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Supporting Information

Sensitizing Explosives Through Molecular Doping

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SI 1. PXRD Data

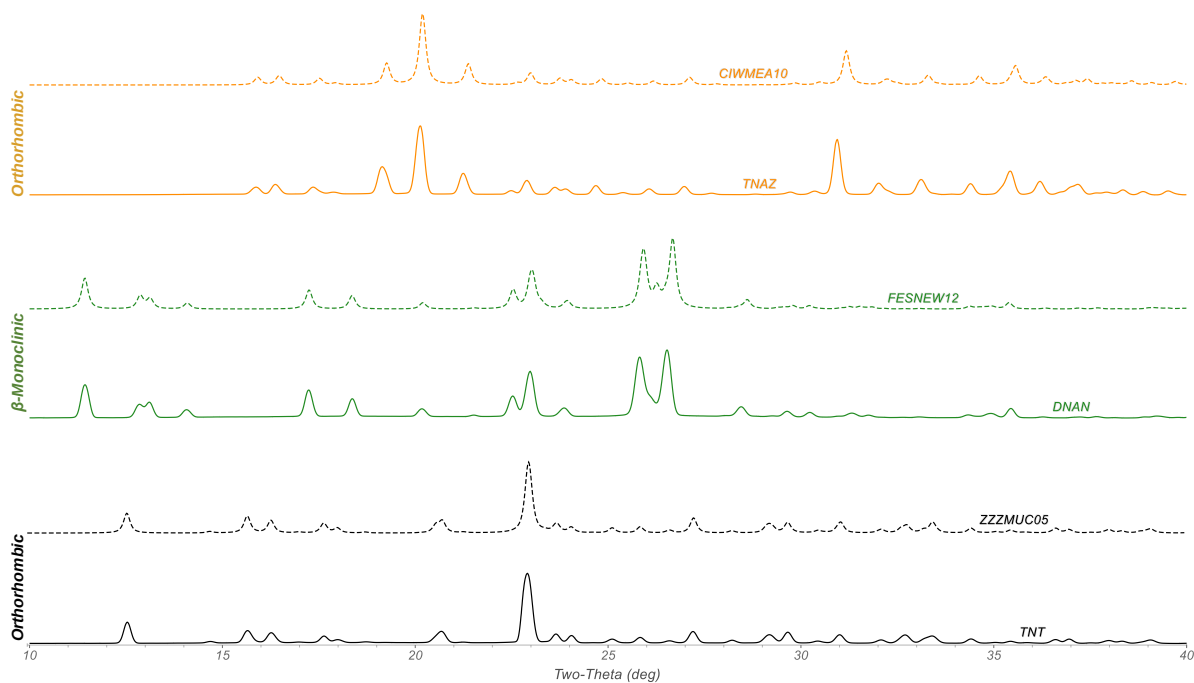


Figure S1. Secondary energetics crystallized from melt. Each adopts a known form as shown by comparison to simulated PXRD patterns (peak setting FWHM: 0.2) corresponding to the Cambridge Structural Database (CSD) reference codes listed.

