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Coal Liquefaction Process Streams Characterization and Evaluation

FIMS Analysis of Direct Coal Liquefaction Process Streams

Topical Report

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PROJECT ASSESSMENT

Introduction

Under subcontract from CONSOL Inc. (U.S. DOE Contract No. DE-AC22-89PC89883), SRI International analyzed selected direct coal liquefaction-derived materials by field ionization mass spectrometry (FIMS). The full report authored by the SRI researchers is presented here. The following assessment briefly highlights the major findings of the project, and describes how FIMS can provide information about the complex chemistry inherent in the conversion of coal to liquid products. These results will be incorporated by CONSOL into a general overview of the application of novel analytical techniques to coal derived materials, and the potential impact of the use of these methods on process economics, at the conclusion of this contract.

Summary

This study was designed to apply the method of field ionization mass spectrometry (FIMS) for the analysis of direct coal liquefaction process-stream samples. The FIMS method was shown to have a high potential for application to direct coal liquefaction-derived samples in a Phase I project in this program.¹ In this Phase III project, the FIMS method was applied to a set of samples produced in HRI bench-scale liquefaction Runs CC-15 and CC-16. FIMS was used to obtain the molecular weight profile of the samples and to identify specific prominent peaks in the low end (160-420 Da) region of the molecular weight profile. In the samples examined in this study, species were identified which previously were recognized as precursors to the formation of high molecular weight structures associated with the formation of coke in petroleum vacuum gas oils.

Program Description

This report describes the work performed at SRI International under a subcontract from CONSOL Inc., Research and Development. CONSOL's prime contract to the U.S. Department of Energy (Contract No. DE-AC22-89PC89883, "Coal Liquefaction Process Streams Characterization and Evaluation") established a program for the analysis of direct coal liquefaction derived materials. The program involves a number of

participating organizations whose analytical expertise is being applied to these materials. The broad objective of this Participants Program is to improve our understanding of fundamental coal liquefaction chemistry to facilitate process improvement and new process development. The specific approach to achieving this objective is to provide a bridge between direct coal liquefaction process development and analytical chemistry by demonstrating the application of various advanced analytical methods to coal liquefaction materials. The methodologies (or techniques) of interest are those which are novel in their application for the support of coal liquefaction and those which have not been fully demonstrated in this application. CONSOL is providing well-documented samples from different direct coal liquefaction production facilities to the program participants. The participants are required to interpret their analytical data in context to the processing conditions under which the samples were generated. The methodology employed is then evaluated for its usefulness in analyzing direct coal liquefaction derived materials. Methods which demonstrate high potential for process stream analysis, and concurrently provide information potentially useful for process design or operation, and thus, those which have the potential for immediate impact on process economics, are further tested by application to a comprehensive set of process-derived materials.

Participant's Methodology

SRI used field ionization mass spectrometry (FIMS) to analyze a set of eighteen process stream samples from HRI CTSL bench unit Runs CC-15 and CC-16. Five of the samples analyzed were filtered process liquids (PFLs). Three samples were viscous process streams obtained from the first-stage internal recycle loop. These samples, designated as "Inter-stage", contain ash and insoluble organic material (IOM). Five samples were pressure filter cakes (PFCs) which contain approximately 50% soluble organic material and 50% ash and IOM. Five samples were light distillates produced by blending the atmospheric still overhead (ASOH) and separator overhead (SOH) materials. The eighteen samples were supplied to SRI with the following analytical information, as available: elemental analyses, ash content, ash elemental analysis, phenolic -OH concentration, calorific value, and hydrogen classes by ^1H -NMR. FIMS spectra were recorded from 48 to 1400 Da. Final ion source conditions were 500 °C and

10⁻⁶ torr. At such conditions, materials with atmospheric equivalent boiling points (AEPB) up to 1400 °C are expected to vaporize completely and materials with AEBPs up to 1600 °C are expected to vaporize at least partially. The FIMS experimental procedure, and a discussion of data quality are described on pages 5-7 of the attached report.

Participant's Major Findings

The following principal observations for the application of FIMS to coal liquefaction materials were reported by SRI. An expanded discussion can be found in the attached report, pages 7-26.

All samples examined gave broad, smooth molecular weight profiles. The distillate sample spectra were confined to the 100 to 300 Da molecular weight range; the other process samples exhibited a molecular weight range of 200 to 1200 Da. The intensity vs molecular weight profiles, excluding those of the distillates, were bimodal in form. No attempt was made to deconvolute the profiles. Chemical structures were assigned to prominent peaks in the 165 to 420 Da range of the FIMS profile. These structural assignments correspond closely to those obtained by other workers with petroleum vacuum gas oils.² They include the compounds identified in Wilsonville two-stage liquefaction resids, which were examined by SRI in a Phase I project in this program.¹

Evidence presented indicates that simple volatilization, not thermal decomposition, is the mechanism for transference of samples from the mass spectrometer inlet to the ionization chamber in the FIMS analysis. SRI reports that the solids-free distillates and PFL samples were 100% (±5%) volatilized and detected, whereas only 44 to 100% (±5%) of the solids-containing PFC and INT samples were volatilized. Thus, the FIMS spectra of the INT and PFC samples may reflect a disproportionate amount of lower molecular weight species than the fully volatilized PFL and ASOH/SOH sample spectra. In addition to the lack of full volatilization, the PFC samples were difficult to sample accurately because of the presence of a lighter oil, possibly filter wash oil.

