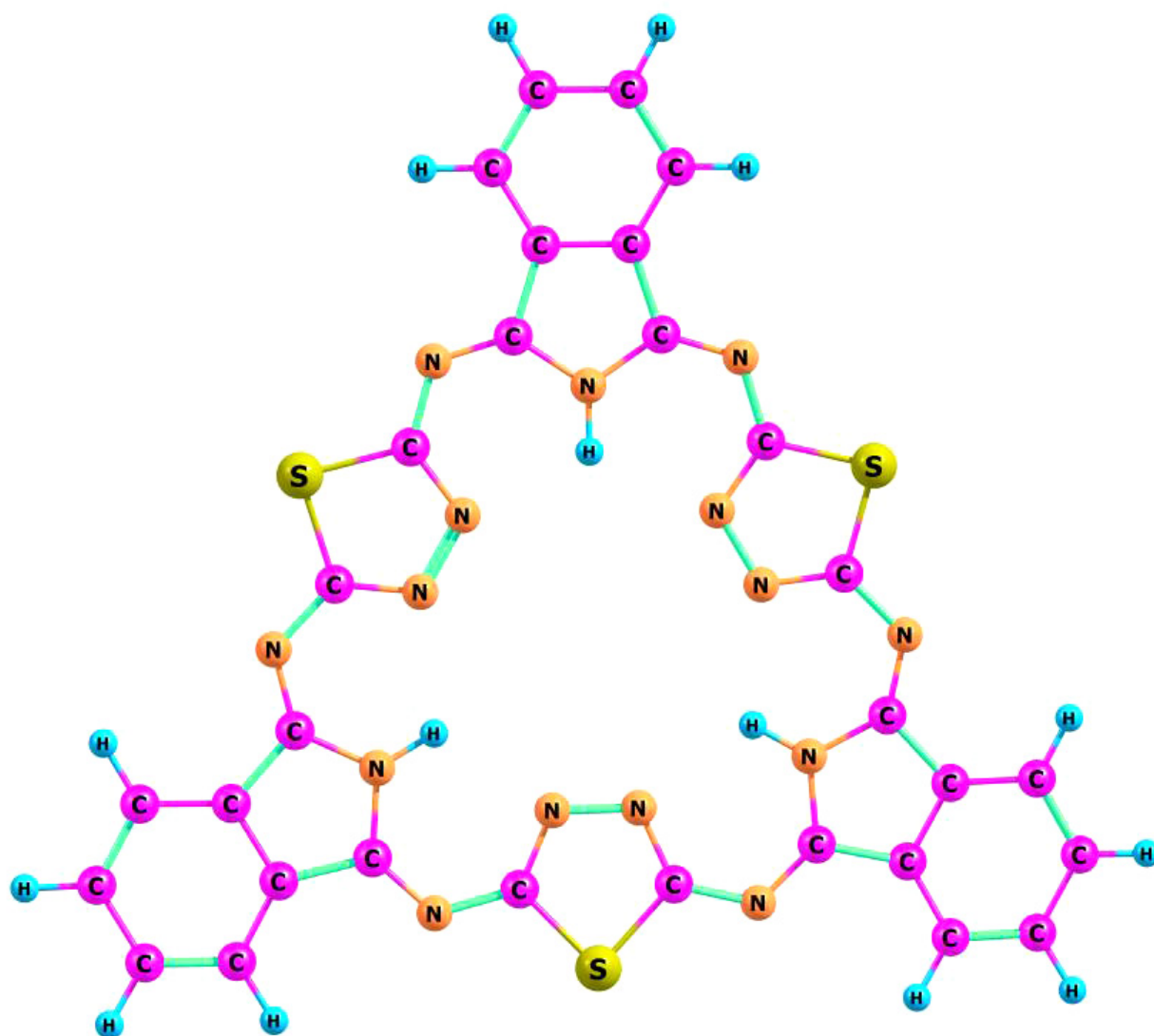


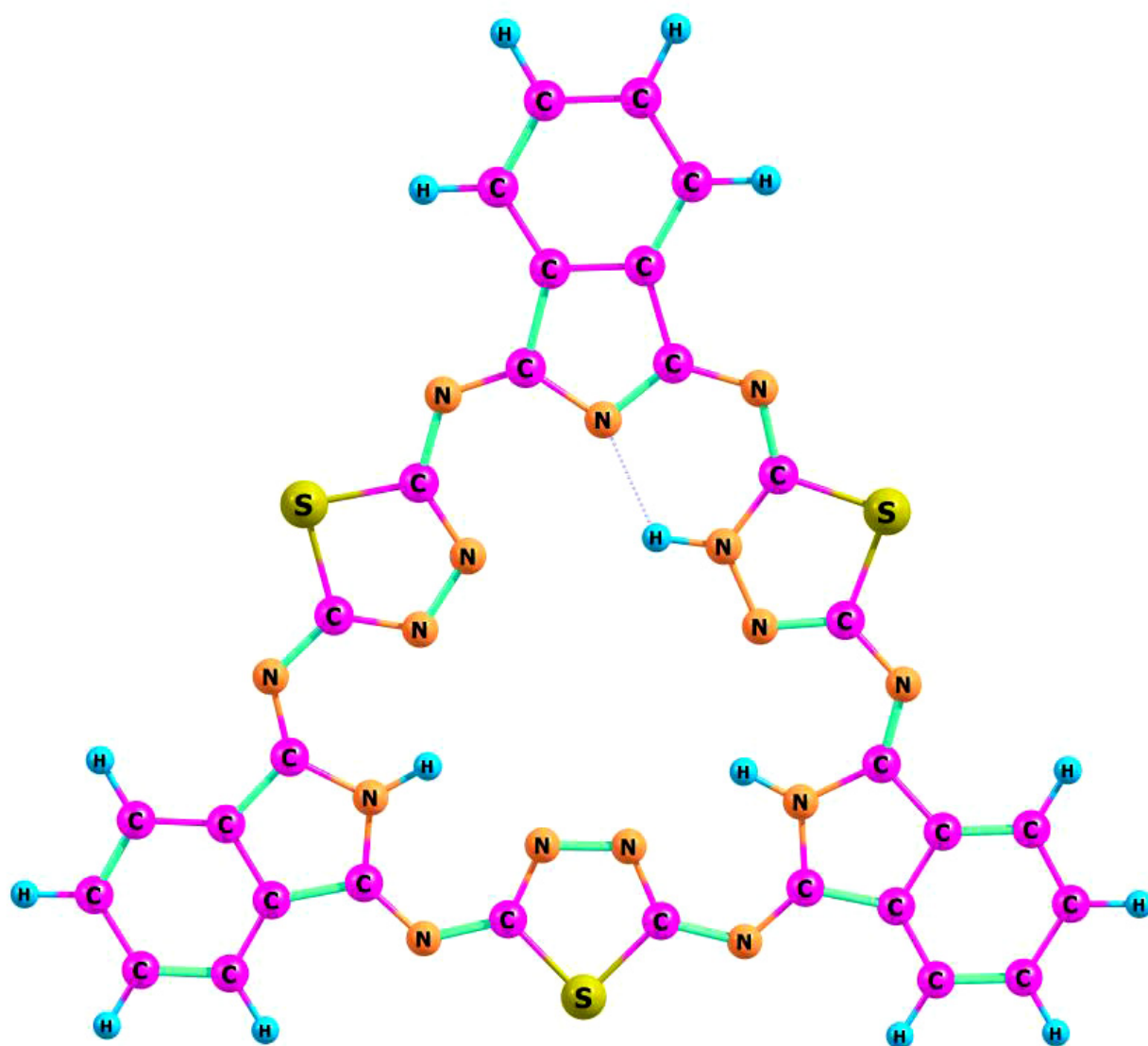


-3168.89675153;

