

New insights on the ESIPT process based on solid-state data and state-of-the-art computational methods

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Table S1. Number of papers (as of September 2020) found on Google Scholar as a combination of the term “ESIPT” + a “keyword”:

Keyword	# of papers combined with the keyword "ESIPT"
DFT	3650
B3LYP	2690
TPSS	59
M06-2X	182
CASSCF	372
CCSD(T)	74
def2	93
6-31G	1620
Molecular Dynamics	905

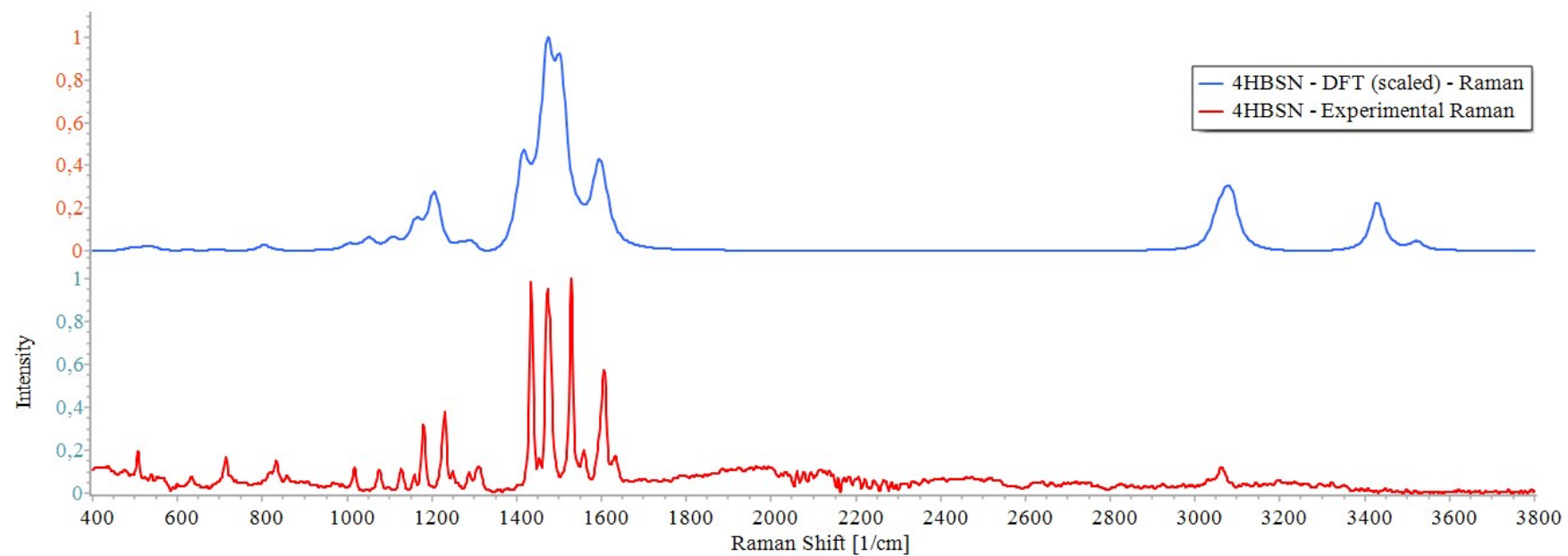


Figure S1. FT-Raman and DFT Raman spectra of the **4HBSN**.

