

Supplementary Material

Destabilisation of Hydrogen Bonding and the Phase Stability of Aniline at High Pressure

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Figure S1: Observed inelastic neutron scattering spectrum of aniline (red)⁶⁷ compared to the one calculated using periodic DFT (blue)

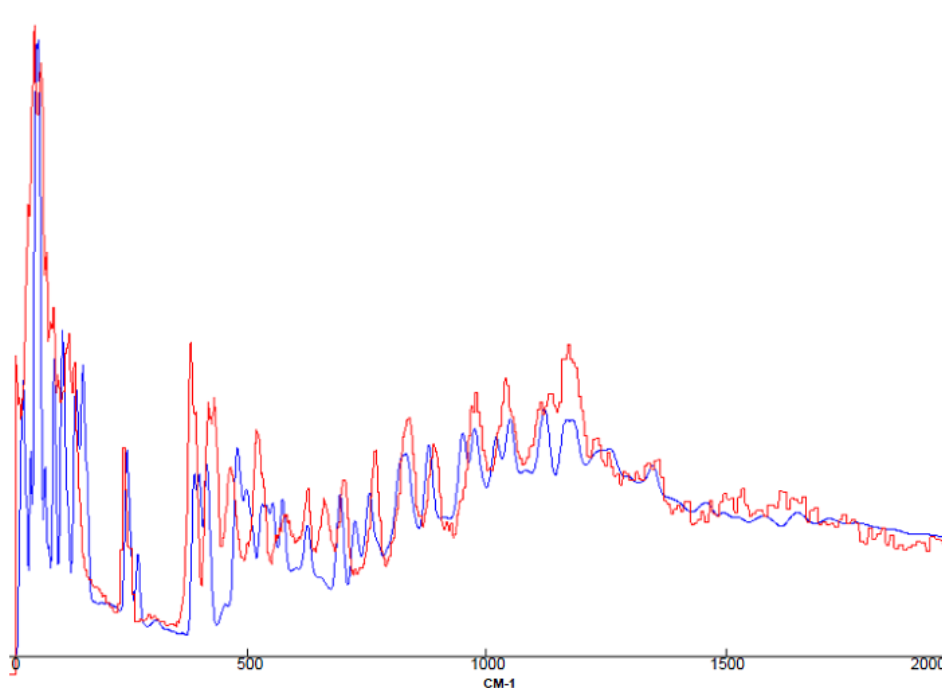


Figure S2: Hydrogen bond geometry in aromatic amines. The search was conducted by constructing two aniline units connected by an NH...N hydrogen bond. Only organic structures were searched, with $R < 0.075$, with 3D coordinates determined and no disorder, errors or powder structures. H-atom positions were normalised, and distance ranges for H...N and N...N contacts were 0 – 3.5 and 0 – 4.0 Å, respectively. Angle limits for NH...N were 120 – 180° (see P.A. Wood, F.H. Allen and E. Pidcock, *CrystEngComm* (2009), **11**, 1563-1571. This search yielded 332 hits and 517 data points.