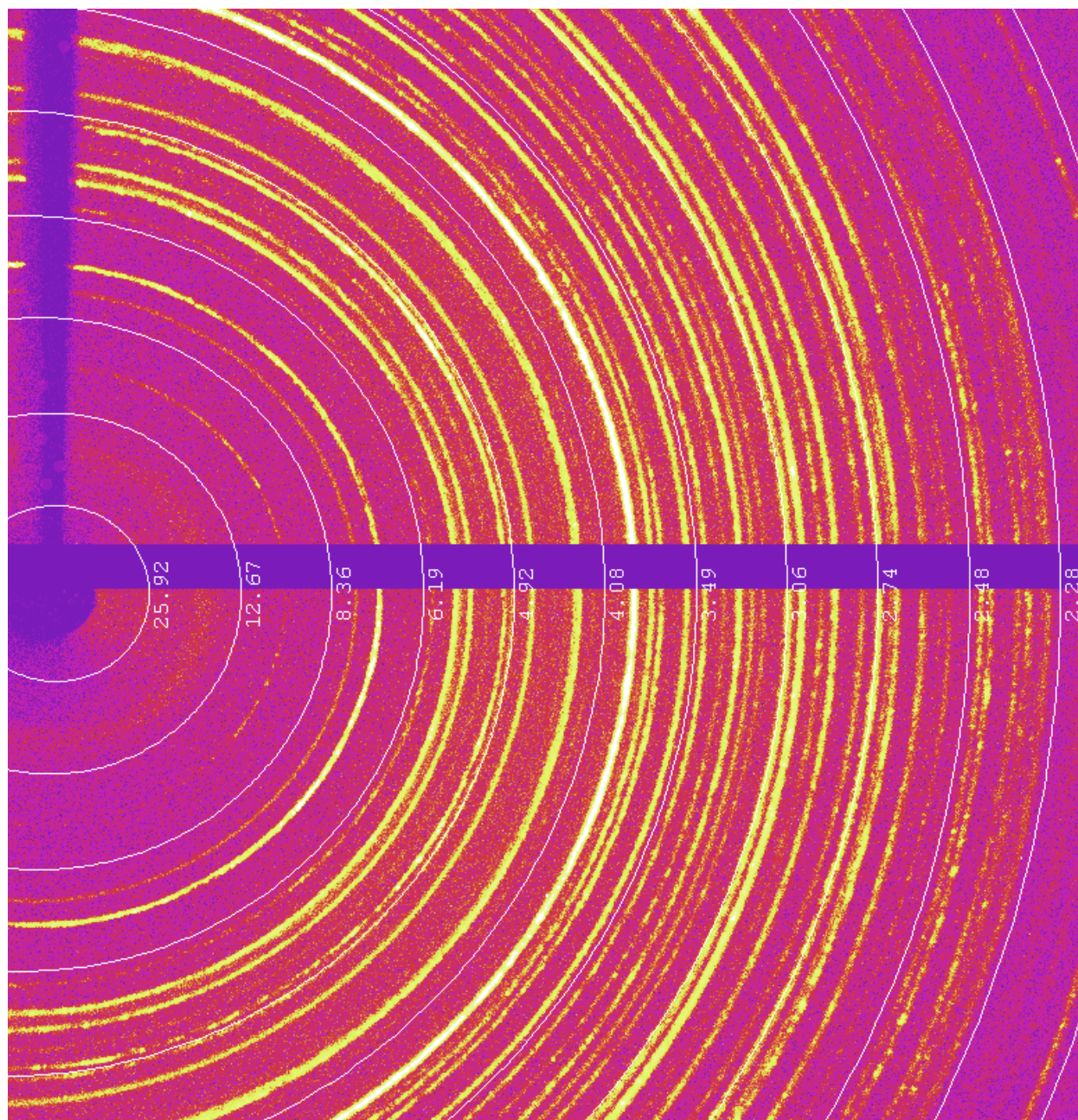


Figure S2. A representative 2D-powder pattern collected using Gandolfi moves for powders to minimize effects of preferred orientation (sample shown is 10% CTA in TNT). 1D-powder patterns were extracted using CrysAlisPro v42.75a for analysis.