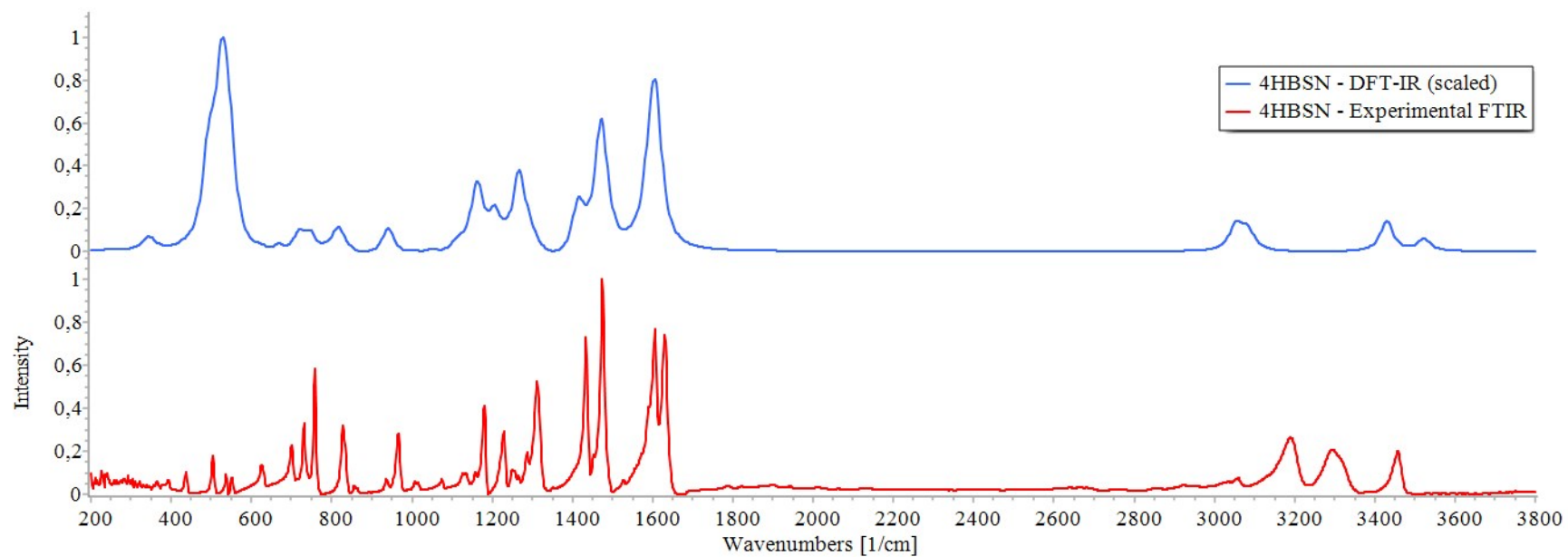


Figure S2. FT-IR and DFT IR spectra of the **4HBSN**.

