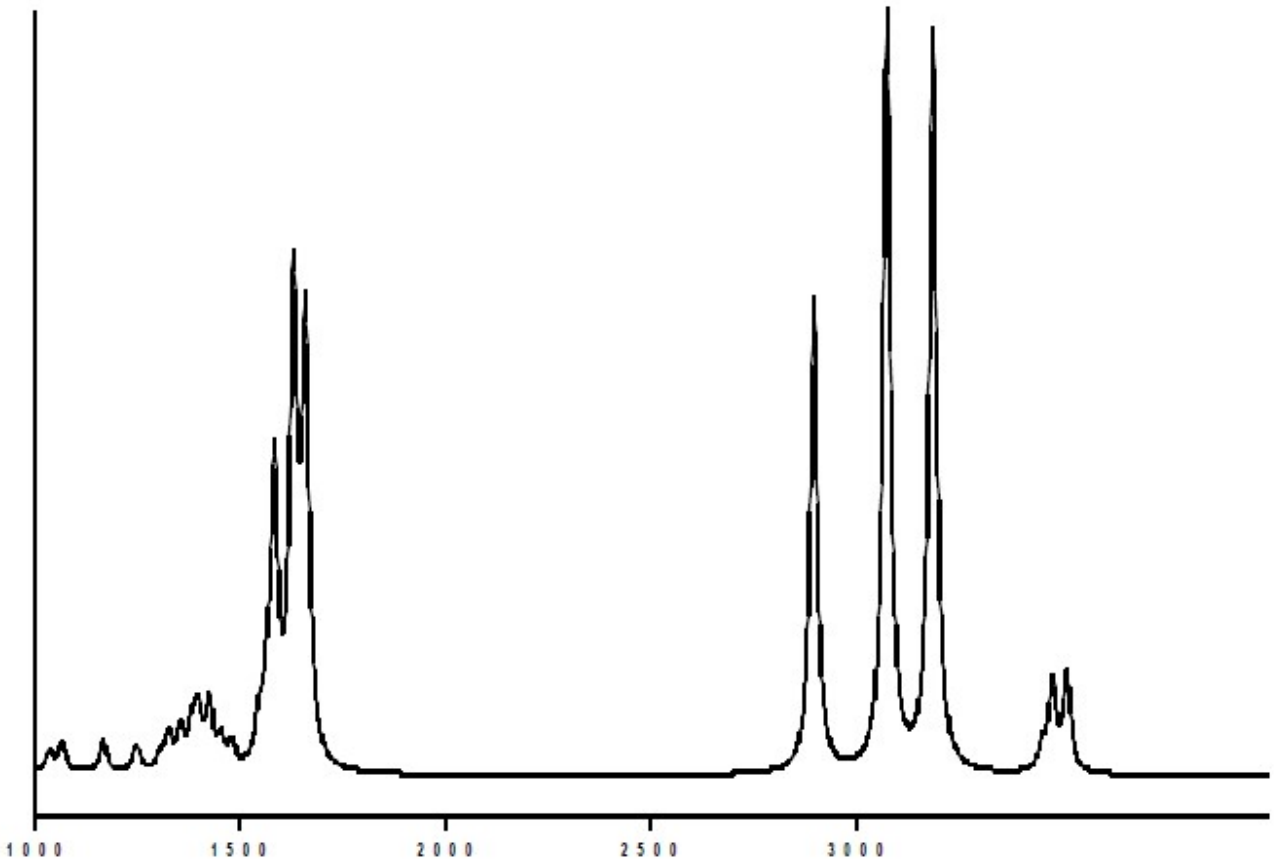


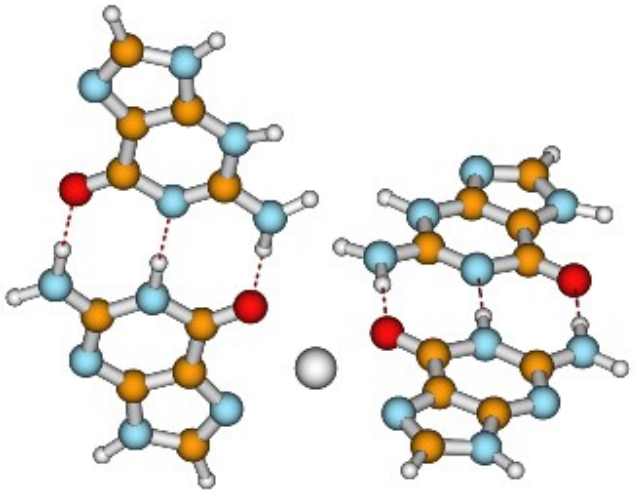
ΔG = 28.4



