Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

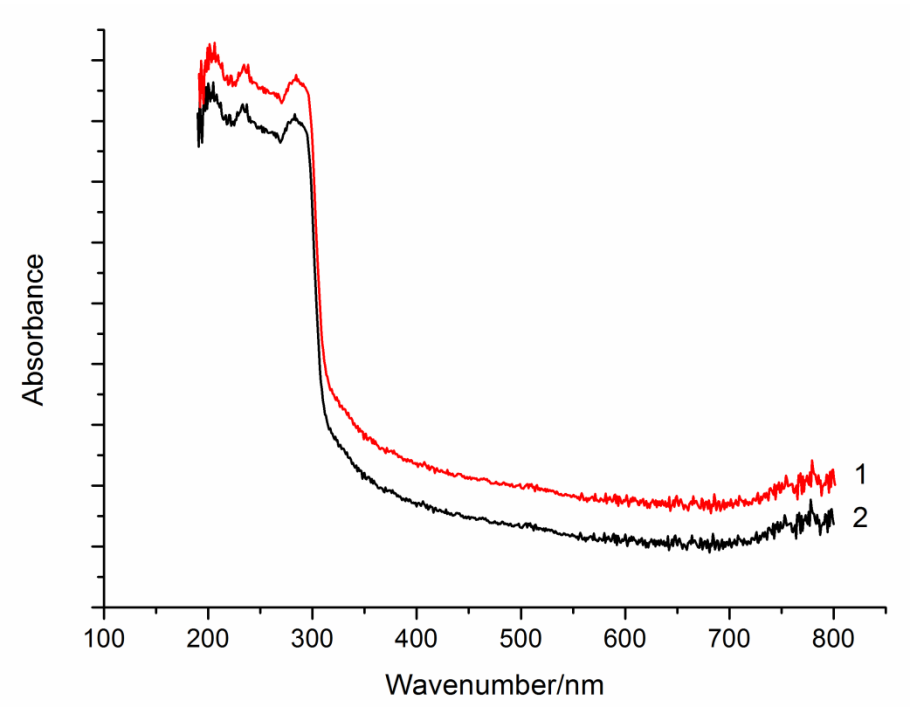

Figure S1: UV/Visible spectra showing the likeness between the form I (1) and form II (2). The plots are staggered along the y-axis for clarity.

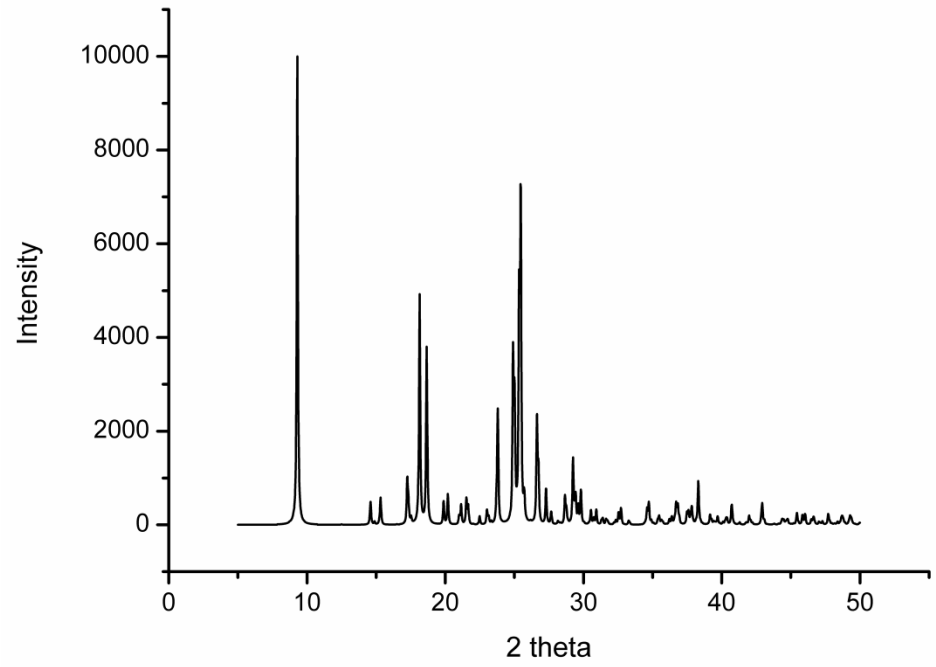

Figure S2. Theoretical powder diffraction pattern calculated from structural data file of Metacetamol II using Mercury 3.0.