SRI established that the sum of the odd mass intensities, as a fraction of the sum of the even mass intensities, correlated with the nitrogen

content in the sample. This correlation corroborates other evidence presented by SRI that very little fragmentation occurs in the FIMS analysis.

The influence of process conditions on the molecular weight profiles was examined. The weight average molecular weights ($\bar{M}_w$) for each sample were compared by run period. The effect of increasing reactor temperature in Run CC-16 between periods 5 and 13 resulted in a decreased $\bar{M}_w$ of both the PFL and PFC samples, and an increased concentration of suspected coke precursors. Although the process distillate yield increased with the elevated reactor temperature, the resid was more refractory (based on CONSOL solvent quality data and proton NMR analyses) with a higher percentage of coke precursors (as determined by FIMS). In both HRI runs, the liquefaction process distillate yield was found to correlate inversely with the weight average molecular weight of the PFL samples. The effects of additional process conditions on the properties of the samples from Run CC-15 also were examined. SRI concludes that because there is no clear evidence of nitrogen incorporation in the FIMS spectra of Run CC-15 samples from Periods 8 and 14 (when a dispersed iron catalyst was impregnated in the feed coal using an ammonium nitrate as a participation agent), the elevated N content (determined by CONSOL) in the samples is due to incorporation of ammonia or an amine of MW <48 Da. Additional discussion can be found on pages 17 and 24-25 of the attached report.

CONSOL Evaluation

FIMS was shown to be useful for the analysis of direct coal liquefaction samples in Phase I of the Participants Program. In this Phase III project, FIMS was applied to eighteen samples from two direct coal liquefaction tests. SRI interpreted the FIMS results in the context of the coal liquefaction run conditions.

The speciation of the lowest molecular weight peaks in the FIMS profile provides some important clues to the fundamental chemistry involved in coal processing. It is likely not coincidental that the same compounds are found in other fossil fuel derived materials (such as petroleum vacuum gas oils), and it is probable that these compounds, as coke

precursors, are indicators of resid reactivity. FIMS appears to be an excellent tool to detect and monitor these materials in process stream samples.

In this project, SRI demonstrated that very little thermal decomposition occurred in the probe and very little ion fragmentation occurred in the FIMS analysis; thus, the distribution of molecular weights is representative of the volatilized sample. SRI's results indicate that the molecular weight profiles obtained in this work are not significantly distorted because of the lack of complete sample volatility. This issue was unresolved at the conclusion of the Phase I project; this work resolved this issue and shows that FIMS can be successfully applied to coal-liquefaction samples in support of process development. The capital investment for FIMS equipment is approximately \$250,000. Operating cost are about \$40 per sample. It requires 1.5 to 3 hours for sample preparation and analysis.

Further Application

There are a number of avenues for further application of FIMS for coal liquefaction materials. The correlation drawn between the nitrogen contents of the samples and the FIMS odd-mass profile may be useful for examining hydrodenitrogenation (HDN) in process-derived samples. Examination by FIMS spectra of samples with a wide range of nitrogen contents may be useful. The use of a curve fitting routine may provide further insight into the subtlety of shifts in the molecular weight distributions attributable to processing conditions. Additional investigation of process derived samples for compounds (those which are considered coke precursors) in the lower molecular weight range of the FIMS profile will provide information useful for kinetic and mechanistic modeling of the coal liquefaction process.

SRI suggests several lines of research derived from this work (p. 26-27 of attached report). All are related to further examining the role of the suspected coke precursors identified here in coke formation.

Participant's Statement of Work

The FIMS technique will be used to analyze eighteen samples obtained by CONSOL from the HRI Inc. bench-scale liquefaction unit. The eighteen samples will be supplied to SRI with the following information, as available: elemental analyses, ash content, ash elemental analysis, phenolic -OH concentration, calorific value, hydrogen classes by ¹H-NMR. Sample size will be at least one gram. Five samples will be filtered process streams, three samples will be viscous process streams which contain ash and insoluble organic material (IOM), five samples will be filter cakes which contain approximately 50% soluble organic material and 50% ash and IOM, and five samples will be light distillates.

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SRI International

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FIMS ANALYSIS OF DIRECT COAL LIQUEFACTION PROCESS STREAMS

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SRI Project PYD 4495
Contract No. 01-001-026582
MP 93-190

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SUMMARY

Under a subcontract with CONSOL Inc., SRI International performed field ionization mass spectrometric (FIMS) analysis of 18 coal liquefaction process stream samples.^{1,2} These samples came from liquefaction of a Black Thunder and an Illinois No. 6 coal at Hydrocarbon Research Inc. (HRI) in HRI's two-stage ebullated-bed bench unit 227.³⁻⁷ The samples covered a wide range of distillability and solubility; they included whole interstage liquids, pressure filtered liquids, filter cakes, and atmospheric still distillates. The primary objective of the FIMS analysis was to provide additional composition data about these samples, including changes that result from differing conditions in different run periods. Of particular interest was compositional information related to factors affecting resid reactivity. Analysis of these samples follows on SRI's earlier FIMS analyses, under this same program, of process stream samples from the Wilsonville liquefaction pilot plant.^{8,9} In this report we will repeatedly make reference to these earlier samples.