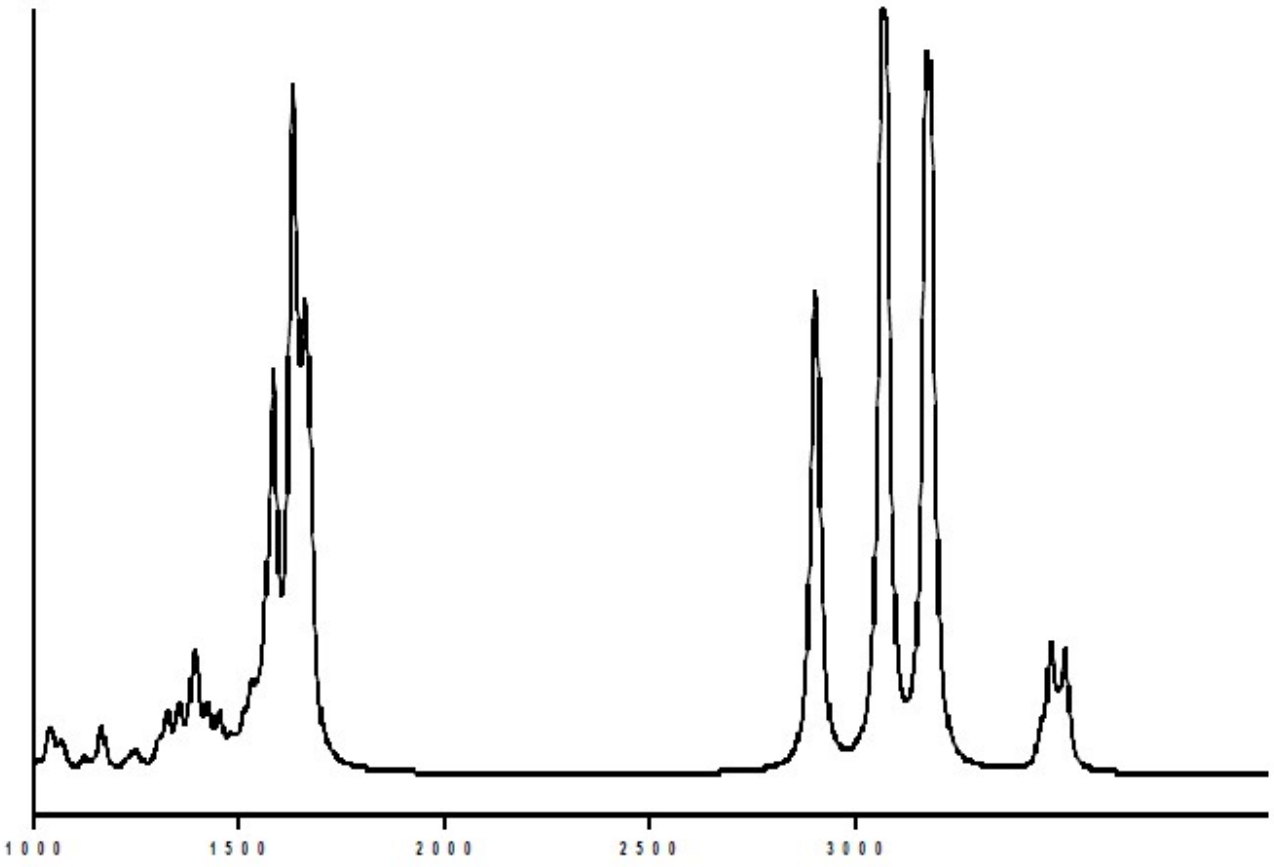


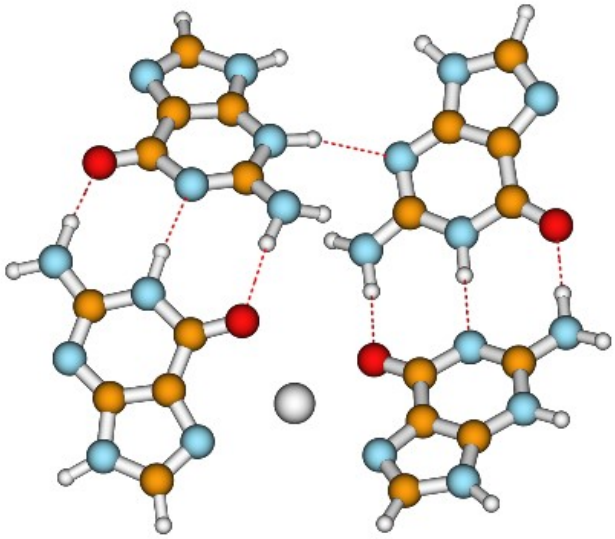
ΔG = 28.3



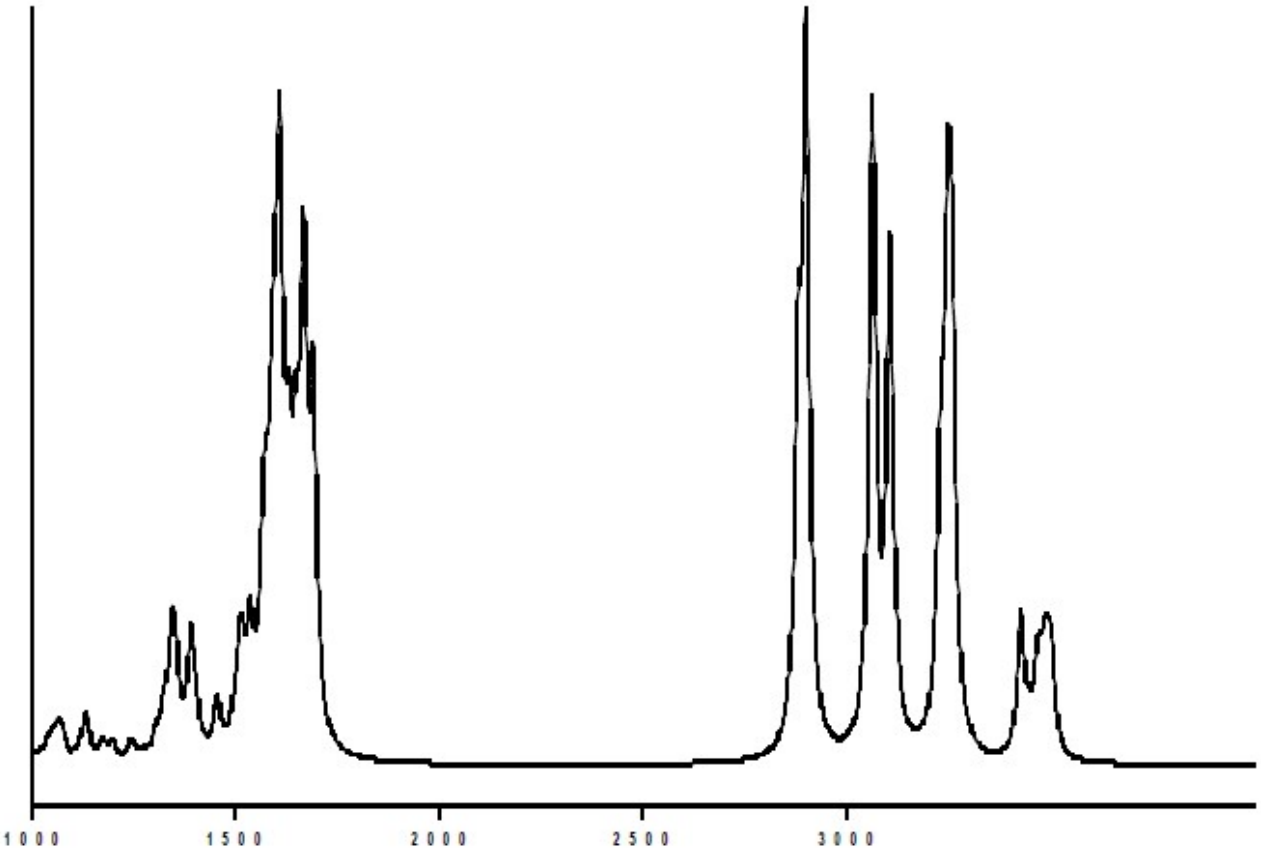