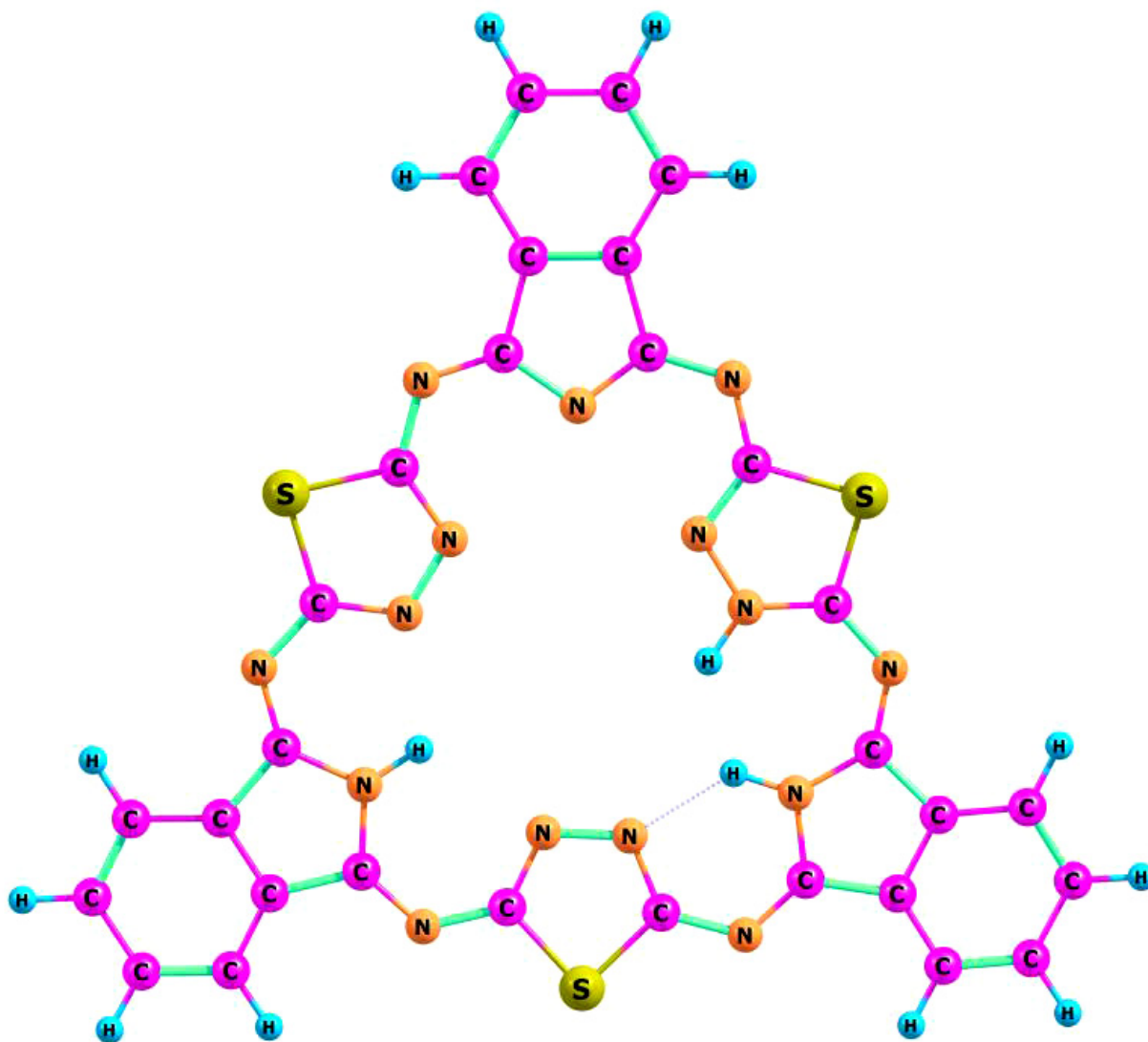
0

NIF=0

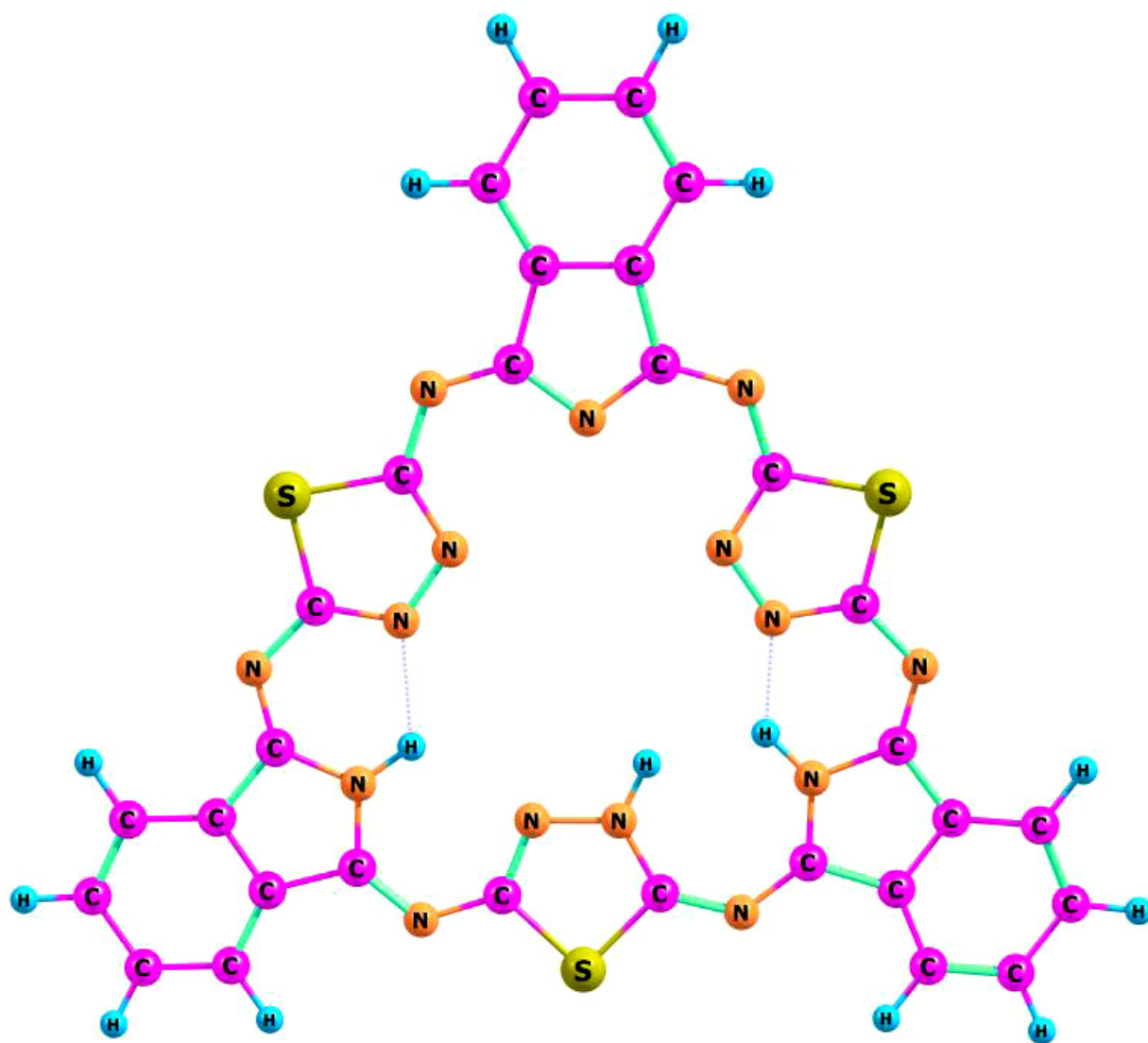
D3h



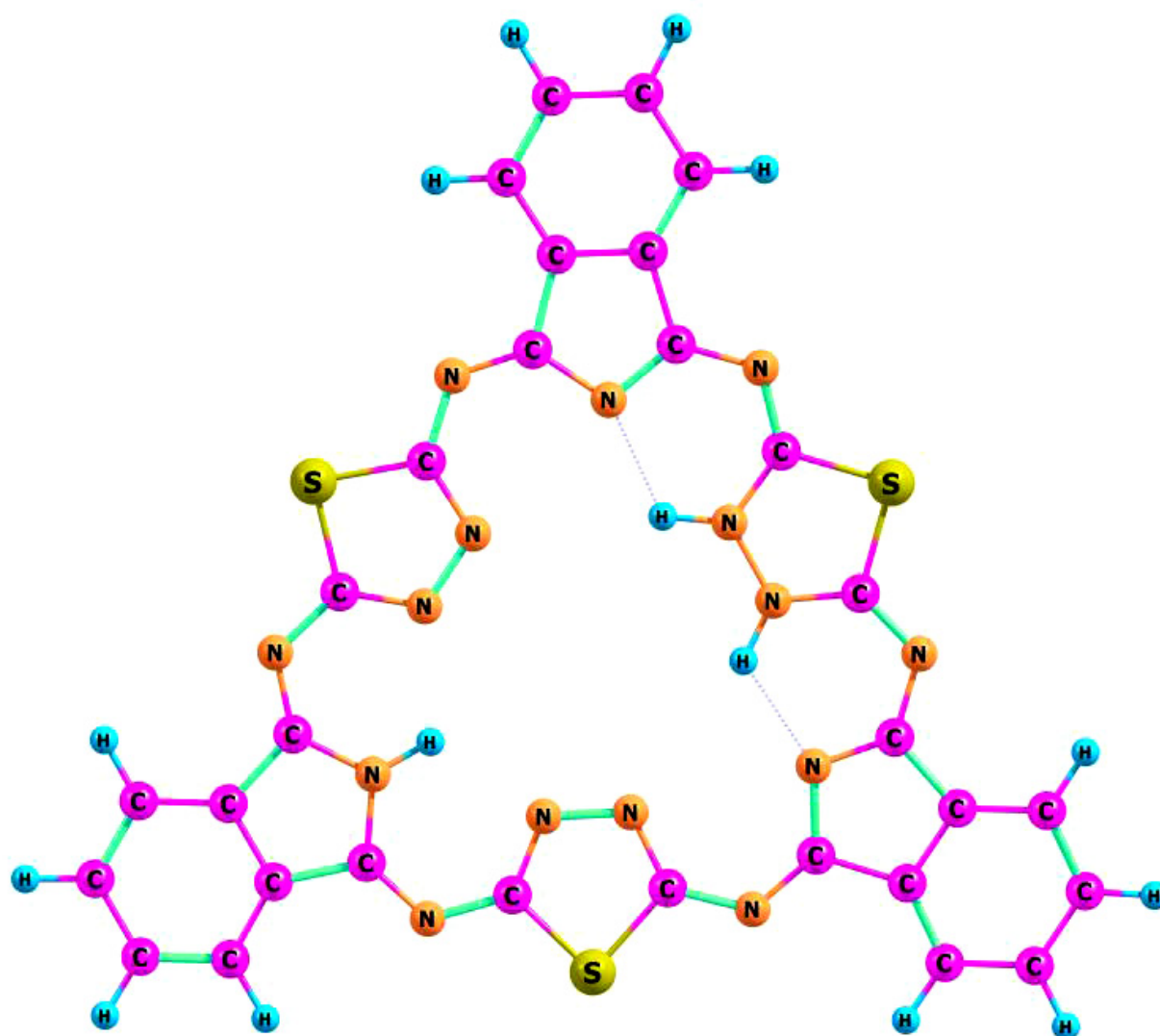
1PT-1
-3168.87935911
45.7