FIMS analysis was found to give reliable and reproducible data for distillates and for filtered liquid samples. We experienced difficulty in getting reproducible spectra with pressure filter cake samples. The problem was attributed to the fact these samples retain varying amounts of soluble wash oils in the insoluble matrix. An examination of the thermal evolution of various peaks in the FI mass spectra revealed that during FIMS analysis volatiles were released purely by evaporation with very little thermal decomposition in the probe. We also observed that the liquids in these samples were essentially 100% vaporized (i.e., 95% or higher with a 5% error limit); the materials insoluble in the process stream or in the wash oil were vaporized from ~50% to 80%.

The HRI process whole oil or filter cake samples showed broad, smooth, molecular weight profiles ranging from 200 to 1200 Da. The distillate samples spanned a MW range of 100 to 300 Da. As in case of Wilsonville liquefaction resids, the HRI whole oils tended to show a bimodal distribution of molecular weights. However, in the present study, we did not perform mathematical deconvolution to quantify the relative amounts of the two components. Such an exercise could provide useful input for lumped kinetic modeling of coal liquefaction. An inverse correlation was observed between the distillate yield of the process in the various periods and weight-average molecular weight ($\bar{M}_w$) of the PFL samples produced in those periods. Also we found that the sum of odd mass intensities as fraction of the sum of all ion intensities correlated with the nitrogen content of the sample. This correlation reiterates the absence of fragmentation during FIMS analysis, and provides a means of assessing HDN activity with FIMS.

As with the Wilsonville samples analyzed earlier,^{8,9} these HRI samples exhibited certain prominent peaks in the lower molecular weight edge of the mass spectra. These peaks correspond to specific analogs of dihydrophenalene (phenelan) that have been previously implicated as coke precursors in petroleum-derived vacuum gas oils.¹⁰ Interestingly, these components tended to be more abundant in oil samples with high insolubles content. These findings suggests that FIMS can be a useful tool in a systematic effort to monitor and elucidate the chemistry in the build up of coke precursors.

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INTRODUCTION

Under a subcontract with Consolidation coal Company (CONSOL),^{1,2} SRI International performed field ionization mass spectrometric (FIMS) analysis of 18 coal liquefaction process stream samples. These samples were generated at Hydrocarbon Research, Inc. in Runs CC-15 and CC-16 on a Black Thunder and an Illinois No. 6 coal respectively.³⁻⁷ This work was conducted under the Participants' Program of CONSOL's contract (Contract No. DE-AC22-89PC89883) with the U.S. Department of Energy, Pittsburgh Energy Technology Center (PETC) on the characterization of coal liquefaction process streams.^{1,2} Under a previous subcontract, SRI had performed field ionization mass spectrometric (FIMS) analysis on resid samples from the Wilsonville facility and had demonstrated the utility of FIMS in providing information that can be correlated with resid reactivity and processing conditions.^{8,9}

The samples spanned a range of materials from different sampling ports during various periods of the HRI liquefaction runs CC-15 and CC-16 made in HRI's two-stage ebullated-bed bench unit 227.³⁻⁷ They included interstage oils, pressure filter liquids, pressure filter cakes, and separator-atmospheric still overheads (INT, PFL, PFC, and SOH-ASOH, respectively). These samples had already been characterized by CONSOL Inc.,¹¹ by methods that range from standard distillation and elemental analysis¹²⁻¹⁴ to ¹H NMR analysis to define the proton type distribution,^{15,16} to FTIR determination of phenolic -OH distribution.^{14,17} In this report we describe primarily the aspects discussed in the previous phase of this study, namely, molecular weight distributions and nitrogen distributions, the occurrence of prominent individual compounds, and the possible importance of these individual compound types in retrograde reactions. Those FI mass spectra most necessary for the discussion that follows are reproduced in the main body of this report. Sum Spectra for Black Thunder PFL and PFC Samples No. 1 and 2 are illustrative of the full boiling-range samples and are shown in Figures 1 and 2. A complete set of the sum spectra, the vacuum evaporation curves, and the sum spectra pattern tables are reproduced in the Appendix. For PFL and PFC Samples 5 and 6, complete sets of the 12 individual mass spectra (and pattern tables) that make up the sum spectra are also reproduced. Table 1 summarizes some of the FIMS values (percent vaporized, average molecular weight, and the ratios of the sums of odd-mass and even-mass intensities), together with other analytical data taken from information supplied by CONSOL, Inc.¹¹

