**Washington State Crime Laboratory**

Infrared Spectral Library of Automotive

Paint Pigments (4000 – 250 cm-1)

Most of the pigments in this library are used in automotive paint, although there are also several related pigments that are not.  The non-automotive pigments are mostly some from the same chemical family as those used in automotive paint and the intent of collecting these was to determine how readily their absorptions could be distinguished from those that are used for automobiles.  Along with the common name of each pigment (which is also the filename), the Colour Index number (which is the universal generic code), the manner in which the pigment was analyzed, the supplier, and the product name are usually given in the description text that accompanies each spectral file.

Spectra of pigment powders were obtained in one of five ways: (1) Analyzed neat in a miniature diamond anvil cell (DAC); (2) Ground with excess CsI, in the DAC; the reference spectrum was a sample of ground CsI in the DAC; (3) Analyzed neat, as a film pressed onto a single anvil of the DAC; (4) Ground with excess CsI and pressed onto a single anvil of the DAC; the reference spectrum was a sample of ground CsI pressed onto this same anvil; and (5) Mixed gently with excess pre-ground CsI and analyzed using DRIFTS; DRIFTS reflectance spectra were transformed to the Kubelka-Munk format (similar to an absorbance spectrum), then converted to a logarithmic (%T) format to give relative absorption intensities similar to those obtained in transmittance.  For all samples, spectra were scaled (in absorbance or in Kubelka-Munk) so that the strongest absorptions had a transmittance value near 10% transmittance and the baseline was set near 99% transmittance.  Baselines were not flattened.

All of the inorganic pigments were analyzed with the DAC and most of the organic pigments were analyzed using DRIFTS.  It should be noted that unlike ATR and some other reflection methods, band peak shifts do not occur using DRIFTS.  In most cases, spectra were compared to data in An Infrared Spectroscopy Atlas for the Coatings Industry for those pigments compiled in this collection (Infrared Spectroscopy Committee of the Chicago Society for Coatings Technology. An infrared spectroscopy atlas for the coatings industry. Philadelphia: Federation of Societies for Coatings Technology, 1980).  The main reason that organic pigments were analyzed using DRIFTS was that several of them—especially the benzimidazolones, but a few others as well—were found to be very sensitive to pressure.  Grinding such powders with CsI or pressing them in the DAC resulted in very noticeable spectral changes, possibly resulting from changes in crystal structures (many of the organic pigments are polymorphic and can occur in two or more crystal forms) or tautomeric transitions.  Some of the spectra in An Infrared Spectroscopy Atlas for the Coatings Industry also show these spectral changes, as many were obtained of CsI pellets pressed from powders ground in a Wig-L-Bug (a mechanical grinder); very strong absorptions of adsorbed water are also evident in some of these Atlas spectra.

Most of the spectra were acquired using a Digilab extended range (4000 to 200 cm-1) FTS-7 FT-IR spectrometer; a few were obtained on a Nicolet Nexus 670 instrument (4000 to 250 cm-1).  All data were collected at a resolution of 4 cm-1.  To minimize noise levels in the far-infrared region below 300 cm-1, at least 1000 scans were averaged for both sample and reference spectra using the DAC and at least 100 scans using DRIFTS.

The titanate pigments are based on rutile (TiO2) and they all have very similar spectra to rutile.  Although there are minor differences between the absorptions of various commercial products of nickel titanate, these are probably not useful for determining manufacturer as it was not determined if lot-to-lot variations within a given product produced reproducible data. Most of the titanate pigments also produced pronounced scattering, as evidenced by the strongly sloping baselines of their spectra.  These are also observed for spectra of most automotive paints containing these pigments.

More information about the pigments in this collection is provided in the PDF reprints of the seven Journal of Forensic Sciences papers that describe their identification and use in automotive paints.