NIF = 0
CS



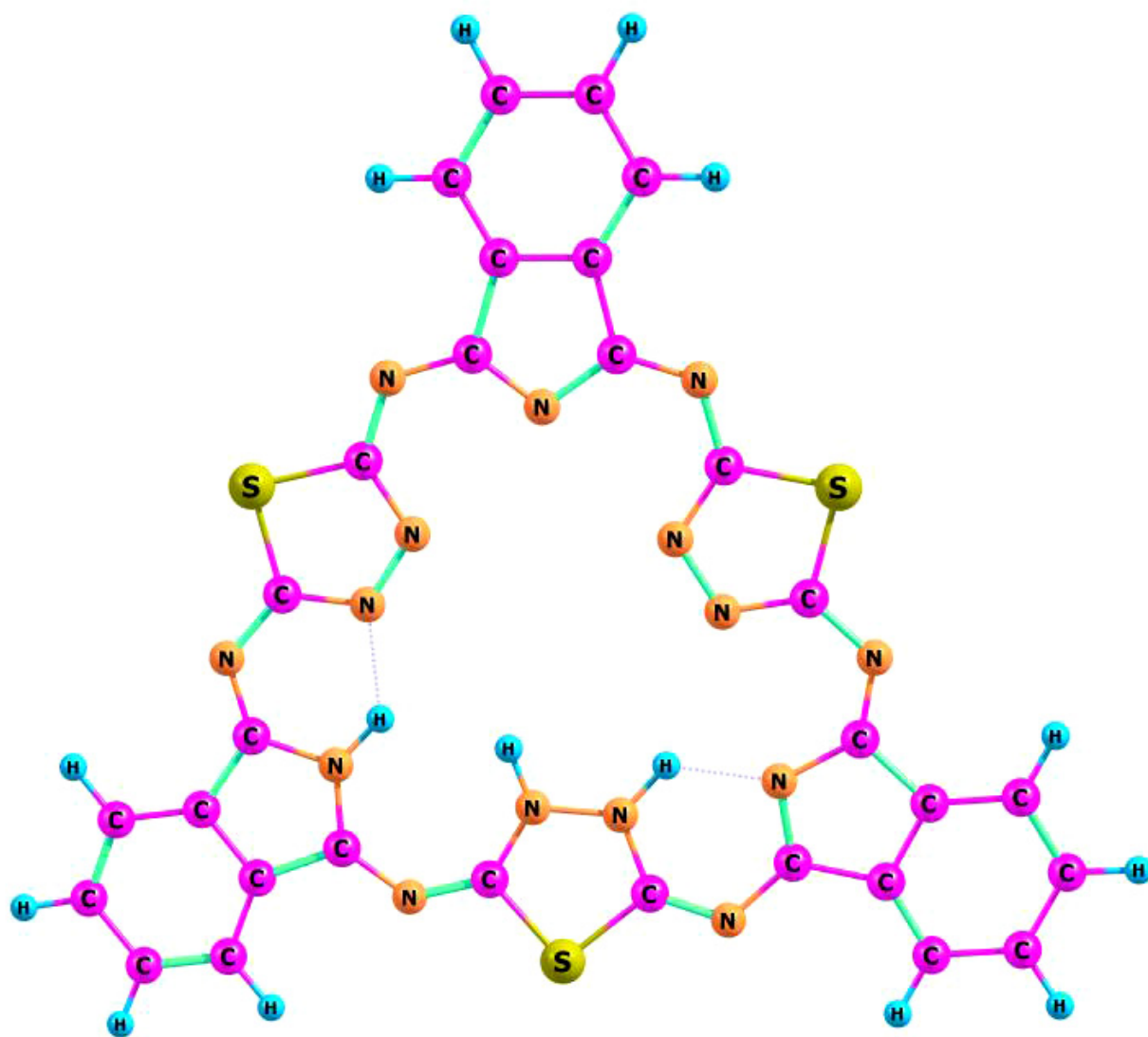
1PT-2
-3168.82719185
182.6
NIF=2
CS



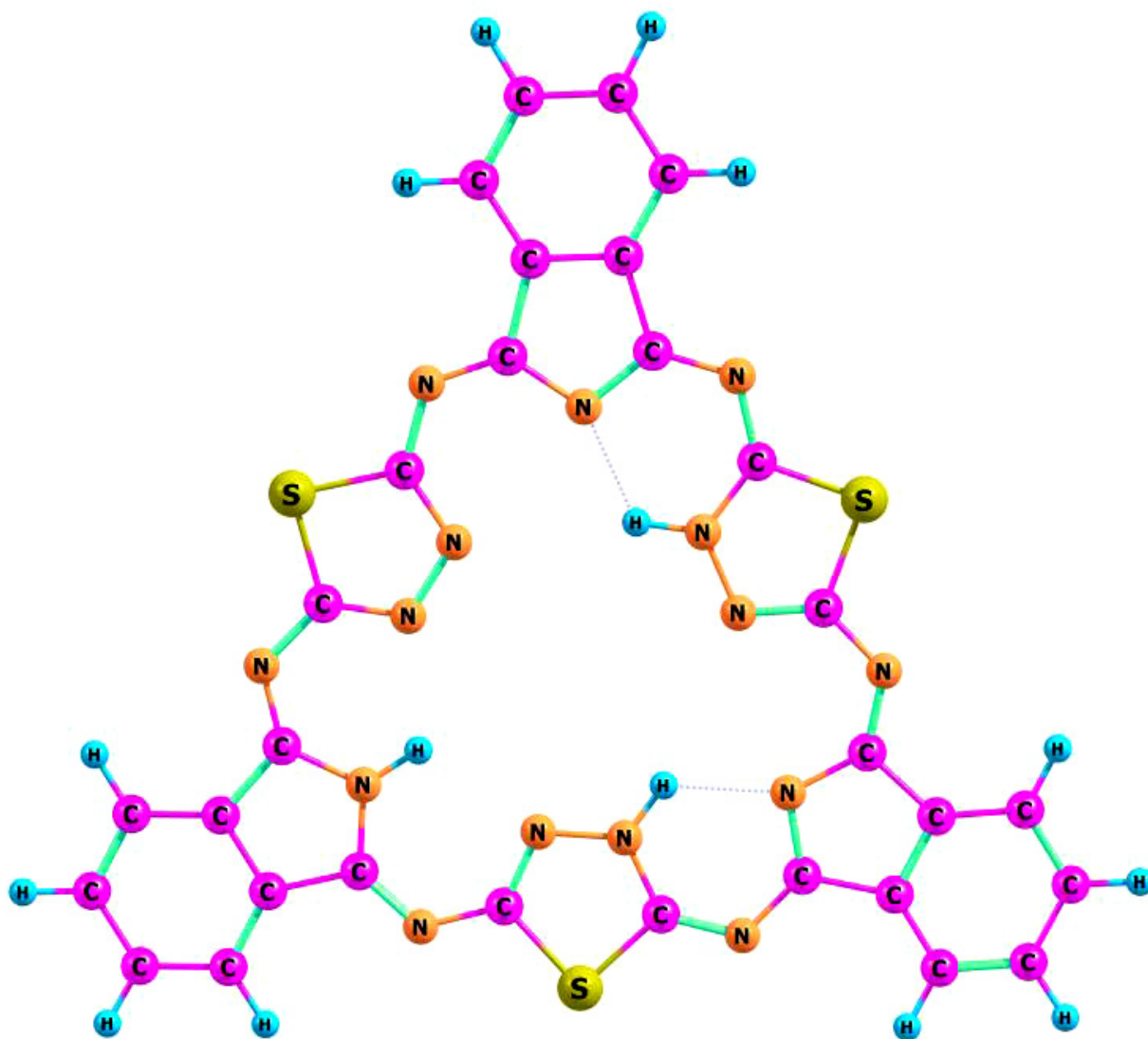
1PT-3
-3168.81875657
204.8
NIF = 2