Table 1
Summary of FIMS Analysis and Other Data for Samples 1-18

Sample No.	Sample Type	Run No./ Period No.	FIMS Volatility (%)	$\bar{M}_W^a$	Sum of (odd/even) ^b	N (wt %) ^c	Distillate Yield (wt %) ^d
CC-15							
1	PFL	8ABC	100 ^e	506	0.37	0.56	64.1
2	PFC	8A	48	450	0.51	0.76	
3	INT	9A	77	529	0.43	0.96	
4	SOH-ASOH	8ABC	(100)	176	0.12	0.40	
CC-15							
5	PFL	11ABC	94	531	0.38	0.54	57.4
6	PFC	11A	50	473	0.55	0.62	
7	INT	12A	100	504	0.46	0.66	
8	SOH-ASOH	11ABC	(100)	179	0.11	0.28	
CC-15							
9	PFL	14ABC	100	526	0.44	0.81	60.2
10	PFC	14A	60	465	0.48	0.81	
11	INT	15A	100	568	0.77	1.05	
12	SOH-ASOH	14ABC	(100)	182	0.20	0.53	
CC-16							
13	PFL	5C	100	557	0.23	0.30	70.2
14	PFC	5C	81	546	0.24	0.39	
15	SOH-ASOH	5C	(100)	192	0.05	0.12	
CC-16							
16	PFL	13C	100	538	0.27	0.35	76.2
17	PFC	13C	44	523	0.34	0.54	
18	SOH-ASOH	13C	(100)	195	0.06	0.09	

a. Weight-average molecular weight.

b. The ratio of the sum of all odd-mass intensities to the sum of all even-mass intensities.

c. Data provided by CONSOL Inc.¹¹

d. C4 - 975°F+ distillate yields were provided by HRI, and represent steady-state performance for that particular run period.

e. The precision of the FIMS total volatility measurement is ± 5 wt%.

B14001.SUM -62 to 501°C No. Av. MW = 395. Wt. Av. MW = 505.
REF NO. 1 (CONSOL) ¹³C-Corrected

Figure 1. Field ionization mass spectrum for Sample No. 1 (Black Thunder Pressure Filter Liquid, HRI Run CC-15, Periods 8A, B, C)

A14002.SUM 30 to 501°C No. Av. MW = 391. Wt. Av. MW = 450.
REF NO. 2 (CONSOL) ¹³C-Corrected

Figure 2. Field ionization mass spectrum for Sample No. 2 (Black Thunder Pressure Filter Cake, HRI Run CC-15, Periods 8A)

WORK PERFORMED AND RESULTS

FIMS INSTRUMENTATION AND PROCEDURES

The analyses were performed using SRI's FIMS instrument, which consists of a foil-type field ionizer interfaced with a 60-degree magnetic -sector mass analyzer and a PDP 11/23 for instrument control, data acquisition, and report production. The spectrometer has a resolving power ($M/\Delta M$) of 1300, although it is capable of scanning up to 3000 Da. In the present study, data were recorded up to 1400 Da, although we have in this report displayed the spectra only up to 1000 Da. The average molecular weights listed are based on data up to 1400 Da. Typically, approximately 30 μg of the sample were taken in a fused-silica capillary tube and introduced into the spectrometer with a heatable direct insertion probe. The samples were heated at a fixed rate (except where a slower rate was dictated by the need to avoid exceeding the ion-counting-rate limits of the instrument) from $\sim -60^\circ\text{C}$ for PFL samples (or from ambient for PFC samples, which were assumed to be much less volatile) to $\sim 500^\circ\text{C}$. The pressure in the ion-source chamber is generally in the 10^{-6} Torr range, although the pressure in the capillary sample is considerably higher. We estimate the sample pressure to be around 10^{-6} Torr. Under these conditions, materials with atmospheric equivalent boiling points (AEBP) up to about 1400°C are expected to vaporize completely, and those with AEBPs between 1400° and 1600°F to vaporize at least partially.^{9,18-20} In practice, what often limits the vaporization of these high boiling materials are the coupling reactions with other species present in the sample. Hence the quoted AEBP limits should be regarded as a rough guide. (Similarly, other pyrolytic reactions can occur that produce volatile species not present as such in the original mixture.) The spectra of the evolving volatiles are continuously recorded, and at the end of a run, they are added to produce a sum spectrum of the total volatiles. Examination of the evolution profiles for any particular mass or group of masses can often indicate the importance of such pyrolytic generation of volatiles and provide additional information about the chemical behavior of the sample.

FIMS VOLATILITY AND REPRODUCIBILITY

As shown in Table 1, the PFL samples were essentially 100% volatile (within the $\pm 5\%$ error limits that the 30- μg sample size places on determination of sample weight loss). In contrast, the PFC samples showed about 50% to 80% volatility under the FIMS analysis conditions, because of the substantial mineral matter and insoluble organic matter they contain. Thus these

data show that materials that are soluble in the process medium are typically 100% volatile under FIMS analysis conditions. This result is entirely consistent with previous experience that *coal-derived* oils are typically close to 100% volatile, while pre-asphaltenes are typically 50% to 80% volatile.

