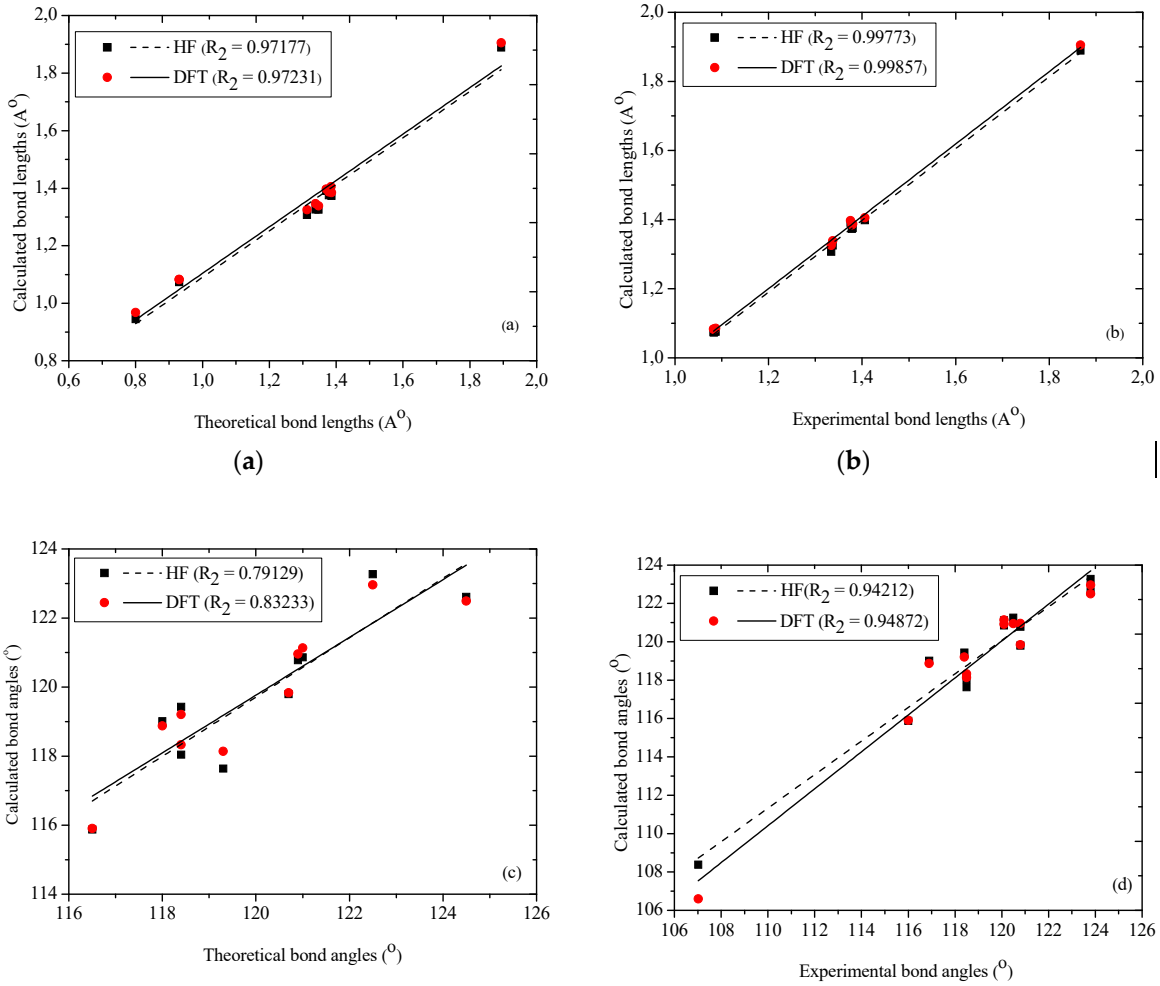

Figure S1. Correlation graphic between the calculated and ((a) and (b) theoretical and experimental bond lengths (c)), and ((d) theoretical and experimental bond angles).

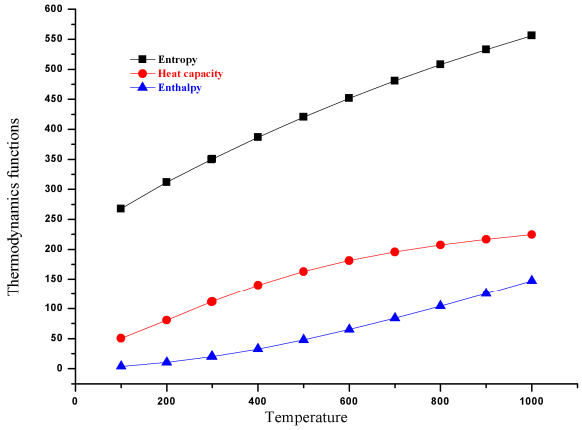

Figure S2. Variation of entropy (S), heat capacity (Cp) and enthalpy (H) with temperature for the 3-Br-2-HPy molecule.

Table S1. Calculated SCF energy, ZPVE, rotational constants, thermodynamic parameters and dipole moment (D) of 3-Br-2-HyP monomer and dimer structures with DFT method.

	Monomer	**Dimer**
SCF energy E(kJ/mol)	–7606473.060	–15213012.632
ZPVE (kcal/mol)	52.10659	104.91781
Rotational constants (GHz)		
A	2.97625	0.71148
B	0.98182	0.11026
C	0.73827	0.09547
Thermal energy (kcal/mol)	56.262	114.086
Specific heat at constant Volume C_v (cal.mol^{-1}.K^{-1})	24.598	52.683
Entropy S (cal.mol^{-1}.K^{-1})	83.583	128.527
Dipole moment (Debye)	2.1152	0.0019