CS



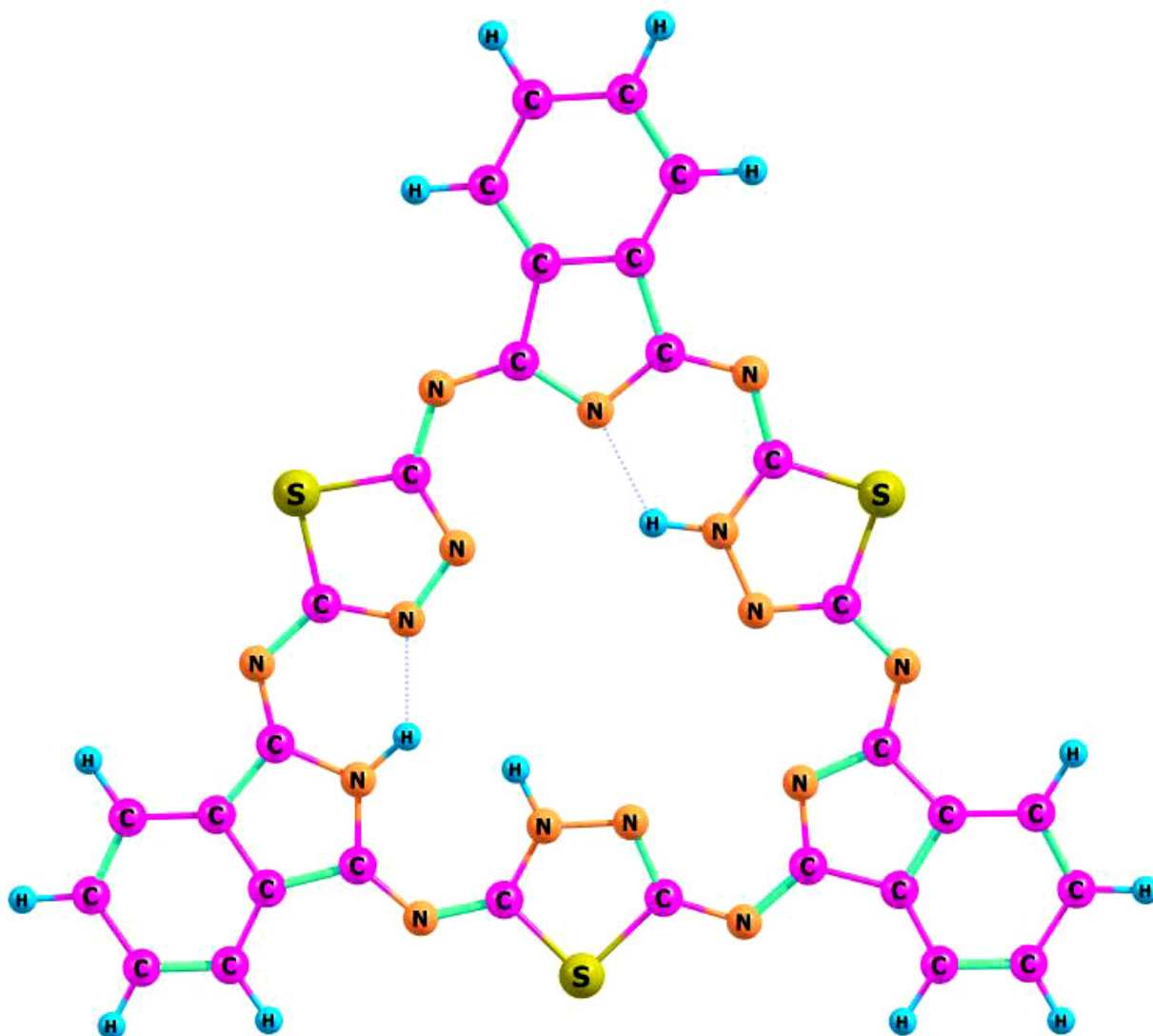
2PT-1
-3168.84303029
141.0
NIF = 0
C2v



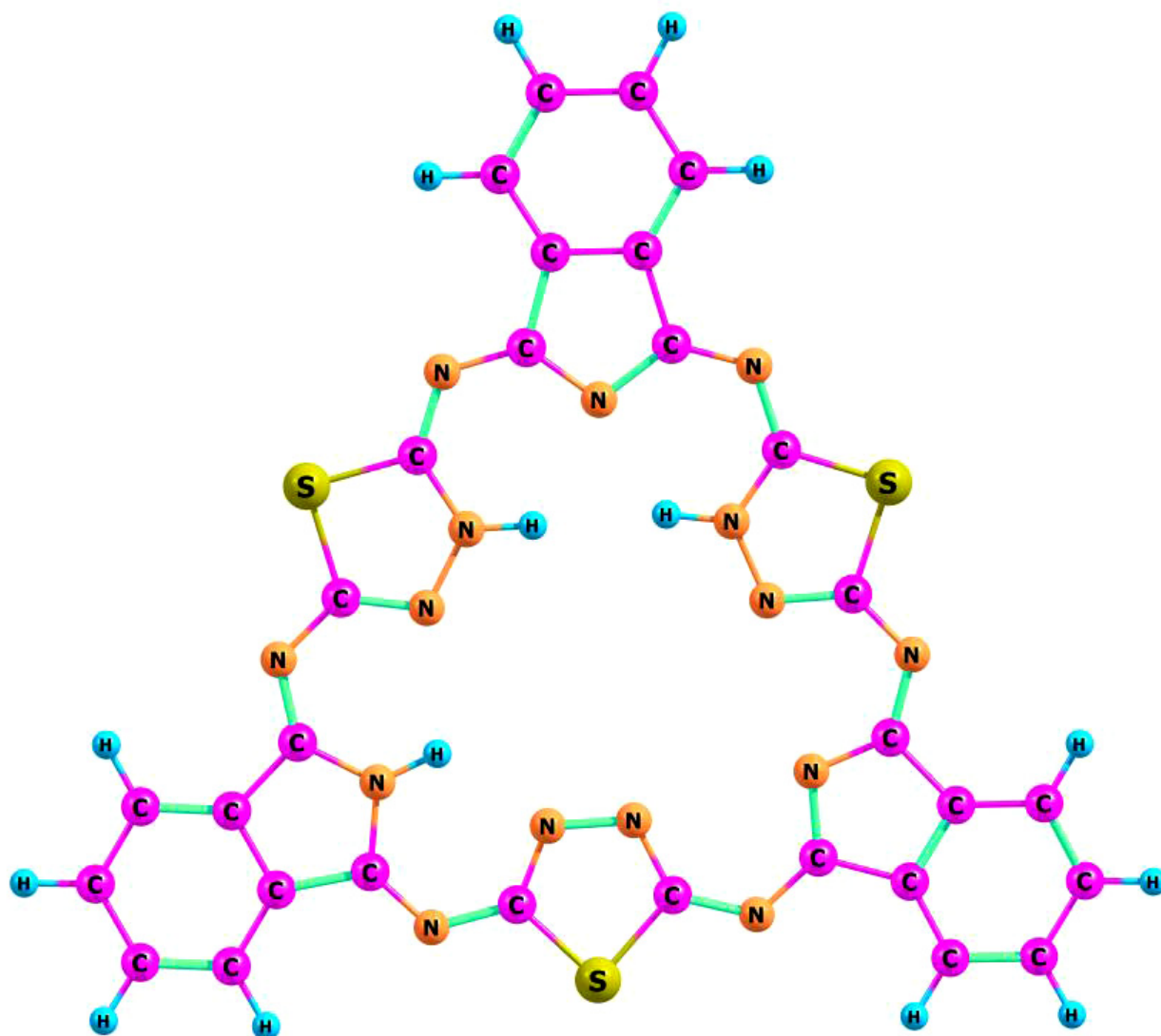
2PT-2
-3168.77406695
322.1
NIF = 2
CS