Typically, FIMS reproducibility is very good for homogenous samples having volatilities in the vacuum gas-oil region. Duplicate or triplicate analyses generally show a standard deviation of no more than 5% to 10% for the intensity of any individual peak.²¹ For low boiling samples (i.e., having substantial material of molecular weight 50 to 150 Daltons), it is usually desirable to perform batch inlet analyses to avoid non-repeatable fractional loss of low-boiling components. This loss can occur during pump-down of the variable temperature probe even though it is cooled to about -50°C. All the SOH-ASOH samples in this set were run with a batch inlet to minimize loss of volatiles. Sample No. 4 was run on two separate days (Analyses B14004 and C14004); the reproducibility was very good, as can be seen by examining the spectra shown in the Appendix, with the average variation in individual peak heights being no more than 5%-10%. (Note that the peak at 92 Da is due to toluene that was purposely added to the batch inlet in Sample B14004, since it, and other similar aromatics, tend to raise and stabilize the ionization efficiency for low molecular weight aliphatics. Because these samples contain low molecular weight components of about the same molecular weight as toluene, and because all samples lack a large indigenous peak at 58 Da, acetone was used in the remaining analyses. For any samples containing substantial amounts of aromatics as large or larger than naphthalene, there is no need for such stabilization.²²)

We anticipated that most problems in nonrepresentative sampling would occur with the PFC samples, which were clearly not homogeneous. Therefore, one of these samples (CONSOL No. 6) was run in triplicate. For the first two runs of this sample, we attempted to ensure representative sampling by thoroughly mixing the contents of the vial. We did this by smashing the particles together, then breaking up the cake and taking many small fragments. This approach however did not succeed, as Spectra A14006 and B14006 illustrate (see Appendix): the overall profiles and odd/even ratios are significantly different. Upon seeing this difference, we reconsidered our procedure and realized that in trying to ensure a well-mixed sample, we were presumably squeezing wash oil out of the solid particles to a varying and uncontrollable degree. Therefore, for the third sample, we simply took many small particles, since it is likely that one portion of the filter cake has a different composition than another portion. This expedient may or may not have worked: the spectrum that resulted (C14006) is different from *either* of the other two.

At this point we learned that expelling of wash oil from the apparent solids was causing problems with other analytical techniques, such as nuclear magnetic resonance (NMR). We could devise no simple and effective way to avoid this kind of behavior, given the small size of sample required for FIMS analysis (20-50 μg), and the possibility that the wash-oil content was not constant throughout the filter cake. Thus, the inevitable variations in PFC sampling prevent us from drawing any fine distinctions between individual spectra for the present PFC sample spectra. However, we can make general comparisons between the PFL and PFC spectra as groups, as we do below when we discuss the existence of a more pronounced "mid-mass" hump (around 500 Da) and the higher ratios of odd to even ions. The interstage samples should be intermediate between the PFL and SOH-ASOH and the PFC samples in terms of homogeneity, and the repeat analysis of CONSOL Sample No. 11 (Spectra A14011 and B14011) shows this to be the case.

Evolution Profiles

One of the questions often raised about FIMS is whether we are observing simple vaporization of pre-existing components or whether the observed peaks are a result of pyrolytic generation of volatiles not present in the original mixture. This question is important, since such thermal fragmentation would distort the molecular weight distribution and possibly cause confusion between the chemical changes that occur during the liquefaction process and those that occur in the mass spectrometer inlet. This question can be addressed by examining a part of the normal FIMS data file that is not often discussed, namely, the 12 to 16 individual spectra that are accumulated during temperature programming of the mass spectrometer probe. These spectra are added to form the "sum" spectrum generally presented. These temperature-dependent data can be examined either by making plots of particular individual ion intensities against probe temperature or by plotting a series of spectra. Both of these approaches were taken here for selected ions and samples, as discussed below.

As an example of the first approach, Figure 3 shows the intensities of six of the prominent molecular ions in PFL Sample No. 1 plotted as a function of probe temperature. (The structures to which these and other prominent ions probably correspond are shown in Table 2.) These plots show that ions at 168, 172, 208, 242, 276, and 300 Da appear in sequence as temperature increases. Therefore, they all come primarily from vaporization of components that are pre-existing in the samples.

Figure 3. Intensities of selected ions vs. probe temperature for CONSOL Sample No. 1.

An example of the second approach can be seen in the Appendix, where all 25 individual spectra for PFC Samples No. 5 and 6 are reproduced (Spectra A 14005.000 to .012 and A14006.000 to .011). For consideration of the possible importance of either ion-fragmentation or in-probe pyrolysis, we will discuss the behavior of Sample No. 6. SRI Sample No. A14006 was chosen because as a PFC it has low volatility and has about 25% THF-insolubles. Furthermore, of the three "duplicates" run of Sample No. 6, Spectrum A14006 shows it to have ion intensity below m/z 150 and weight-average molecular weights similar to those of the other two PFC samples, Nos. 2 and 10. A PFC sample was chosen, because in addition to significant non-volatile material, they show as much or more fragmentation as any of the samples, and therefore are the "best" candidates for thermal- and/or ion fragmentation during the heating process. Even with this PFC sample, however, the summed intensity of all ions below 174 Da is only 1.1% of the total ion intensity (see Sum Spectrum A14006). Furthermore, inspection of the 12 individual spectra shows that once the wash-oil remnant is vaporized (i.e. at about 150°C), there is essentially no intensity below 200 Da until temperatures above 400°C are reached. Thus, even with the most non-volatile sample, there is very little fragmentation of any kind, and that which does occur, occurs almost entirely at temperatures above 400°C. Therefore, neither ion- nor thermal fragmentation is significantly distorting the spectra of *any* of the 18 samples included in this study.