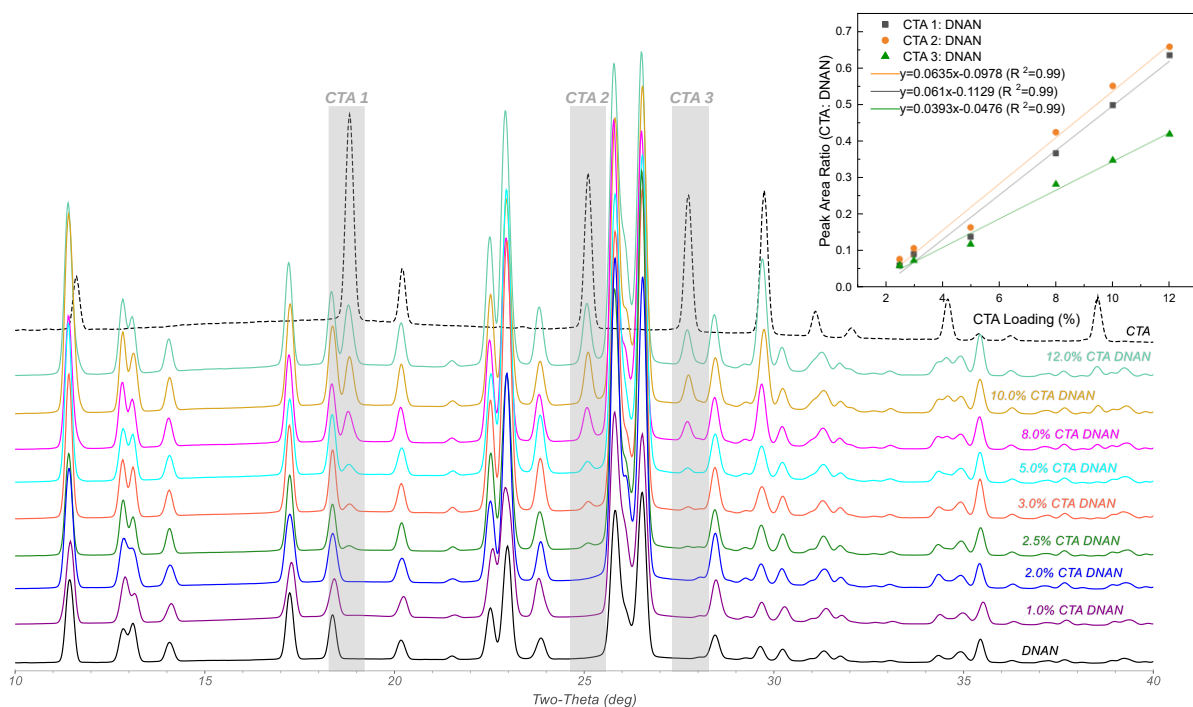


Figure S3. PXRD patterns of pure DNAN, pure CTA, and various loadings of CTA into DNAN (grey boxes emphasize unique diffraction peaks of CTA). The inset image represents maximum dopant loading extrapolation based on peak area ratios of three CTA peaks to a DNAN reference peak.