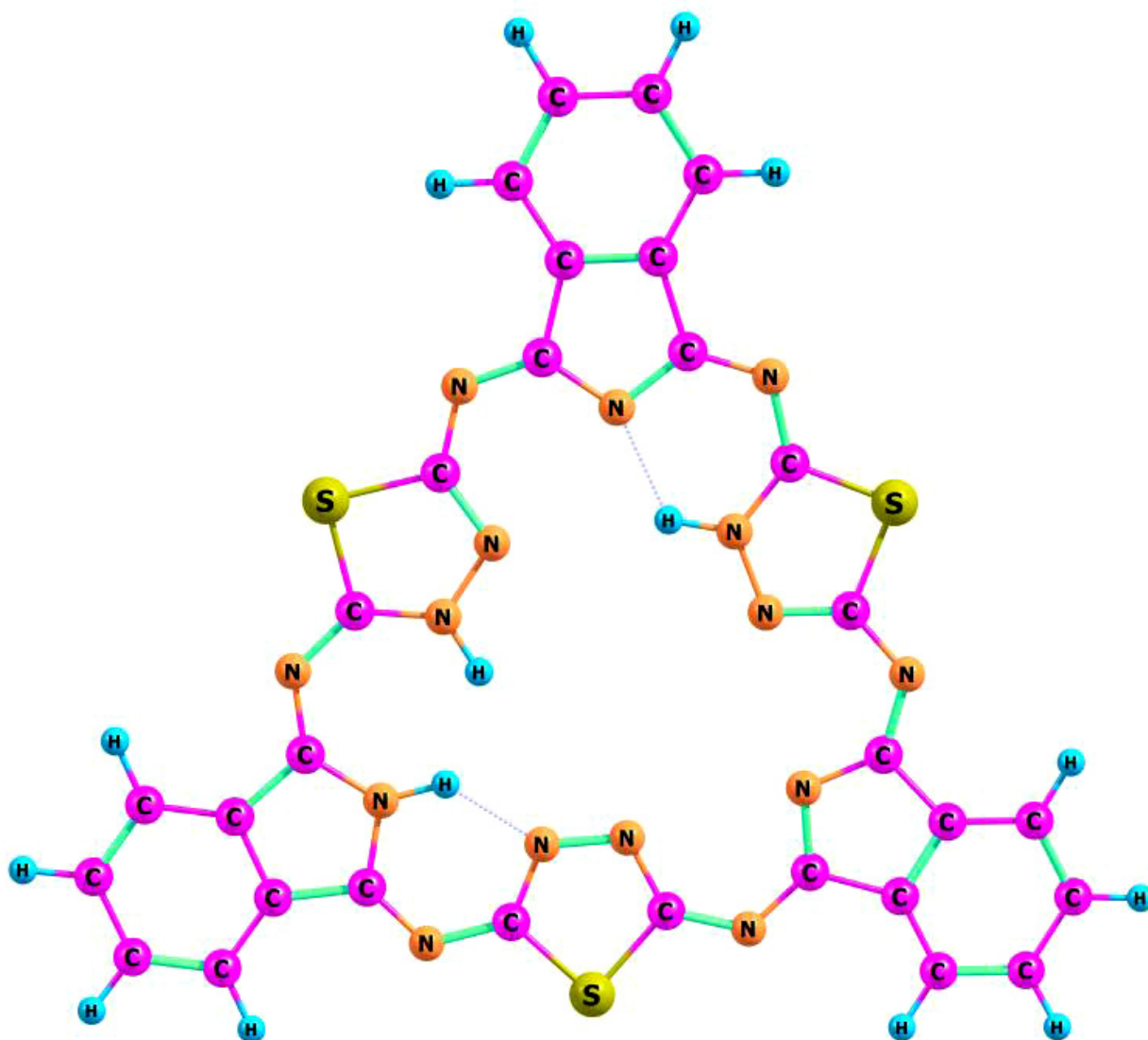
2PT-3
-3168.86569682
81.5
NIF = 0
CS



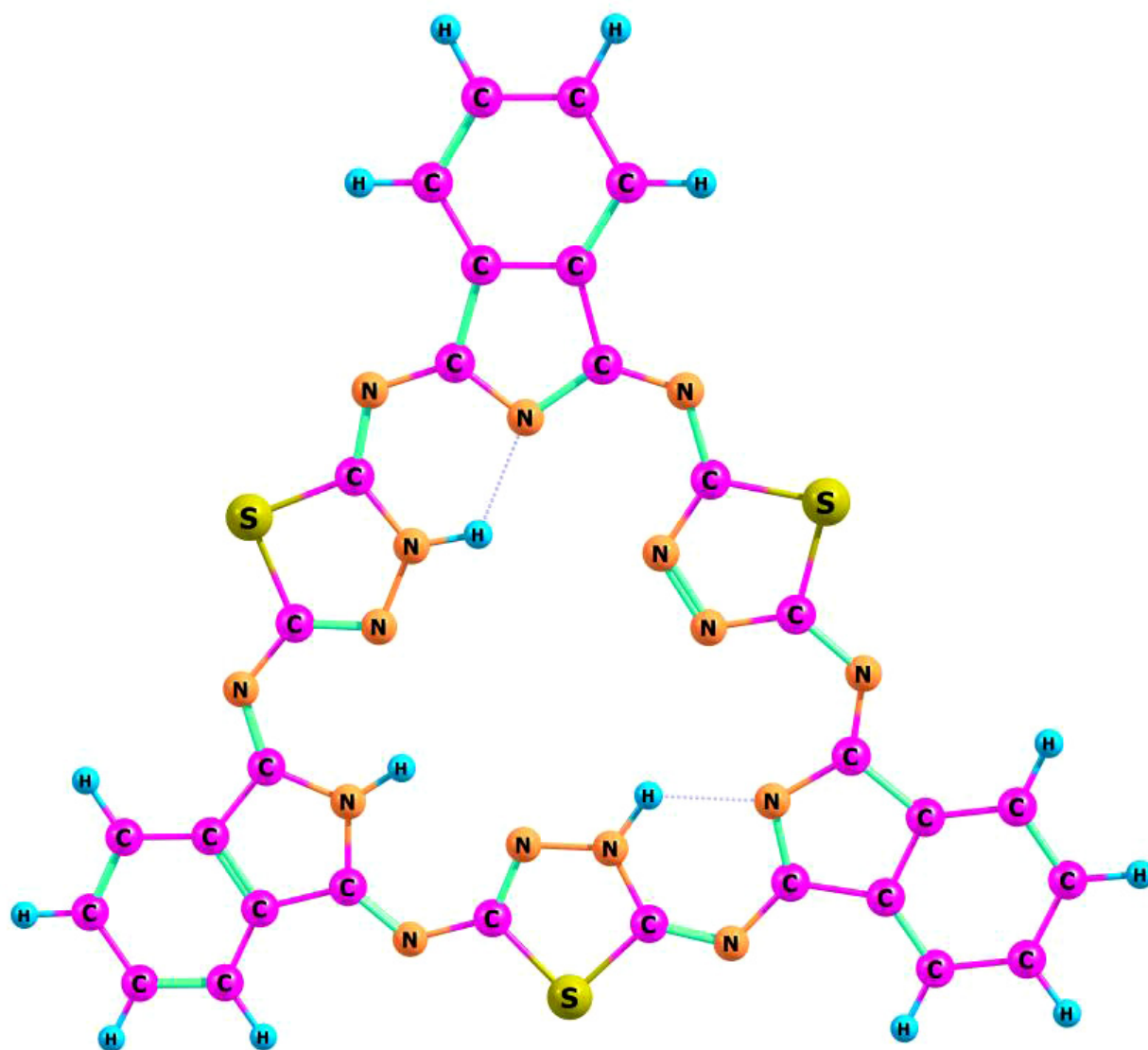
2PT-4
-3168.81971126
202.3
NIF = 1
CS



