

**Materials Characterization Using A Novel Simultaneous Near-Infrared/X-ray
Diffraction Instrument**

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X-ray powder diffraction (XRD) is utilized for determination of polymorphism in crystalline organic materials. Though convenient to use in a laboratory setting, XRD is not easily adapted to in situ monitoring of synthetic chemical production applications. Near-Infrared spectroscopy (NIR) can be adapted to in situ manufacturing schemes by use of a source/detector probe. Conversely, NIR is unable to conclusively define the existence of polymorphism in crystalline materials. By combining the two techniques, a novel simultaneous NIR/XRD instrument has been developed. During material's analysis, results from XRD allow for defining the polymorphic phase present, and NIR data are collected as a fingerprint for each of the observed polymorphs. These NIR fingerprints will allow for the development of a library, which can be referenced during the use of a NIR probe in manufacturing settings.