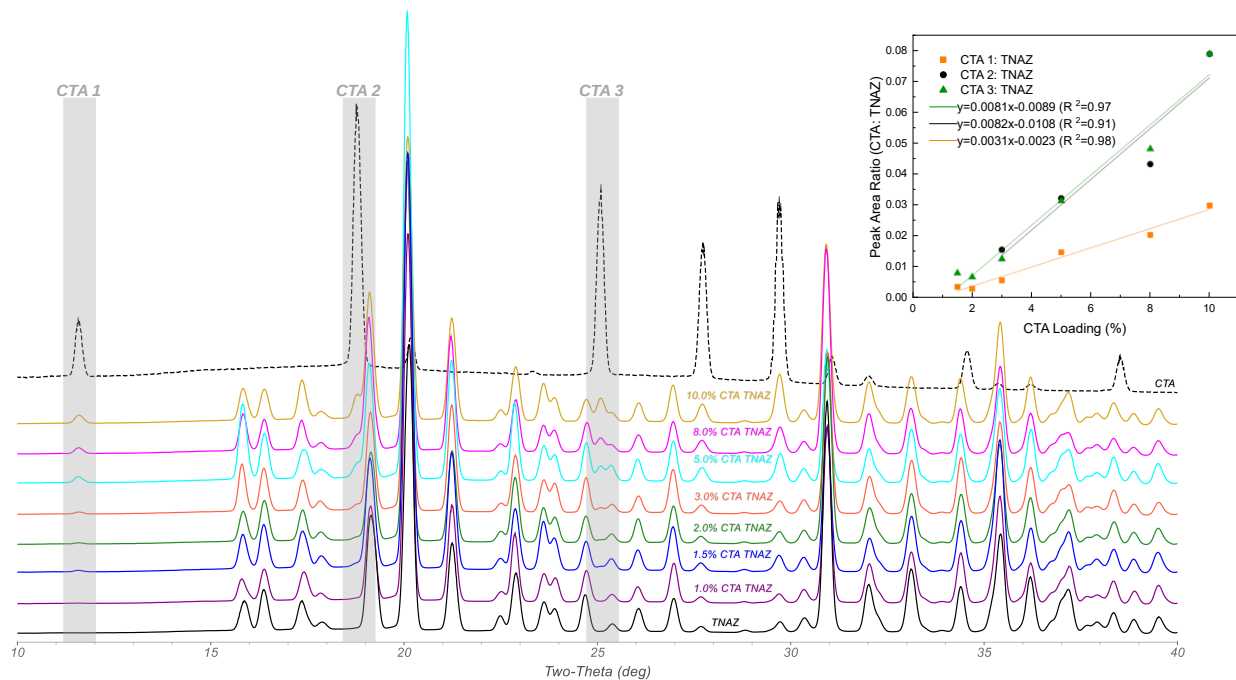


Figure S4. PXRD patterns of pure TNAZ, pure CTA, and various loadings of CTA into TNAZ (grey boxes emphasize unique diffraction peaks of CTA). The inset image represents maximum dopant loading extrapolation based on peak area ratios of three CTA peaks to a TNAZ reference peak.

SI 2. IR Data

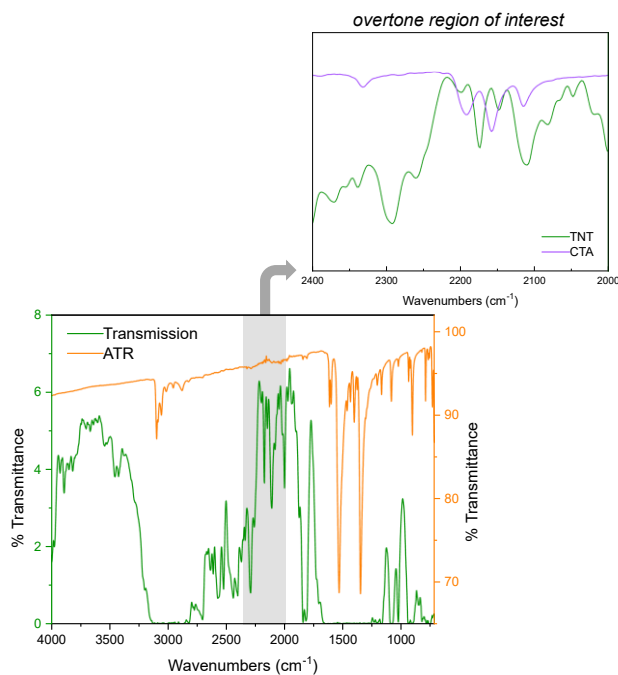


Figure S5. Transmission infrared spectroscopy collection mode of TNT (host compound) saturates mid-infrared regions when compared to an ATR collection. CTA is an excellent model dopant because it possesses strong and unique vibrational stretches in the overtone region of the host which are not saturated in transmission mode.