The absence of substantial pyrolysis in the probe at temperatures below 400° to 450°C is generally the case when a material has previously been subjected to conditions of equal or greater thermal severity. It is in distinct contrast to the situation, for instance with raw coals, where most of the observed ion intensity is from pyrolysis, rather than from simple vaporization.²⁰

The essential absence of ions from in-probe pyrolysis for the samples in this study does *not* mean that there is no *selection* for low molecular weight components in the FIMS process. Where vaporization is incomplete, those materials that are not vaporized are of course not ionized. What the absence of significant in-probe pyrolysis means is that the ions seen are representative *at least* of those components in the original sample volatile enough to simply vaporize under the high vacuum conditions of the mass spectrometer. As shown in Table 1, the PFL samples were essentially 100% volatile, while the PFC samples showed about 50% to 80% volatility under the FIMS analysis conditions. Thus, for the PFC samples, the vaporization process could very well be selecting for lower molecular weight components. This possibility is discussed in the following section.

Table 2
Prominent Ions in FI Mass Spectra and Their Probable Structures

MZ (Da)	Intensity ^a in Sample No. 1	Probable Structures
168	471
172	576
174	352
180	237
202	1293
208	894
242	1082

Table 2 (cont)
Prominent Ions in FI Mass Spectra and Their Probable Structures

M/Z (Da)	Intensity ^a in Sample No. 1	Probable Structures
276	664
300	337
316	377
340	288
398	188
414	196

^a Intensities are given here in the same units as in the pattern tables, that is, normalized to 100,000 counts as the sum of all ion intensities, after ¹³C correction. Thus an intensity of 1000 corresponds to 1% of the total of all ions.

Molecular Weight Distribution

The PFL materials, as the only full boiling range samples that are homogeneous (and therefore where the possibility of non-representative sampling is eliminated), should have the molecular weight distributions (Table 1) that are most straightforwardly related to coal conversion, distillate yield, and distillate composition. This does appear to be the case. Within these limited sets of PFL samples, there are good inverse correlations between the weight-average molecular weight ($\bar{M}_w$) and the distillate yield of the process, as shown in Table 1 and Figure 4. [Note that for samples of this type (i.e., having mass distributed principally between 200 and 1000 Da), a change of 30 mass units in weight-average molecular weight is a substantial change.*]

Figure 4. Weight-average molecular weight vs. distillate yield for three PFL samples from HRI Run 15 (Black Thunder) and two PFL samples from Run 16 (Ill. No. 6).

*In the sets of PFL samples for Black Thunder and Illinois No. 6 coals, we do not see as regularly the pronounced bimodal distributions we observed in the set of 850°F+ samples from Wilsonville.^{8,9} However, the Run Periods 11 and 14 PFLs do show more discernable high molecular weight "humps" than Period 8 PFL.

In all five sample sets, the $\bar{M}_w$ of the PFC samples are *lower* than the respective PFL samples (Table 1). In contrast to this result, one might have expected the filter cake samples to have *higher* average molecular weights, since they are material insoluble in the reaction medium, and therefore less converted. Thus we need to ask if the observed lower weight-average molecular weight values for the PFC samples are simply an artifact. Are highly polar materials of high mass present in the sample, but simply are not volatile, and therefore not detectable? (Since, as Table 1 shows, the PFCs range from 20 to 55% non-volatile under FIMS conditions, we are not discussing here the question of whether some material is unseen — clearly it is — but only the question of whether the non-volatile and unseen materials substantially *distort* the molecular weight profile from what it would be if all of the components were seen.)

In the PFC sample analyses, ions in the tail of the molecular weight profile (i.e., around 800 Da) begin appearing at probe temperatures of about 300°C, and have begun to decline substantially before 500°C. In fact, when we construct a series of plots of intensity at 100, 200, 300 Da, etc., vs. probe temperature (Figure 5), we see that the intensity at all mass regions above

Figure 5. Ion intensity as a function of temperature at 100, 200, 300, 400, 500, 600, 700, and 800 Da for PFC Sample No. 6 (SRI spectrum A14006).

