Abbreviations

2BBA 2-bromobenzoic acid  
3A5HP 3-amino-5-hydroxypyrazole  
4AAP 4-aminoantipyrine  
6APA 6-aminopenicillanic acid  
ANB 5-amino-2-nitrobenzoic acid  
AP Antipyrine  
ATR Attenuated Total Reflectance  
B3LYP Becke 3Lee Yang Parr  
CCD charge-coupled device  
cc-pVTZ correlation consistent polarized valence triple-zeta  
CECRI Central Electrochemical Research Institute  
DFT Density Functional Theory  
FT Fourier Transform  
FT-IR Fourier Transform Infra-Red  
FT-Raman Fourier Transform Raman  
HF Hartree-Fock  
ipb In-plane bending  
m Medium  
MMTU Morpholine-4-ylmethylthiourea  
MOPAC Molecular Orbital Package  
MP2 Møller-Plesset 2nd Order  
NIR Near Infra-Red  
NMR Nuclear Magnetic Resonance  
opb Out-plane bending  
PES Potential Energy Surface  
RMS Root Mean Square  
s Strong  
SD Standard Deviation  
t Twisting  
vs Very strong  
vw Very weak  
w Weak  
XRD X-Ray Diffraction  
ZPVE zero-point vibration energies  
δ Scissoring  
v Stretching  
νas Asymmetric stretching  
νs Symmetric stretching  
ρ Rocking  
τ Torsion  
β In-plane bending  
γ Out-plane bending  
ω Wagging