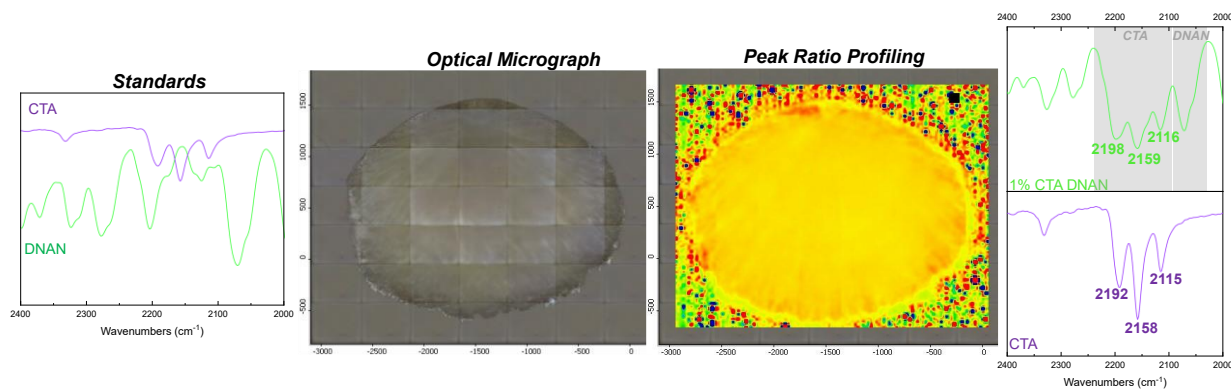


Figure S6. DNAN melt cast with 2% CTA is mapped using transmission IR microspectroscopy to verify CTA incorporation into host. Peak ratio profiling is used to check for CTA present throughout the entire sample. The uniform color distribution of the profile represents uniform peak area ratios of the CTA region of interest to DNAN overtone (highlighted in grey boxes). A representative 2% spectrum is analyzed for shifts in CTA primary bands to further support molecular doping.

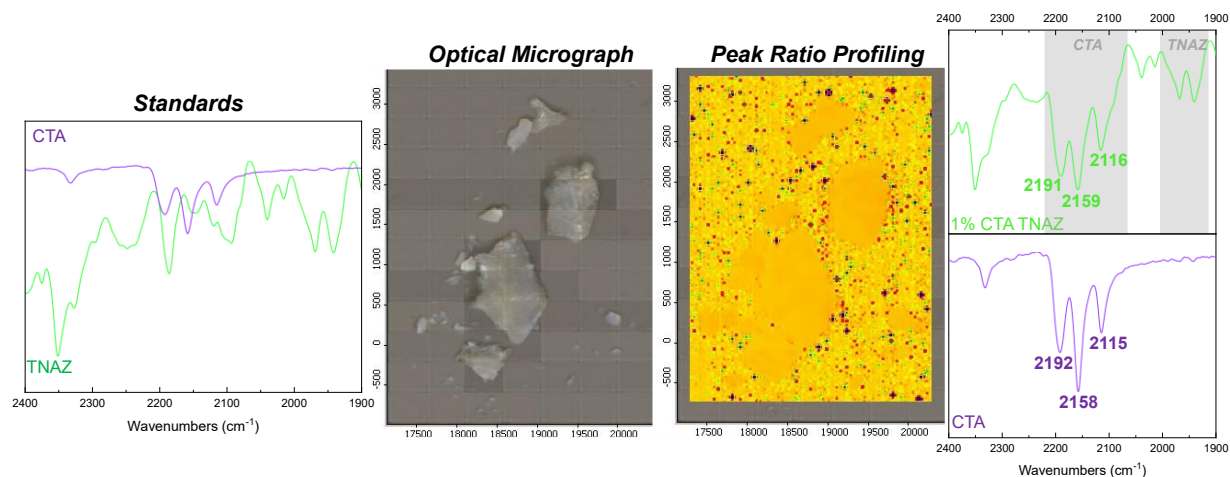


Figure S7. TNAZ melt cast with 1% CTA is mapped using transmission IR microspectroscopy to verify CTA incorporation into host. Peak ratio profiling is used to check for CTA present throughout the entire sample. The uniform color distribution of the profile represents uniform peak area ratios of the CTA region of interest to TNAZ overtones (highlighted in grey boxes). A representative 1% spectrum is analyzed for shifts in CTA primary bands to further support molecular doping.