200 is declining roughly similarly as the final temperature of 500°C is approached. This decline in concert means that unless the mass 800 material exhibits a bimodal distribution with temperature, it would continue to decline above 500°C (assuming for sake of argument that material boiling at higher temperatures could be accessed without substantial pyrolysis and additional crosslinking). Thus, it does not appear likely that *selective* inability to see involatile, high molecular weight material is making the apparent weight average molecular weights for the PFC samples spuriously low. We conclude that the PFC materials are involatile *not* primarily because they are bigger than the volatiles, but because they are more polar, and thus that the weight average molecular weight values shown in Table 1 and on the individual spectra are not substantially distorted by high-molecular weight non-volatile material. This situation is somewhat parallel to that described by Boduszynski for heavy petroleums.^{18,19}

A separate question about the PFC average molecular weights is whether they are lower than those of the PFL samples just because of the presence of the wash oil in the filter cake. Although the presence of this wash oil must indeed lower the average molecular weights of the filter cake samples, examination of the data suggests the lowering is not very great. Table 3 shows that the first five individual spectra recorded for Sample No. 6 were accumulated over a temperature range of only 35°C (29 to 64°C), and that the weight-average molecular weight for material vaporized during each of the six intervals remained relatively constant, increasing from 210 to only 255 Da [This constancy can be easily seen by examining the individual spectra (A 14006.000 to A 14006.004).] The materials vaporized in this region could be comprised primarily by the wash oil. Examination of the vacuum evaporation profile for this sample (A 14006) indicates that material in these first five spectra constituted only about 8 wt% of the total volatile material. Even if all of this 8% of low-mass components were from the wash oil, and is therefore excluded from the average molecular weight calculations, the M_w value computed for Sample No. 6 is only increased to 506 Da, or about one-half the distance to the 531 M_w value computed for the entire PFL Sample No. 5. Nevertheless, in any future analyses, it would probably be appropriate to (1) separately analyze a sample of the wash oil, so that if desired its contribution can be subtracted out of the sum spectrum, and (2) begin the PFC analyses at -67°C, just as was done for the PFL samples.

Interestingly, the amount and molecular weight range of apparent wash oil, or low-molecular weight material (ca 150 - 350 Da) in PFC Sample No. 6 is not greatly different from the lighter fractions of PFL Sample No. 5, also shown in Table 5. Inspection of the pattern tables for each of the individual spectra accumulated for each of the two samples reveals that there are some differences in compound class distribution for PFL and PFC spectra accumulated in equivalent temperature regions. However, a more thorough examination would be necessary to see if these

differences are really characteristic of differences between the wash oil and low-boiling portions of the PFL samples.

Table 3
Temperature Intervals and Weight-Average Molecular Weights
for the Individual Spectra for Samples 5 and 6.^a

Spectrum No.	PFL Sample No. 5		PFL Sample No. 6	
	Temperature Interval, °C	Weight-Average Molecular Weight, Daltons	Temperature Interval, °C	Weight-Average Molecular Weight, Daltons
000	-62 to -29	188	30 to 29	210
001	-32 to -17	197	29 to 37	218
002	-19 to -7	210	38 to 46	225
003	-8 to +17	220	47 to 53	239
004	22 to 56	250	53 to 64	255
005	58 to 93	299	65 to 89	289
006	98 to 159	386	94 to 156	349
007	173 to 227	486	161 to 239	426
008	233 to 293	589	244 to 305	501
009	299 to 359	672	310 to 399	572
010	365 to 471	720	408 to 468	614
011	483 to 501	739	474 to 501	576
Sum	-62 to 501	531	30 to 501	473

a. Data taken from Individual Spectra A14005 and A14006, reproduced in the Appendix.

Nitrogen Distributions

Interpretation of Even- Versus Odd-Mass Profiles. Here, as in previous coal product analyses,²³ the ratio of odd/even ions is a reliable reflection of the nitrogen content of the (ionized portion) of the sample. First, in the spectra (Figures 1 and 2, or the pattern tables in the Appendix), which extend down to 48 Da, the t-butyl cation (at 57 Da) together with its homologs

at 71, 85 etc. Da, while visible, typically constitute only about 0.1% of the total ion count. That is, virtually no ion fragmentation occurs, not even to produce the most stable category of ion fragments, namely, butyl, pentyl, etc., tertiary ions. Thus, after correction for ^{13}C , the odd-mass profiles should accurately represent the molecules containing odd numbers of nitrogen atoms. This conclusion is reiterated by the fact that the ^{13}C -corrected FI mass spectra of the SOH/ASOH samples show minimal odd-mass profiles, which indicates that ion fragments and nitrogen-containing compounds are both insignificant.

Correlation with Nitrogen Contents. The Run CC-15 PFL samples show a fair positive correlation between the wt % nitrogen and the ratio of the sums of odd and even molecular ions, as shown in Table 1 and Figure 6. From the point of view of nitrogen content (both as reflected in the CONSOL wt% nitrogen values, reproduced in Table 1, and in the odd/even intensity ratios), Run Period 14 appears to suffer from catalyst degradation and/or buildup of polar (nitrogen-containing) materials to a considerably greater degree than in the otherwise equivalent Run Period 8. A similar phenomenon is observed for the two Run CC-16 periods for which we obtained samples. In this latter case, Run Period 13, even though the temperatures were higher and the distillate yield was 6 percentage points higher, the nitrogen content and odd/even ratios were increased considerably.