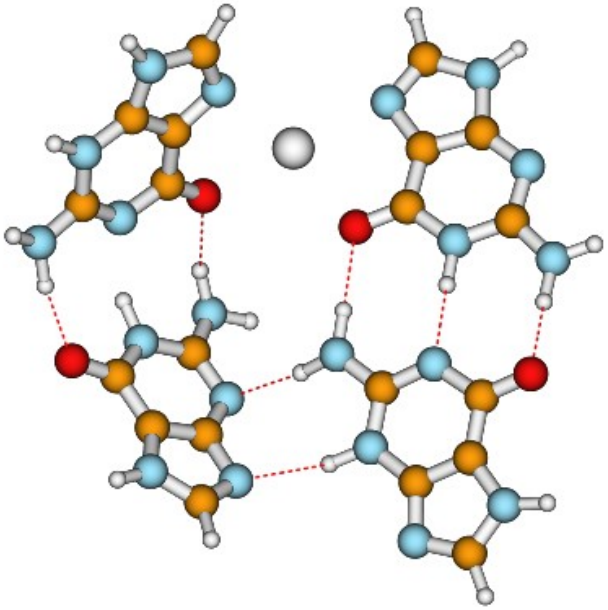
ΔG = 40.1



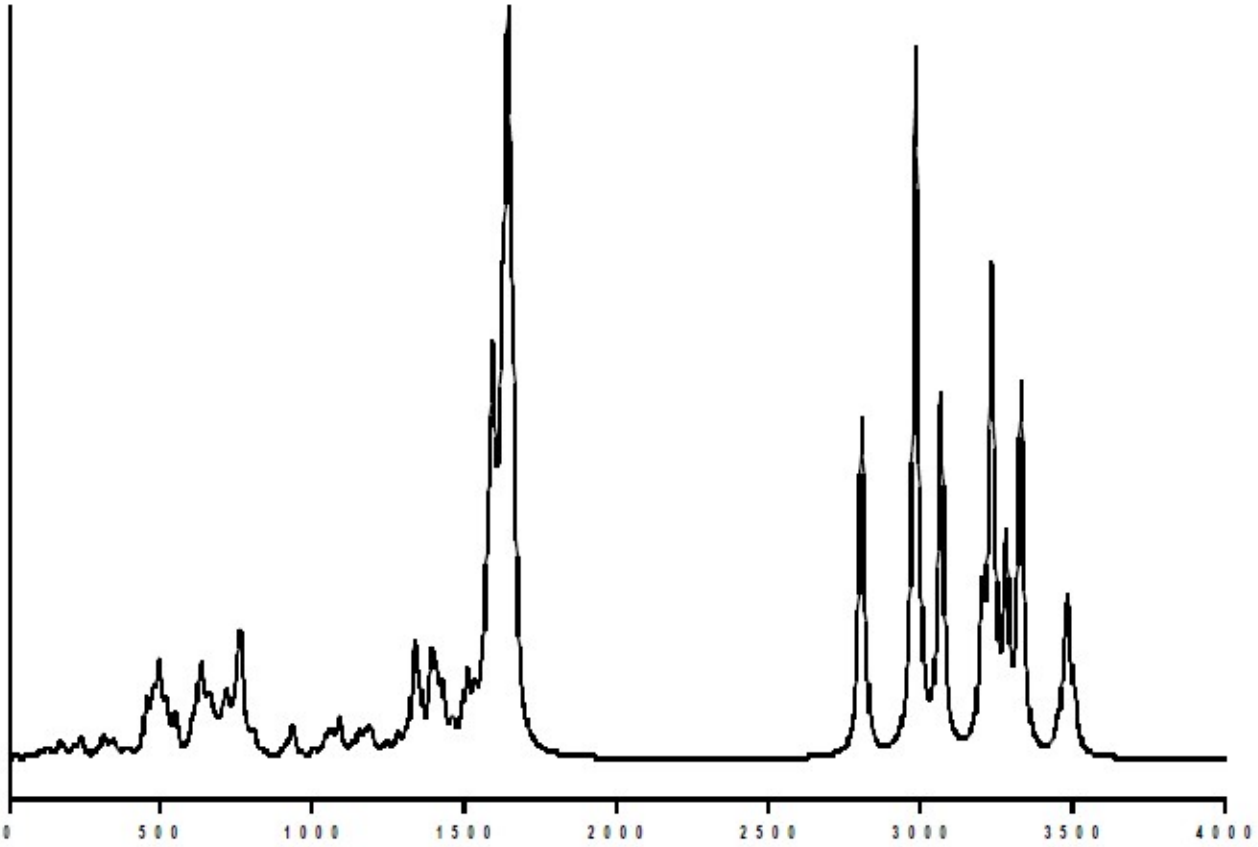


