Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

In-situ high pressure study of an elastic crystal by FTIR spectroscopy

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S1. Experiments details:

Materials. All the compounds were purchased from Sigma-Aldrich. Commercially available solvents were used as received without further purification.

Single crystal preparation: Long and acicular, 3-5 mm long and 0.02-0.05 mm thick, elastic bendable crystals of DBA were prepared by adding one equivalent each of the corresponding 2,3-dichlorobenzaldehyde and 4-bromoaniline in hot methanol followed by slow evaporation of the solution at ambient conditions.

In-situ high pressure FTIR experiment:

Defect free selected crystals were used for single crystal X-ray (SCXRD) and HP-FTIR studies. In-situ high pressure FTIR spectra were recorded using Bruker's VERTEX80V Fourier transform infrared spectrometer attached with a HYPERION 2000 infrared microscope with 15x objectives equipped with a mid-infrared globar source and HgCdTe detector. The reference spectra were recorded using pure KBr inside DAC (diamond anvil cell). The resolution was kept 4 cm^{-1}. The high pressure FTIR measurements on DBA crystals were carried out using a short symmetric DAC (diamond anvil cell), equipped with type IIA diamonds and KBr as a pressure transmitting medium. Figure S1 shows lowest pressure (~0 GPa) FTIR spectrum of DBA crystal recorded inside DAC. The sample was filled inside a 150-micron size hole in 50-micron thick gasket. Pressure was measured by ruby calibration system.[1] Both the sample as well as reference spectra were normalized for diamond contribution. The sample transmittance spectra were obtained after background correction using the reference spectra.

Figure S1. FTIR spectrum of DBA crystal recorded inside DAC at 0 GPa.

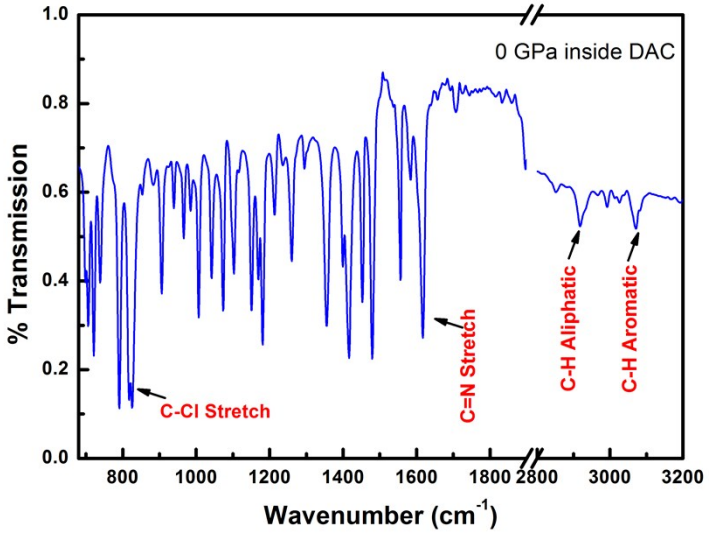


Figure S2. FT-IR spectra in the 600-3600 cm^{-1} region of the DBA crystal on compression to 13.8 GPa pressure from ambient pressure.