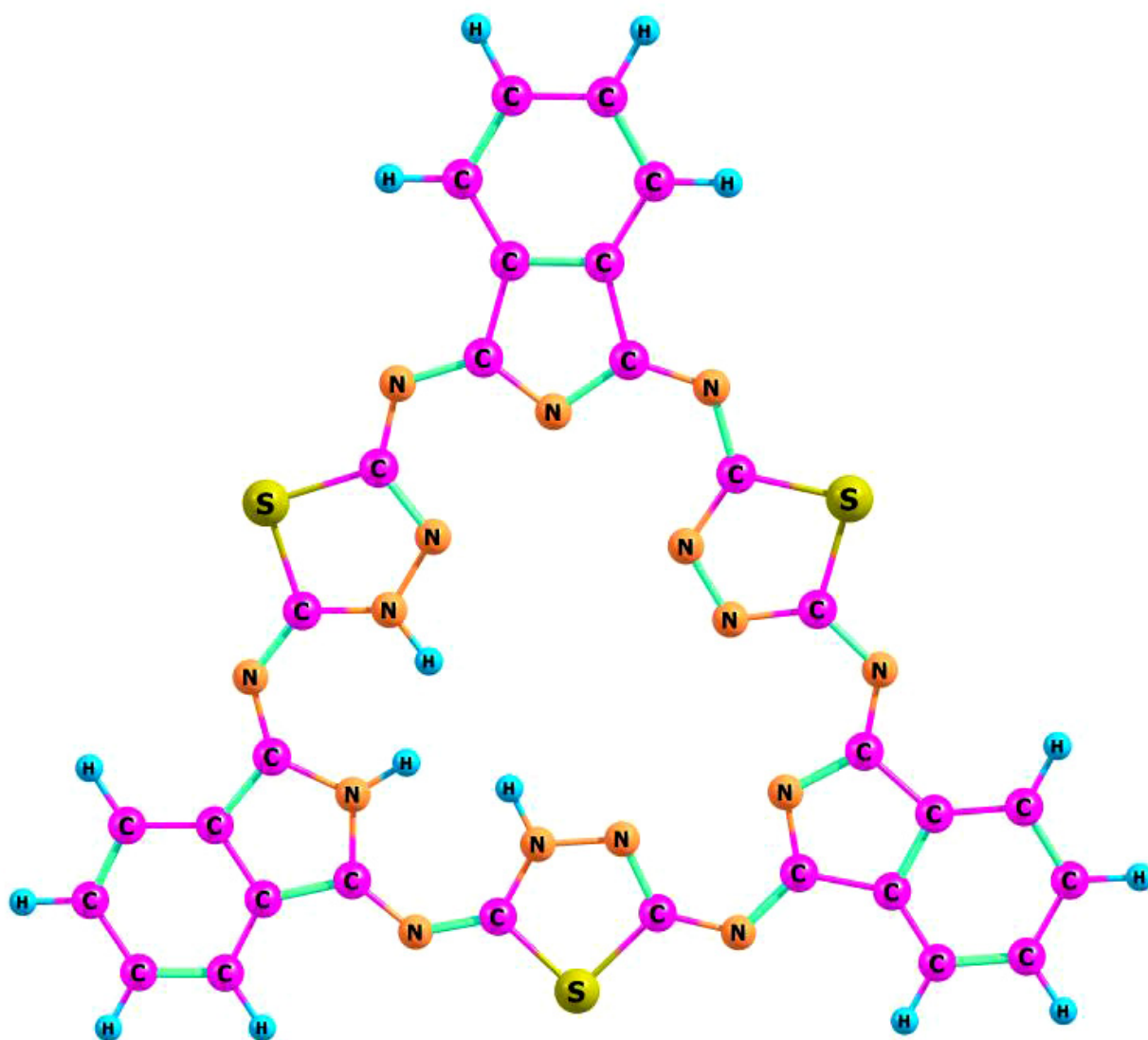
2PT-5
-3168.83098571
172.7
NIF = 2
CS



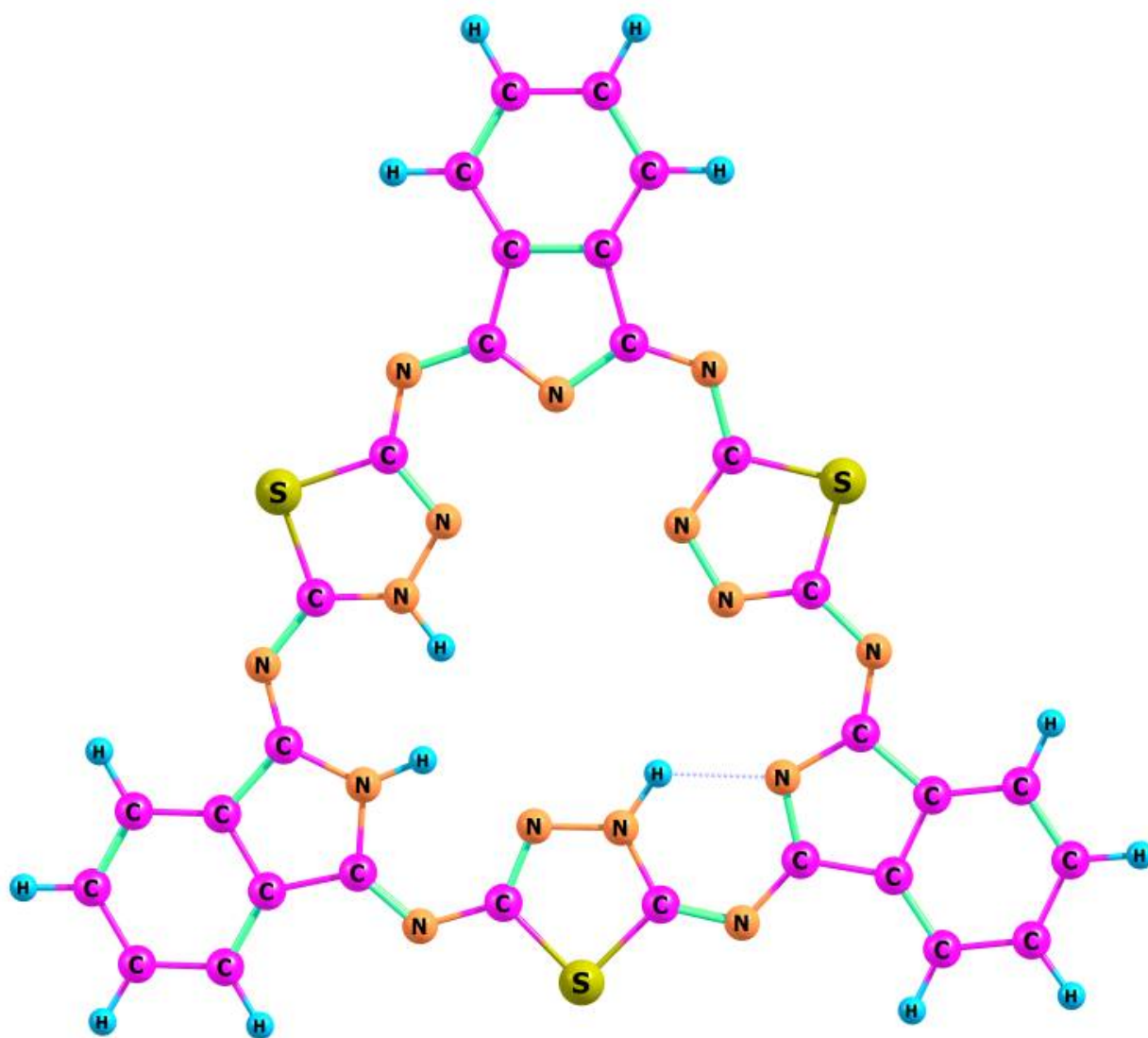
2PT-6
-3168.81654547
210.6
NIF = 2
CS