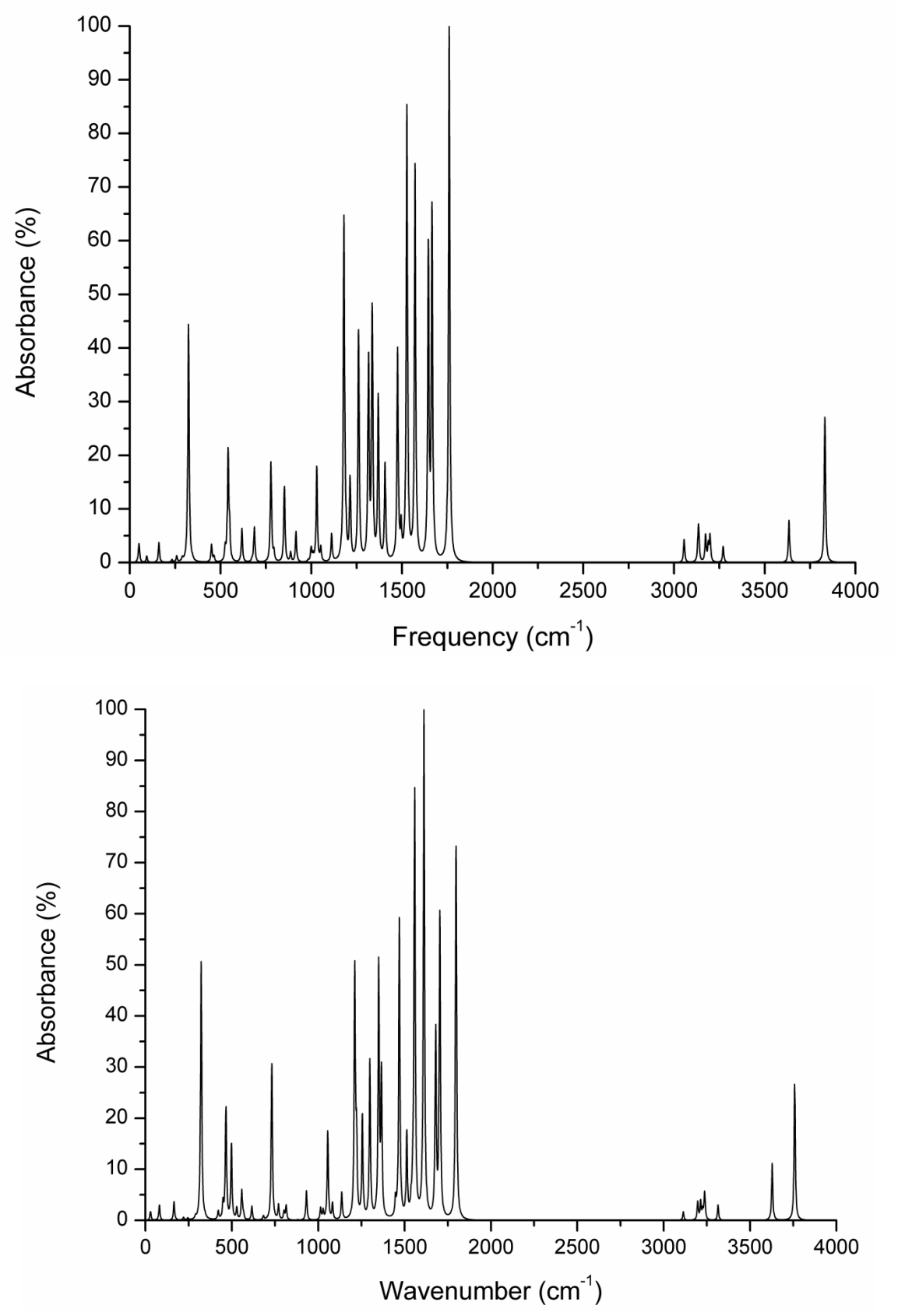

Figure S3. Calculated spectra for Metacetamol molecule in gas phase using B3LYP 6-31+G(d,p) (upper plot), and MP2, 6-31G(d)) (lower plot) level of theories. Highest vibrational modes are assigned to the vibrations of free NH and phenyl -OH groups. Modes are 3633cm^{-1} - NH, 3831cm^{-1} - OH using B3LYP and 3627cm^{-1} - NH, 3758cm^{-1} - OH using MP2. In gas spectra -OH group that is not involved in any H-bond has higher wavenumber; this gives a strong reason to assign 3327 cm^{-1} and 3398 cm^{-1} bands to -NH vibration mode. Vibration modes were assigned from normal mode animation.