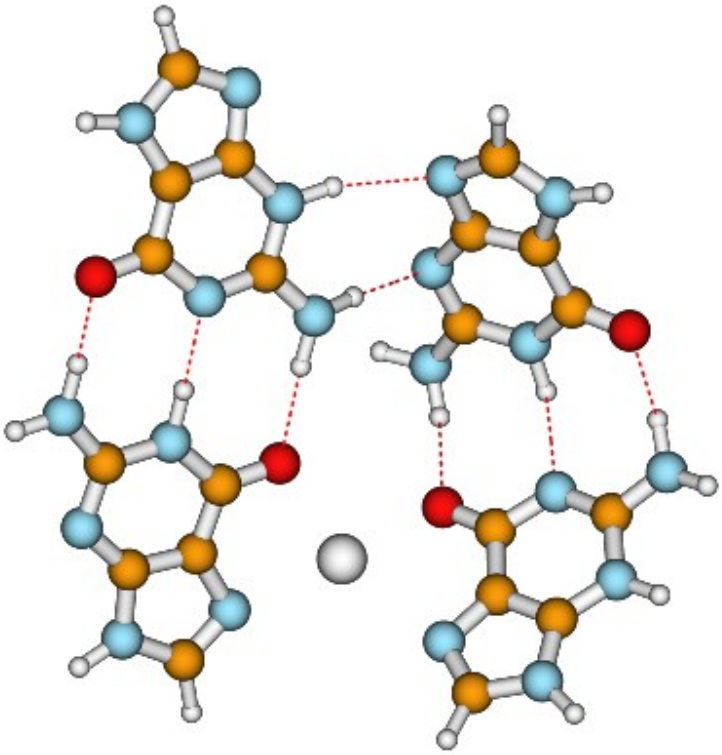
ΔG = 57.8





ΔG = 43.7





ΔG = 43.5

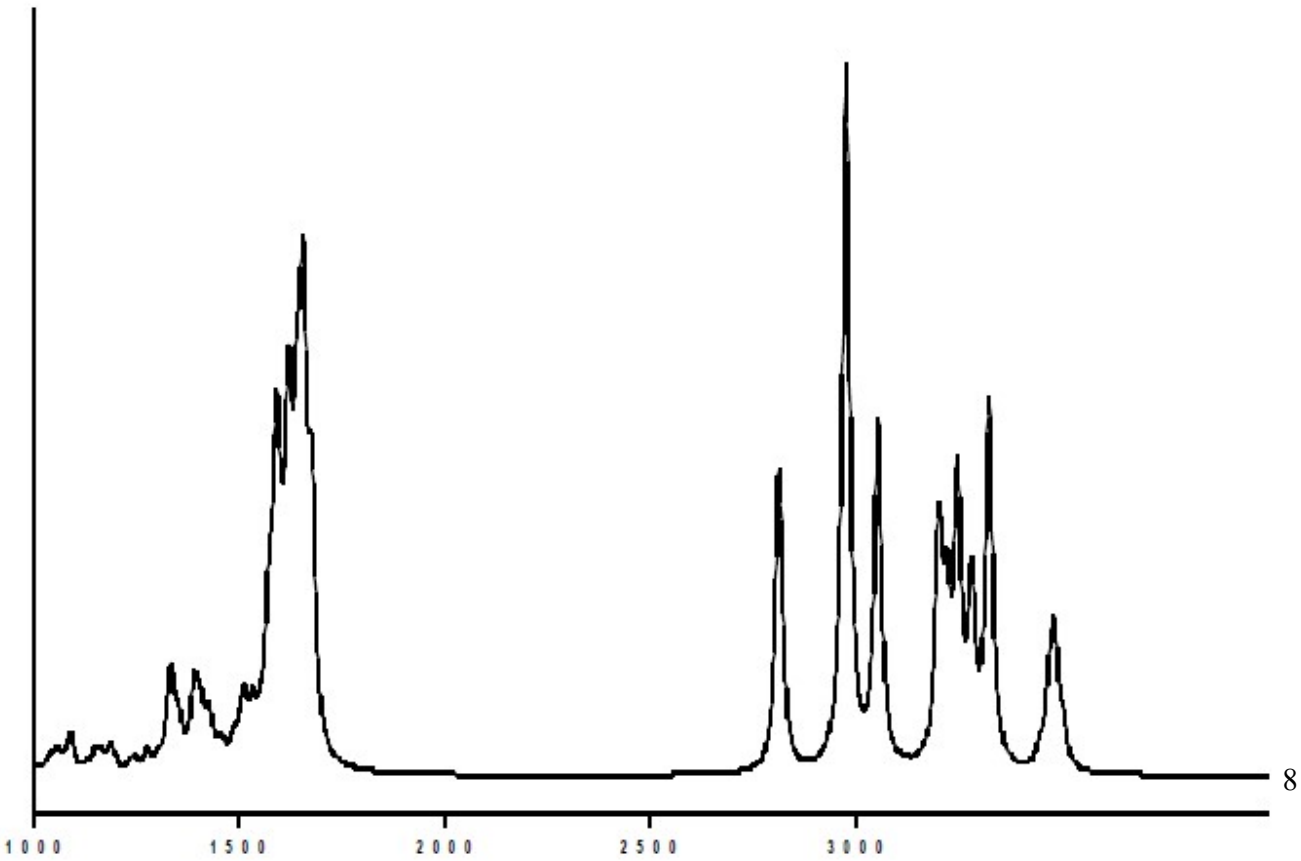