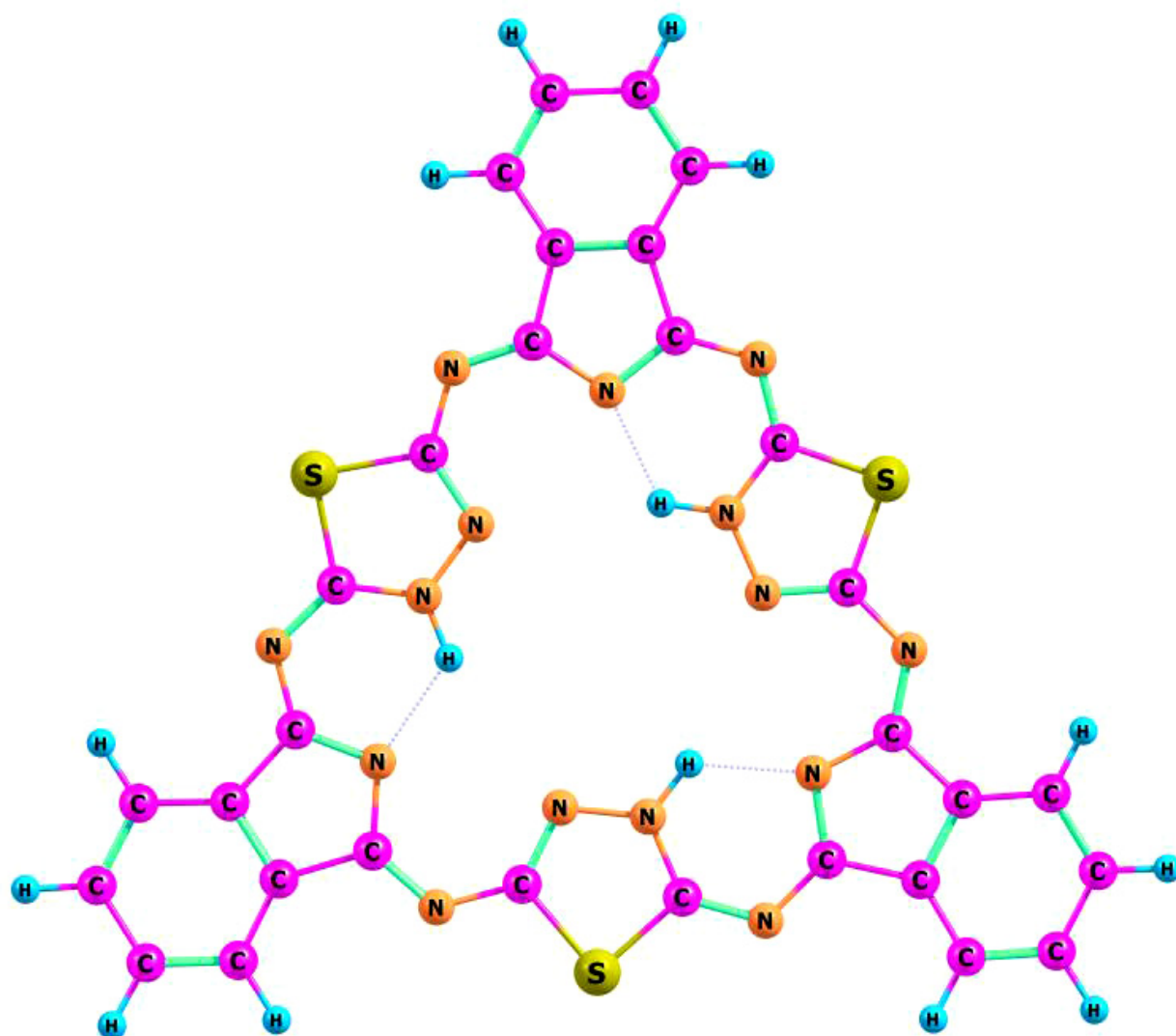
2PT-7
-3168.85944451
97.9
NIF = 0
C_{2v}



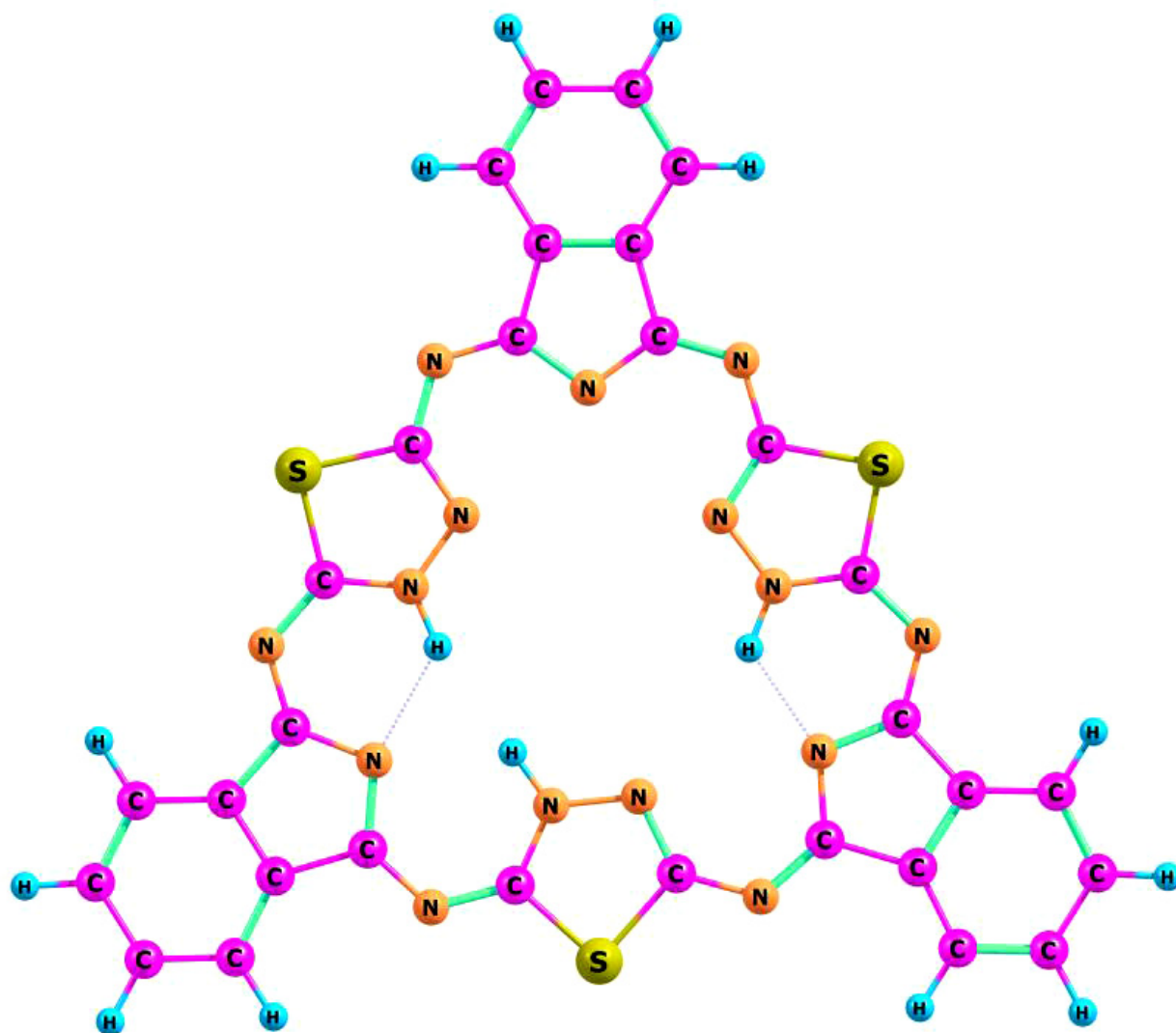
2PT-8
 -3168.72138492
 460.4
 NIF = 4
 C_{2v}