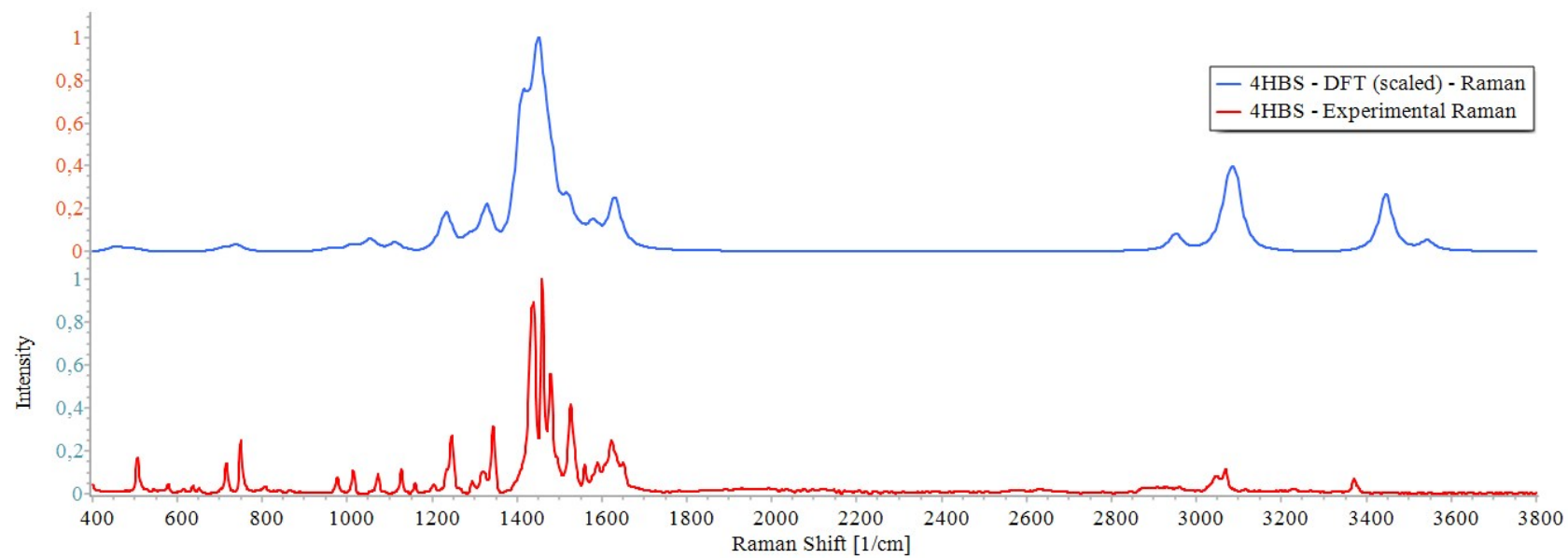


Figure S3. FT-Raman and DFT Raman spectra of the **4HBS**.

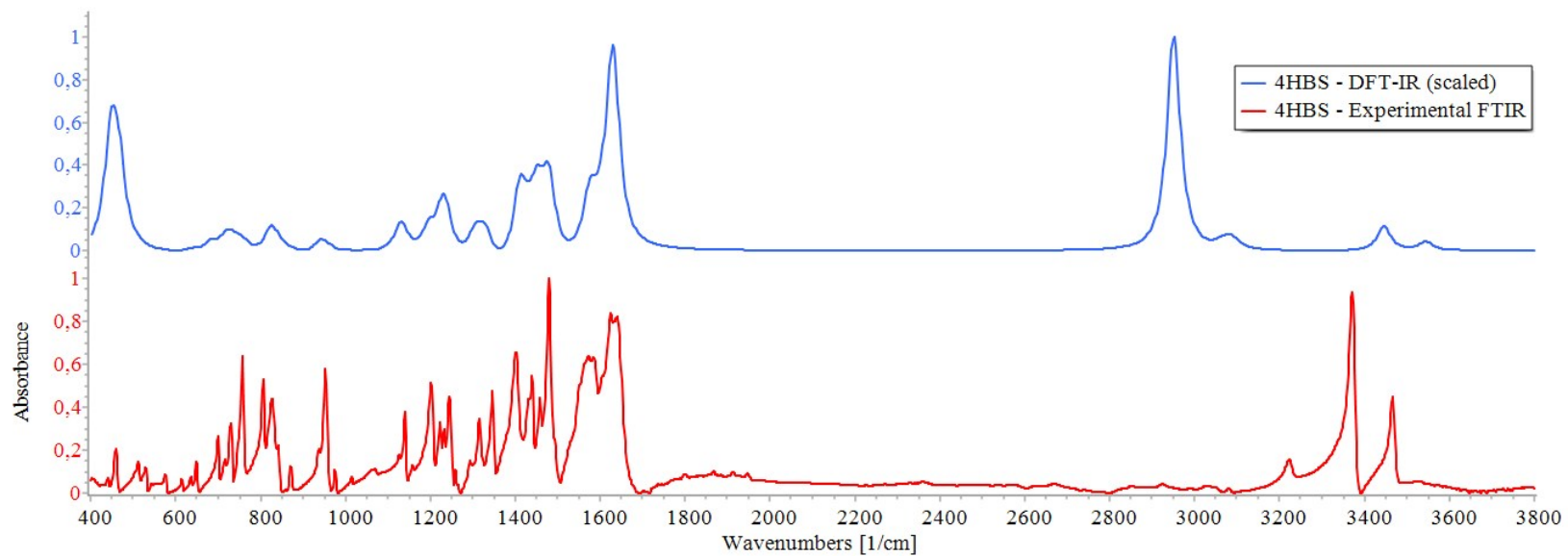


Figure S4. FT-IR and DFT IR spectra of the **4HBS**.