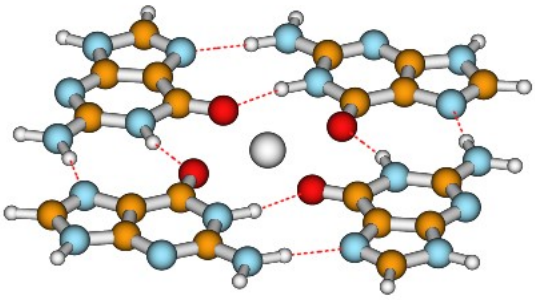
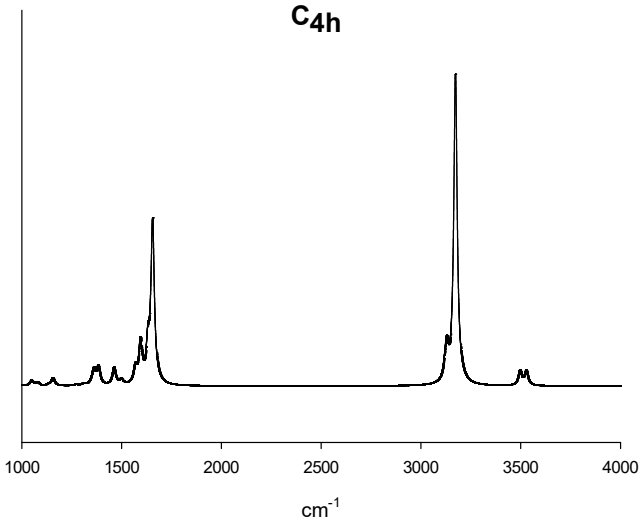
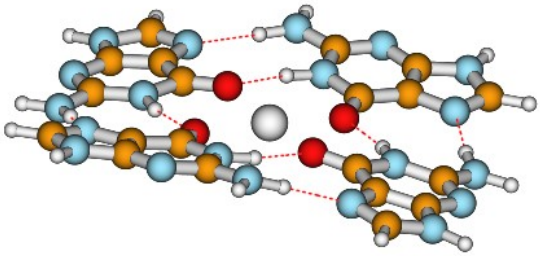