SI 3. Raman Data

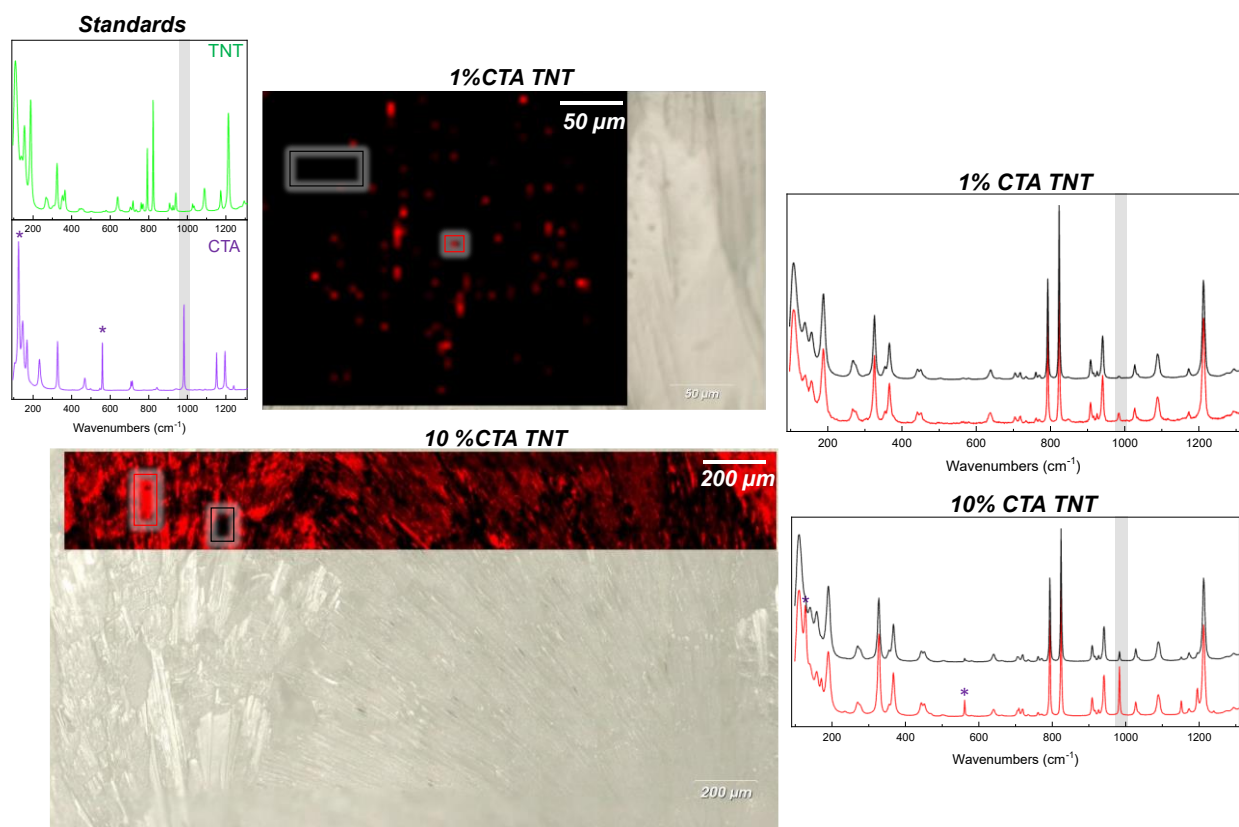


Figure S8. Raman mapping of 1% vs. 10% CTA in TNT that shows distribution of CTA across melt. Representative spectra are shown for each loading based on regions of average CTA signal (color-coded black) and high CTA signal (color-coded red). In addition to the main CTA peak identified in average signal (grey box), additional CTA peaks (*) can be found in higher concentration areas.