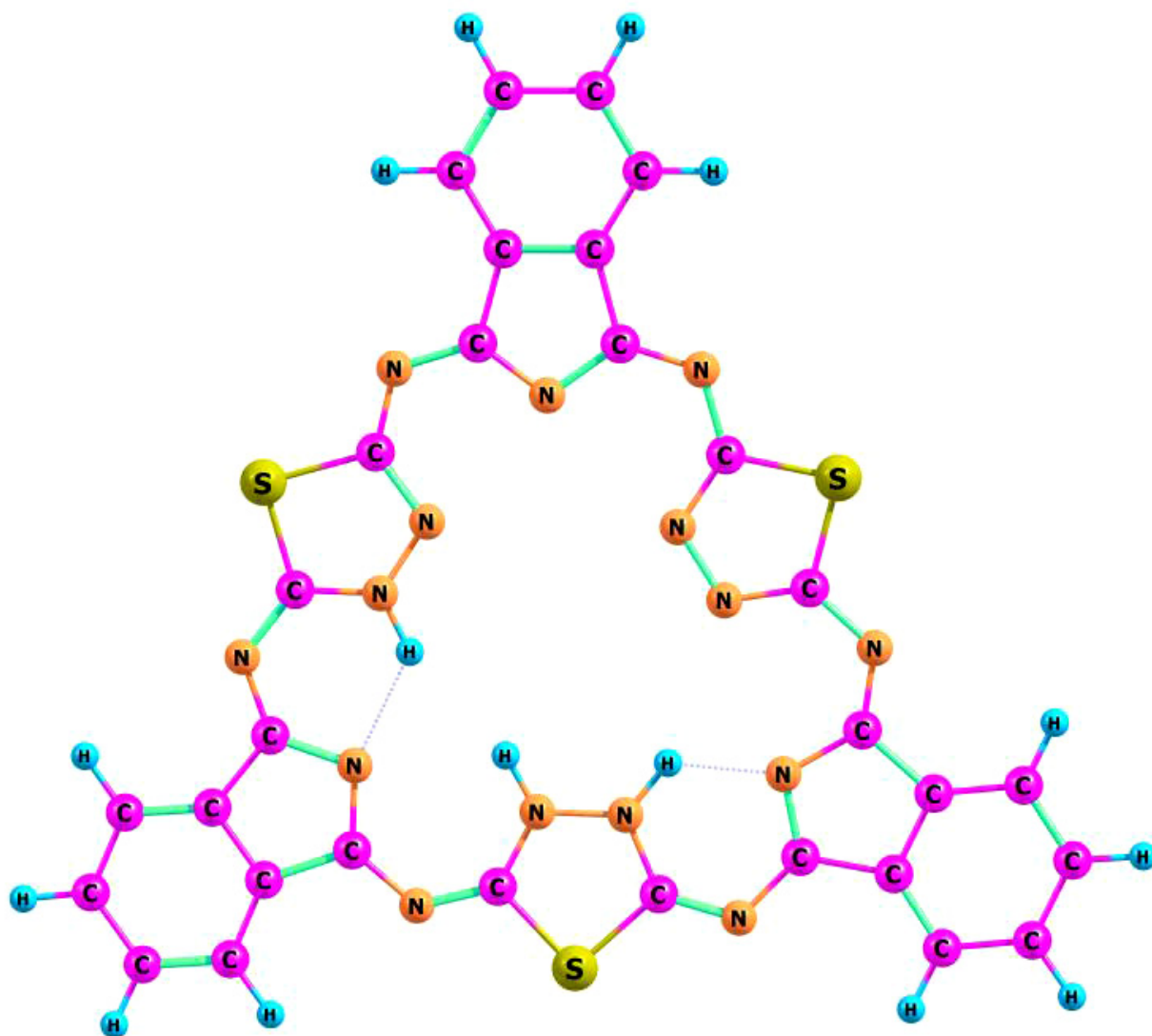
2PT-9
-3168.79858449
257.7
NIF = 2
CS



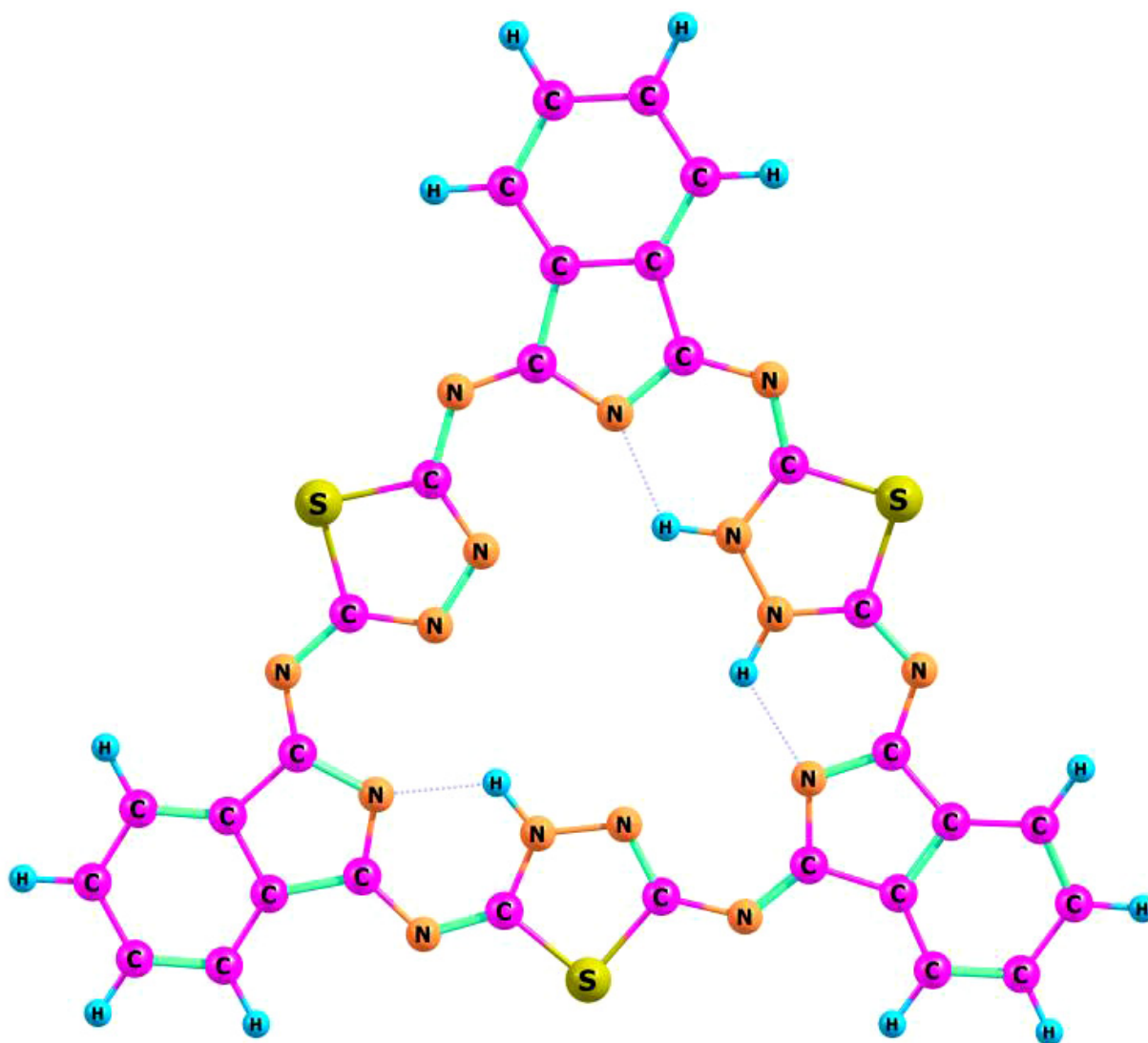
3PT-1
 -3168.85582960
 107.4
 NIF = 0
 C3h



3PT-2
-3168.82717636
182.7
NIF = 1
CS



3PT-3
-3168.78639750
289.7
NIF = 2
CS



3PT-4
 -3168.82740766
 182.1
 NIF = 0
 CS

Figure S1. The considered tautomers of HHP, their total energies (in Hartree), relative energies (in kJ mol^{-1}), numbers of imaginary frequencies (NIF) and symmetries.

Model	HHp	1PT-1	1PT-2	1PT-3	2PT-1	2PT-2
ΔE , kJ mol ⁻¹	0	45.7	182.6	204.8	141.0	322.1
NIF	0	0	2	2	0	2
Model	2PT-3	2PT-4	2PT-5	2PT-6	2PT-7	2PT-8
ΔE , kJ mol ⁻¹	81.5	202.3	172.7	210.6	97.9	460.4
NIF	0	1	2	2	0	4
Model	2PT-9	3PT-1	3PT-2	3PT-3	3PT-4	
ΔE , kJ mol ⁻¹	257.7	107.4	182.7	289.7	182.1	
NIF	2	0	1	2	0	

Table S1. Relative energies (at B3LYP/pcseg-2 level) and numbers of imaginary frequencies (NIF) for all considered tautomers of **HHp**.