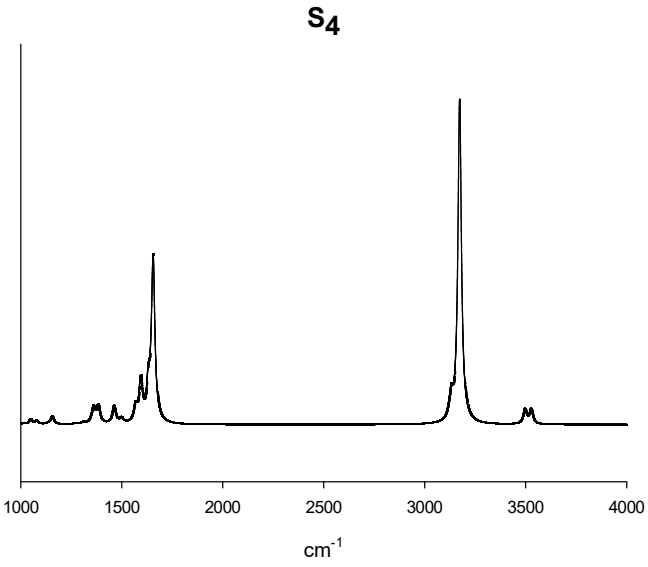
Figure S3





C_{4h} (1.2)





S_4 (0.0)

