TERAHERTZ PULSED SPECTROSCOPY OF PHARMACEUTICAL MATERIALS

D. A. NEWNHAM, P. F. TADAY, D. D. ARNONE, and M. PEPPER, *TeraView Limited, 302/304 Science Park, Cambridge, CB4 0WG, United Kingdom*.

Terahertz pulsed spectroscopy (TPS) is a recently developed quick, simple, and versatile technique for analyzing the chemical composition and physical form of a wide range of solid, liquid, and gaseous materials. Portable TPS systems using room temperature sources and detectors can now readily access the 'terahertz gap' with broadband coverage from 50 GHz to 4 THz (1.3 cm^{-1} to 133 cm^{-1}). For the first time the unique properties of terahertz radiation can be readily exploited in spectroscopy and imaging.

TPS accesses low energy transitions including large-amplitude torsional vibrations (intra-molecular), intermolecular interactions such as hydrogen bonding, molecular rotations, and phonon bands. For solids it is often uniquely sensitive to the amorphous/crystalline state, hydration or water content, and polymorphic form of the material. This has allowed us to present a detailed investigation of the polymorphs of the important drug compounds ranitidine hydrochloride and carbamazepine. Full exploitation of TPS requires new spectrum libraries for identifying materials, evaluation of chemometric algorithms for quantitative analysis, and technical developments including accessories for non-contact online sampling in real-time.

Recent developments in TPS will be presented including examples from a database of terahertz absorbance spectra for common materials. The unique terahertz signatures of target chemicals are complemented by the highly transmissive properties of common packaging materials including many plastics, allowing new sampling strategies to be considered. Quantitative studies demonstrate how multivariate analysis of terahertz spectra with established spectroscopic software can yield valuable multi-component information about active ingredients and excipients in pharmaceutical raw materials and products.