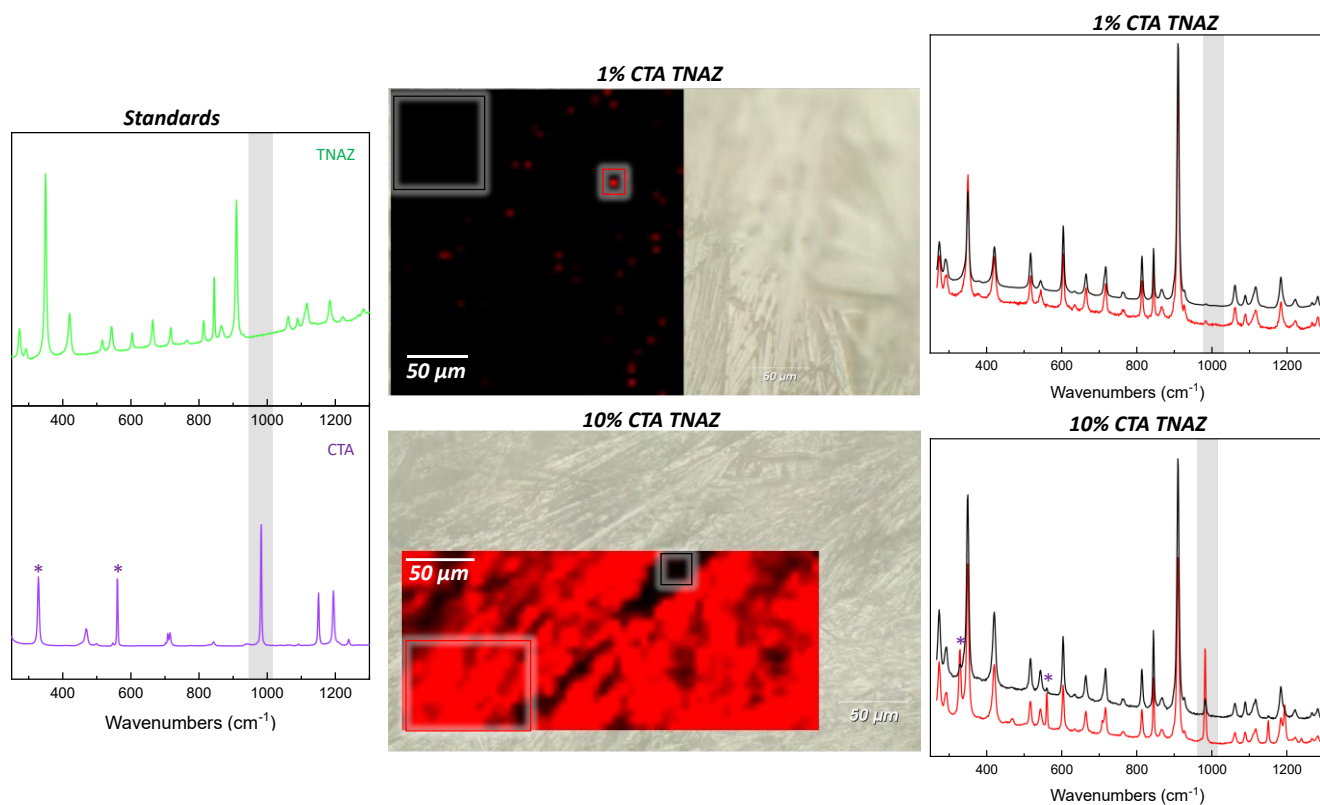


Figure S9. Raman spectra of TNAZ vs CTA, with peak of interest highlighted by a grey box. Mapping of 1% vs. 10% CTA in TNAZ shows distribution of CTA across melt. Representative spectra are shown for each loading based on regions of average CTA signal (color-coded black) and high CTA signal (color-coded red). Additional CTA peaks (*) can be found in higher concentration areas.