Figure S4

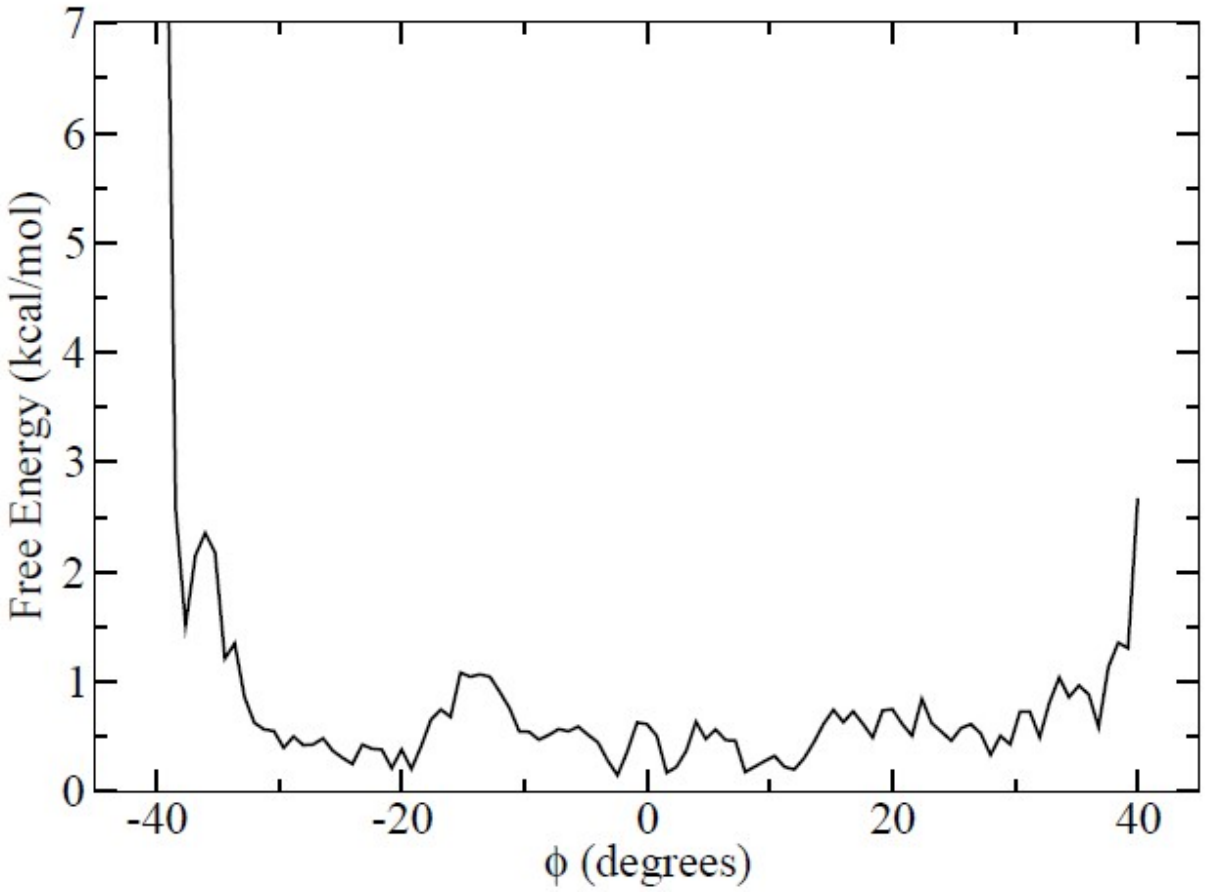


Figure S5

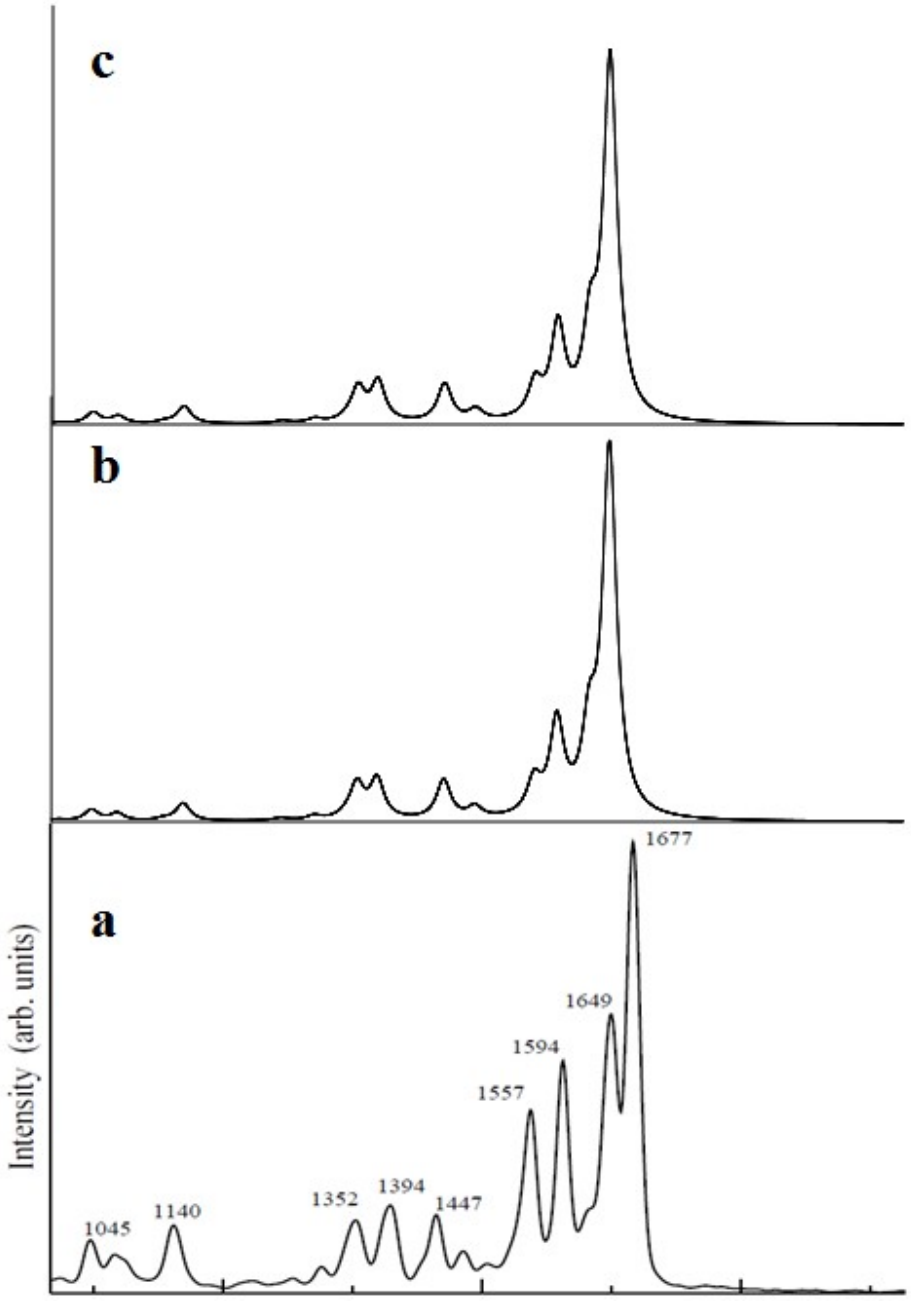
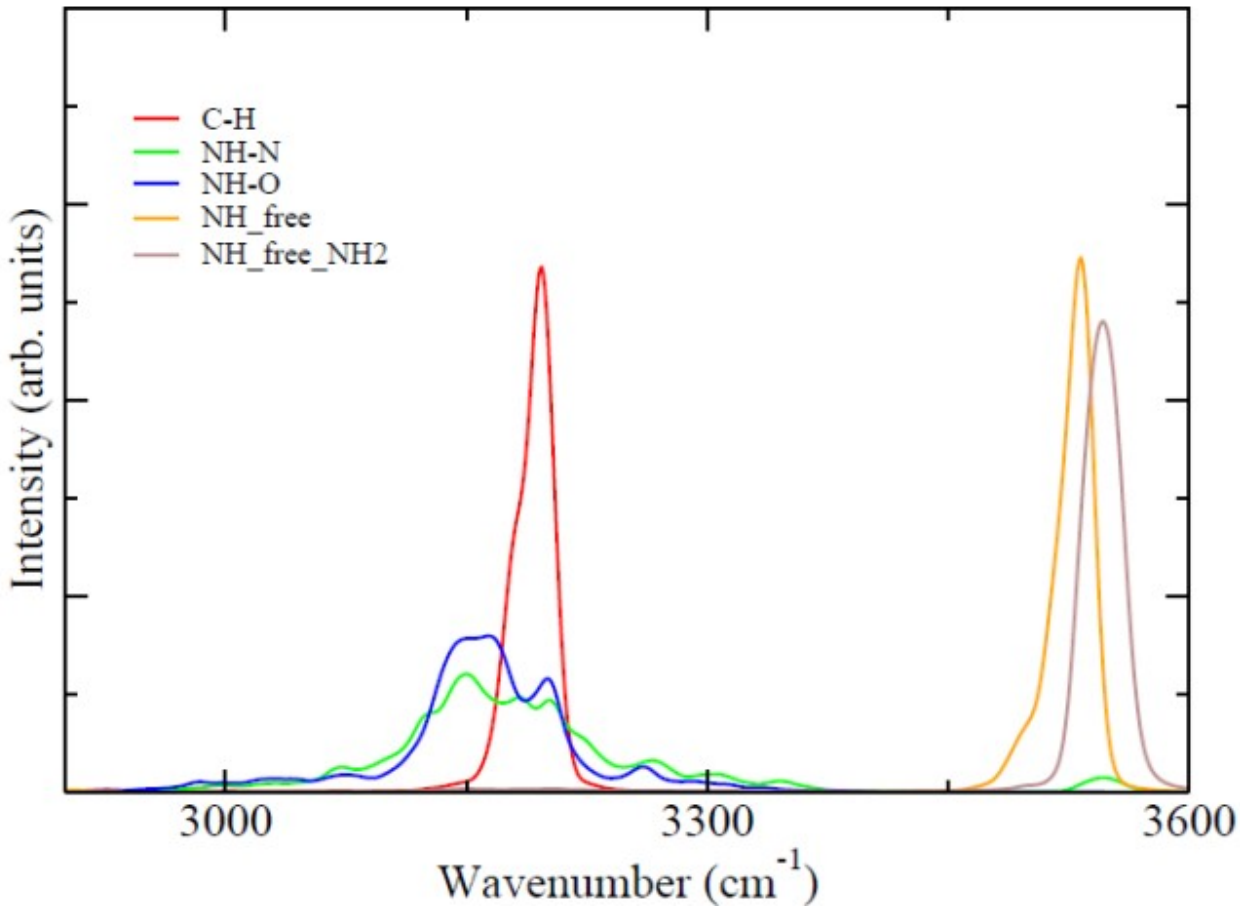

c
b
a
Intensity (arb. units)
1045
1140
1352
1394
1447
1557
1594
1649
1677

Figure S6


C-H
NH-N
NH-O
NH_free
NH_free_NH2
Intensity (arb. units)
3000
3300
3600
Wavenumber (cm-1)