CHEMIR
Analytical Services

December 5, 2007

Mr. Christopher Kringle
Santa's Workshop
12 Days Lane
North Pole

Re: Deformulation of a Christmas Tree
Chemir Analytical Job #: 65754

Dear Mr. Kringle

Per your request, we have completed the qualitative deformulation of a Christmas tree using Gas Chromatography with Mass Spectrometry (GC/MS), Gel Permeation Chromatography (GPC), Nuclear Magnetic Resonance Spectroscopy (NMR), Fourier Transform Infrared Spectroscopy (FT-IR) and Scanning Electron Microscopy with Energy Dispersive X-Ray Analysis (SEM/EDXA).

SAMPLE LOG-IN

The sample was logged as follows:

SAMPLE DESCRIPTION	CHEMIR ANALYTICAL SAMPLE NUMBER
Tree, Christmas	957235

PROJECT OBJECTIVE

The project objective was to qualitatively deformulate Chemir #957235 for components above 1%.

ANALYSIS CONCLUSIONS

The chief material found in Chemir #957235 was poly(vinyl chloride).

ANALYSIS RESULTS AND DISCUSSION

Sample Receiving

Chemir #957235 was received at Chemir Analytical Services. CHART 1 shows a picture of Chemir #957235 after assembly.

SEM/EDXA Analysis

A Scanning Electron Microscope equipped with an Energy Dispersive X-ray Analyzer (SEM/EDXA) is used to detect and spatially map elements present in a sample. For analysis, the sample is placed into a vacuum chamber and irradiated with a focused, high-energy electron beam. The resulting X-rays emitted from the sample possess discrete energy levels. Because each element emits its own characteristic "fingerprint" of

discrete energy levels, it is possible to identify the elements present in the sample. When used with known standards, a semi-quantitative composition of elements from boron to uranium can be determined.

A portion of Chemir #957235 was analyzed by EDXA. The major element detected was chlorine. Other elements detected at trace levels include cerium, magnesium, silicon, gold and titanium. Confirmation of these trace elements through a quantitative Inductively Coupled Plasma (ICP) analysis may be required. Resulting spectra are attached as CHART 2.

GC/MS Analysis

In Gas Chromatography/Mass Spectrometry (GC/MS), GC resolves the sample components based on volatility, and MS detects and identifies the components. Sample components that interact less with the stationary phase spend less time in the chromatographic column. In MS, the resolved sample components are ionized and separated in a mass analyzer. The fragmentation pattern of a sample component and its computer library match enables sample identification.

A specimen of Chemir #957235 was dissolved in dichloromethane and the solution analyzed by GC/MS. The chromatographic results and corresponding mass spectral matches are shown in CHART 3.1-3.3 and summarized in Table 1.

Table 1 Summary of GC/MS Results for Sample #957235

Retention Time (min)	Tentative Identification	Amount Found
6.27	2-Ethyl-1-hexanol	Trace
10.29	2,6,7-Trimethyldecane	Trace

GPC Analysis

Gel Permeation Chromatography (GPC) is used to determine the molecular weight distribution of polymers. In GPC analysis, a solution of the polymer is passed through a column packed with a porous gel. The sample is separated based on molecular size with larger molecules eluting more quickly than smaller molecules. The retention time of each component is detected and compared to a calibration curve, and the resulting data is then used to calculate the molecular weight distribution for the sample.

A specimen of Chemir #957235 was dissolved in tetrahydrofuran and the solution was analyzed by GPC. As only a single peak is observed in the GPC chromatogram, there is likely only a single polymer in the sample. GPC results are shown in CHART 4 and summarized in Table 2 below.

Table 2. GPC Results for Sample #957235

Parameter	Determined Value
M_n	62224 Da
M_w	125327 Da
M_P	104290 Da
M_z	221284 Da
M_{z+1}	343298 Da
Polydispersity Index	2.014141

NMR Analysis

Nuclear Magnetic Resonance Spectrometry (NMR) is an extremely useful method for material characterization. NMR is a physical phenomenon based upon the magnetic property of an atom's nucleus. NMR studies a magnetic nucleus (most commonly that of a hydrogen atom), by aligning it with a very powerful external magnetic field and perturbing this alignment using an electromagnetic pulse. The response to the perturbation is recorded, with each individual nucleus giving a response specific to its chemical, electronic, and spatial environment.

A portion of Chemir #957235 was dissolved in deuterated tetrahydrofuran and analyzed by ^{1}H-NMR spectroscopy. The ^{1}H-NMR spectrum showed two clusters of signals. The first ranges from 2.0 to 2.6 ppm. The second ranges from 4.2 to 4.7 ppm. The NMR spectrum is a good match for poly(vinyl chloride), considering chlorine as a major component (SEM/EDXA data, see above). The signals at 3.58 and 1.73 ppm are due to the solvent. Also, please note that there are no resonances in the aromatic (7-9 ppm region). This limits the type of materials that could be in the sample. The ^{1}H-NMR spectrum of Chemir #957235 is included as CHART 5.

FT-IR Analysis

Fourier Transform Infrared Spectroscopy (FT-IR) is a tool of choice for identification of materials. In FT-IR, the infrared absorption bands are assigned to characteristic functional groups. Based on the presence of a number of such bands, a material under consideration can be identified. Availability of spectra of known compounds increases the probability of making a positive identification.

A portion of Chemir #957235 was analyzed by FT-IR spectroscopy. The resulting spectrum is a good match for poly(vinyl chloride). In particular, the bands at approximately 1730 cm^{-1}, 1440 cm^{-1}, 1260 cm^{-1}, and 960 cm^{-1} are noted. The spectrum and a reference spectrum of poly(vinyl chloride) are included as CHART 6.1-6.2. The bands in the FT-IR spectrum are assigned in Table 3.

Table 3. FT-IR Spectrum Assignments for Sample #957235

Band Frequency (cm^{-1})	**Band Assignment**
1440	CH_2 symmetric deformation
1260	CH bend
960	CH_2 rock

POTENTIAL FUTURE WORK

- **Inductively Coupled Plasma (ICP) Analysis** – This analysis would provide further detail and precision for the metals and other inorganic components of the sample.
- **Customized Extraction Scheme** – Using a customized extraction scheme, we would attempt to separate minor components from the poly(vinyl chloride) in the sample. This may allow for the identification of plasticizers and other additives.
- **Heated Headspace Analysis** – A heated headspace analysis would allow us to identify any materials that are outgassed from the sample.
- **Colorant Analysis** – Analysis of the colorant by Liquid Chromatography/Mass Spectroscopy (LC/MS) may allow for identification of the colorant.
- **Differential Scanning Calorimetry** – DSC can be used to confirm the presence of poly(vinyl chloride).