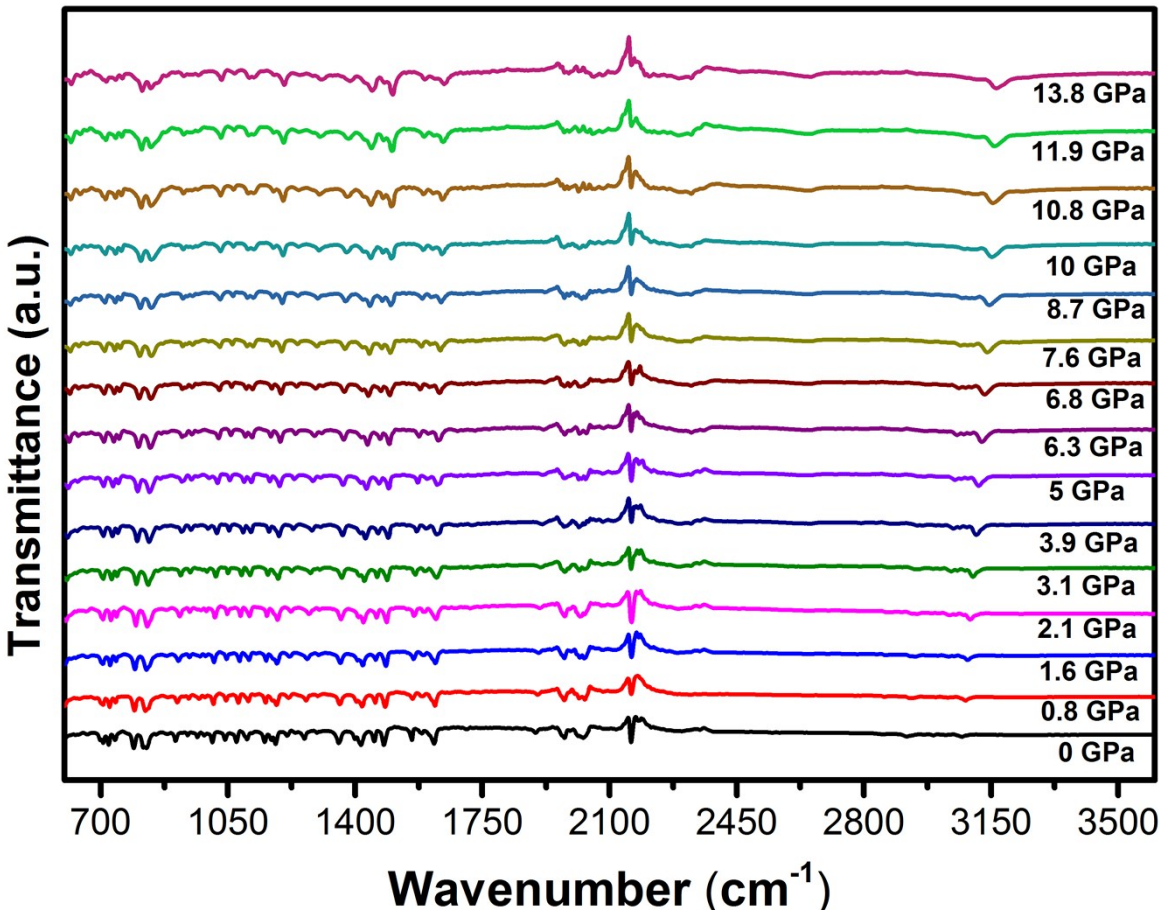


Figure S3. Selected FT-IR spectra in the 600-1000 cm^{-1} region of the DBA crystal on compression to 13.8 GPa pressure from ambient pressure. The orange shaded bar represents the C-Cl stretching mode on compression.