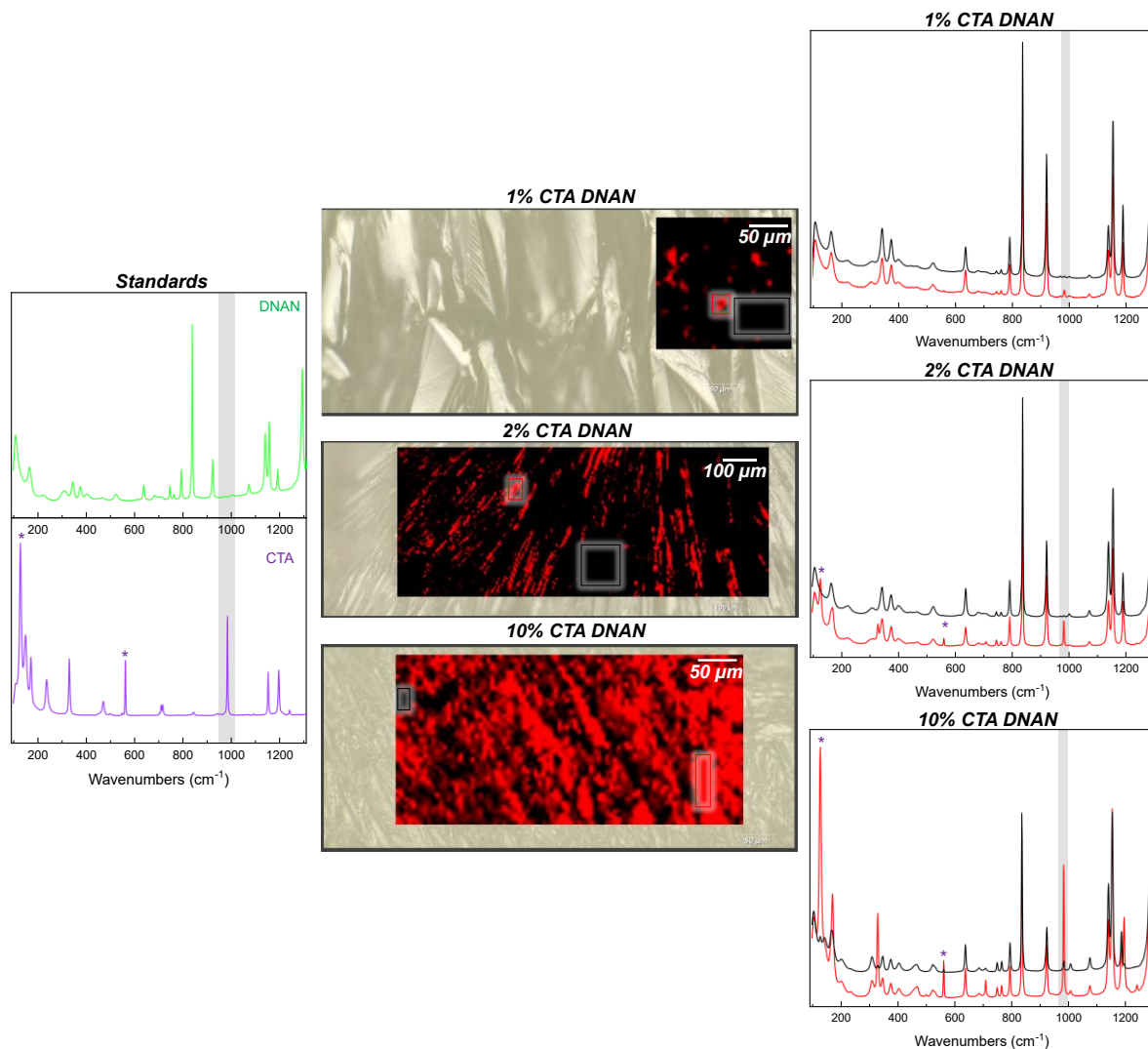


Figure S10. Raman spectra of DNAN vs CTA, with peak of interest highlighted by a grey box. Mapping of 1% vs. 2% vs. 10% CTA in DNAN shows distribution of CTA across melt. Representative spectra are shown for each loading based on regions of average CTA signal (color-coded black) and high CTA signal (color-coded red). Additional CTA peaks (*) can be found in higher concentration areas.