Introduction
IR spectroscopy is a useful tool for group chemical species identification of a wide variety of sample materials, particularly for the classification of "organic" chemical materials based upon carbon atoms being present in the molecular structure. Many plastic and polymeric type samples which can be included in the category of organic molecular materials can be classified into a particular “family” groupings and it is possible to identify the sample family types both qualitatively and quantitatively by use of the Attenuated Total Reflectance (ATR) technique as an IR measurement.

Application
The Specac Quest ATR accessory with diamond crystal puck was used for measurement of a variety of plastic/polymer sample types. Use of this accessory and the ATR technique for measurement obviates the need to specifically prepare the sample types for analysis, which may usually be the case for allowance of a transmission spectral analysis to be performed. In many instances for an ATR measurement, the polymer sample form if presented as a bead, pellet, fragment, shard or rod, etc., can simply be positioned correctly over the ATR crystal as is and clamped into position to make excellent contact with the ATR crystal using an anvil and force arm assembly to obtain a reproducible and consistent ATR spectrum for the sample type.

Equipment and Method
For the ATR measurement of various polymer samples chosen and to obtain a spectral range for the sample between 4000cm⁻¹ to 400cm⁻¹, the Quest ATR Accessory (p/n GS10800-B) was used with the single reflection AR coated diamond crystal puck on its optical unit. The stainless steel flat anvil option was fitted to the force arm assembly for use against each sample type for correct and consistent contact to the diamond ATR crystal.

The ATR spectra were collected on a Thermo Nicolet iS5 instrument using the standard room temperature detector system set a resolution of 4cm⁻¹ for 32 scans.

13 plastic/polymer type materials were taken as examples to be studied using the Quest ATR Accessory. The sample types used for the studies are listed in table 1.

The samples used for this study are shown from the following images as to their form for sample handling with the Quest ATR Accessory.
From the 13 different samples chosen to study and use, there are 7 different basic polymer family types. They have been colour coded as similar family types for their sample number as seen in the table (e.g. the 2 polycarbonate type samples of the the sample types are coded for a red colour).
Spectrum Quest1 - Sample 1 - PVC Classified Type Material

Spectrum Quest2 - Sample 2 - PVC Classified Type Material
Spectrum Quest3 - Sample 3 - Polycarbonate Classified Type Material

Spectrum Quest4 - Sample 4 - Polypropylene Classified Type Material
Spectrum Quest5 - Sample 5 - Polyester Classified Type Material

Spectrum Quest6 - Sample 6 - Polypropylene Classified Type Material
Spectrum Quest7 - Sample 7 - Polyethylene Classified Type Material

Spectrum Quest8 - Sample 8 - Polyethylene Classified Type Material
Spectrum Quest9 - Sample 9 - Polycarbonate Classified Type Material

Spectrum Quest10 - Sample 10 - Cellophane Classified Type Material
Spectrum Quest11 - Sample 11 - Polystyrene Classified Type Material

Spectrum Quest12 - Sample 12 - PVC Classified Type Material
**Discussion**

The 13 individual ATR spectra collected for the plastic/polymer samples are indicative of the family type of the polymer material. The spectra representative of the same family type of polymer material show them to be similar, but there are some subtle unique features for each spectrum to enable the particular sample to be distinguishable from another sample type.

Of the 7 different polymer family sample types of spectra collected, 4 types can be compared from an overlay of their individual spectra (only one sample type for polyester, cellophane and polystyrene family type for the examples taken were measured). The sample spectra were compared for overlay are:-

- Samples 1, 2 and 12 for a PVC family type polymer material.
- Samples 3 and 9 for a Polycarbonate family type polymer material.
- Samples 4, 6 and 13 for a Polypropylene family type polymer material.
- Samples 7 and 8 for a Polyethylene family type polymer material.

The overlaid spectra have been presented between 3800cm⁻¹ to 500cm⁻¹ and have all been fully scaled for the strongest absorbance peak in the spectrum.
Samples 1 (blue), 2 (purple) and 12 (red) for a PVC family type polymer material

Samples 3 (red) and 9 (pink) for Polycarbonate family type polymer material
Samples 4 (purple), 6 (green) and 13 (red) for a Polypropylene family type polymer material.

Samples 7 (blue) and 8 (red) for Polyethylene family type polymer material.
Conclusion
The Specac Quest ATR Accessory using a diamond ATR crystal puck can be used to discriminate for different plastic/polymer types from a surface reflectance measurement. Use of the ATR technique allows for minimal sample preparation and in all cases for the sample types examined here, they were introduced “as is” for contact to the ATR crystal from the specific sample form as presented.

Comparison of the polymer family types (e.g. PVC with PVC and polypropylene with polypropylene), shows both similarities and differences from the ATR spectra alone. The differences seen in the ATR IR spectrum may be used to discriminate from one particular sample type to another and as such, an ATR IR measurement may be all that is required as a measurement technique to identify and determine for a particular polymer type material.

The ATR technique is a surface measurement of a sample type with typically a penetration depth of circa 2 microns into a sample surface using a diamond (or ZnSe) crystal, giving an effective pathlength measurement distance of circa 4.5 microns for the sample for a single reflection event of the sample area under study. From an ATR measurement of a plastic/polymer type sample, although it may be possible to determine the polymer family type, the sensitivity of the measurement for the effective pathlength allowed may be insufficient to determine any specific sample constituents (additives, fillers, etc.) in the make-up of the polymer material that are present at a low concentration. Therefore it may be necessary to create a thin film of the plastic/polymer sample for transmission study from a suitable film making accessory (See - Specac Application Note 43).

Acknowledgement
The study was carried out by: C. Moss, Specac Limited, Orpington, Kent, UK.