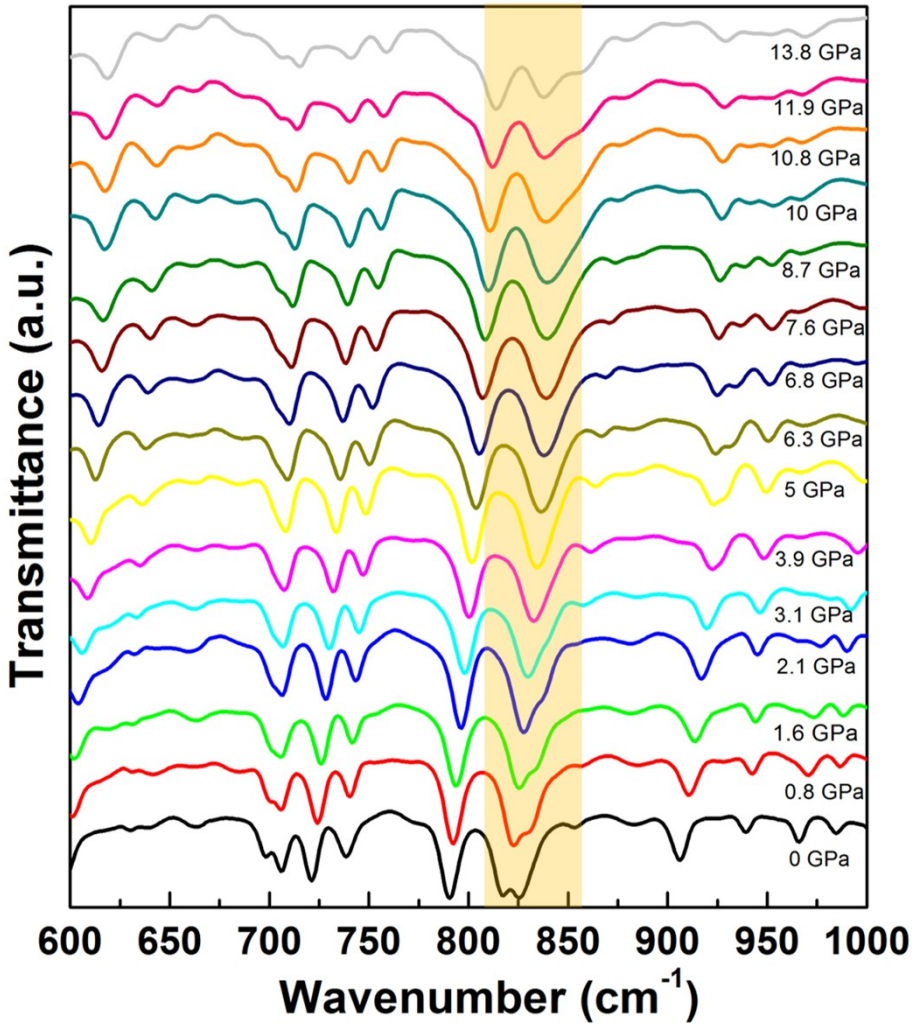
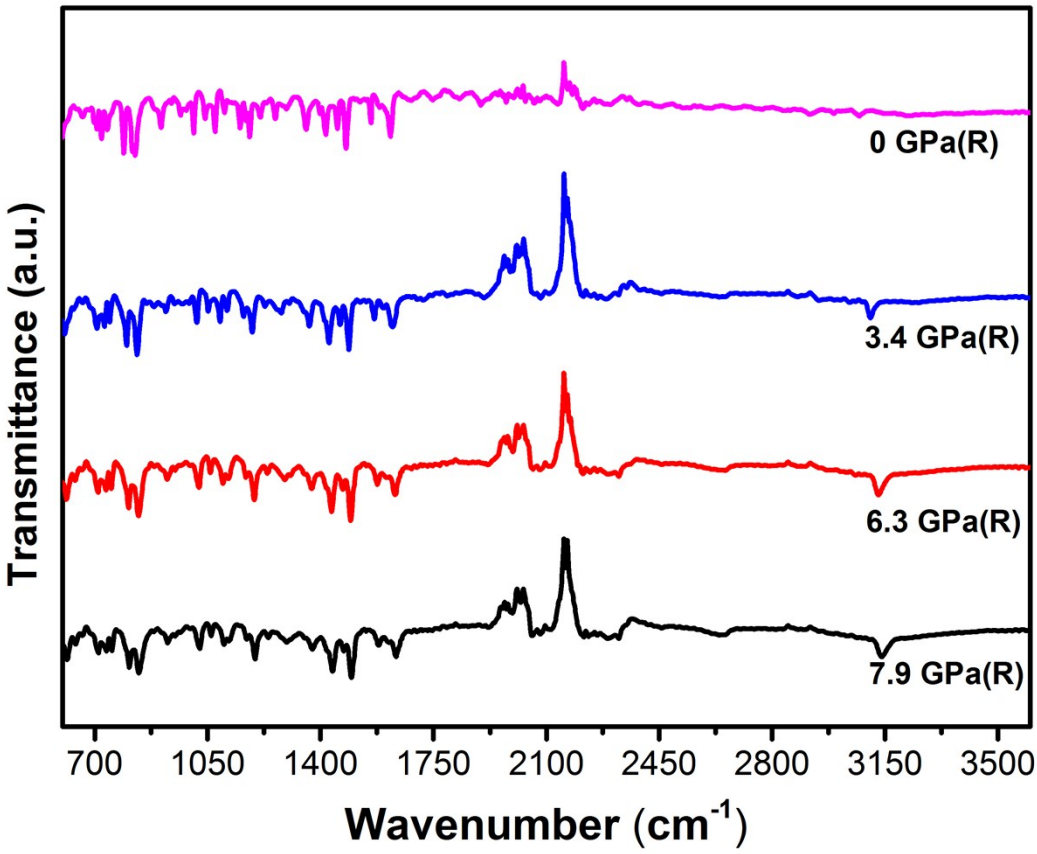


Figure S4. FT-IR spectra 600-3600 cm^{-1} region of DBA crystal on decompression to an ambient pressure from 13.8 GPa. Here, we shown the pressure range from 7.9 to 0 GPa because no major difference appeared from the range of 13.8 to 7.9 while decompression.



References:

1. R. A. Forman, G. J. Piermarini, J. D. Barnet and S. Block, *Science*, 1972, **176**, 284-285.