Figure 6. The ratio of the sum of even-mass intensities to the sum of odd intensities versus nitrogen content by ultimate analysis for Samples 1-18 [N-contents taken from CONSOL data (see Table 1)].

Relative Odd/Even Ratios for PFL and PFC Samples. The values of the odd/even ratio and the wt % nitrogen content are both larger and more scattered for the PFC and INT samples, where varying amounts of the insoluble organic matter (IOM) may be taken in any one 40- μ g FIMS sample. An additional reason for expecting less regularity for the PFC samples is that the FIMS analysis counts nitrogen only in volatile (or pyrolyzable to volatile) material, whereas the nitrogen analysis counts everything in the sample.

Comparing the PFL to the PFC samples, the area occupied by the odd profiles, as a fraction of the respective even-mass profiles, is considerably larger in the PFC samples and clearly indicates that the nitrogen is concentrated in the more polar and more insoluble products, where it would be expected from previous studies of deposit formation in fossil fuels.²⁴ There is no clear indication of the nitrogen incorporation during iron-pretreatment procedure of HRI¹ for Periods 8 and 14. The mass spectra do tell us that whatever nitrogen incorporation did occur must have involved ammonia or an amine of molecular weight less than 48 (where the standard scan begins), or must have been of a covalently bound sort, since hydrogen-bonded amine absorption would be reliably and unambiguously reflected in a prominent peak for the molecular ion for whatever nitrogen-containing solvent that had been used. As has been previously discussed²³ in the context of nitrogen-containing liquefaction solvents, even the strongest of hydrogen bonds is not sufficient, under the high-vacuum FIMS conditions, to keep the equilibrium between hydrogen-bonded and dissociated species from shifting well to the side of the dissociated species as the molecules vaporize in the mass spectrometer inlet.

Odd/Even Profiles of Black Thunder Versus Illinois No. 6 Samples. The odd-mass profiles and the odd/even summary ratios are generally lower in the case of the Illinois No. 6 (Run 16) samples, than they are for the Black Thunder coal, notwithstanding the fact that the Illinois coal originally contained more nitrogen (1.30 wt% vs. 1.04 wt % for Black Thunder). This result (which is seen most reliably in the homogenous PFL and SOH-ASOH samples) is completely consistent with the CONSOL nitrogen analyses (Table 1), and it explained by the nitrogen-removal effectiveness of the first stage supported catalyst in run periods 8, 11, and 14 of Run CC-15, as contrasted the first stage of Run CC-16 for the Black Thunder coal, which contained no supported catalyst. A contributing factor could also have been the detrimental impact of the high -OH content of the Black Thunder coal on the second stage catalyst, suppressing its hydrodenitrogenation activity.

Prominent Individual Compounds

As in our previous analyses of Wilsonville resids,^{8,9} we can readily see substantial "structure" in the FIMS profiles at the lower-molecular-weight or "leading" edge of the envelopes, at about 200 Da. Although in the 400 Da region the intensity of any individual ion does not differ by more than 20% from any of its near neighbors, at about 200 Da the intensity of a particular ion may differ by a factor or two or more from that of its neighbors. This enhanced structure at the low molecular-weight limit occurs because separation of the atmospheric still overhead removes the more volatile compounds at borderline molecular weights (i.e., 200 to 300 Da); these more volatile compounds are the less aromatic and less condensed materials (aliphatics and cycloaliphatics). When they are removed, they leave behind only the least volatile materials in that mass range, i.e., the most condensed or most aromatic species.

Probable Coke Precursors. Table 4 lists the intensities of some of the prominent ions observed in the 160 to 300 Da range for the PFL, PFC, INT, and SOH-ASOH samples. Some of the structures expected to contribute to these ions are shown in Table 2 above. Apart from 202 (pyrene, fluoranthene) and 208 (hexahydropyrene) and some other moderate molecular weight aromatics and hydroaromatics, well known and desired components of recycle streams, the most prominent ions include a number that appear to be undesirable. These include compounds at 168 and 172 Da, as well as most of those products we identified earlier^{8,9} in the 850°F+ resids from Wilsonville runs, particularly at 242, 276, 300, and 316 Da.

Although the peaks at each of the above masses are not comprised entirely by a single structure, we again believe, based on the careful HPLC/FIMS work of Sullivan, Boduszynski, and Fetzer¹⁰ on petroleum resids, that they (1) are dominated by the structures shown in Table 2 and (2) are very probably precursors to coke formation. Furthermore, in preliminary model compound studies at SRI, we have observed^{25,26} that peaks at 242 and 316 Da, and presumably other of these suspected coke precursors, are in fact generated during the pyrolysis of long chain alkylpyrenes. We looked for these components in alkylpyrene pyrolysis products because we expected that their formation was key to the thermal disproportionation that occurs during resid upgrading: their formation makes hydrogen available to give reduced (i.e., alkane-rich) distillate materials, but then this hydrogen is available only at the cost of producing oxidized products, namely, these coke precursors. Inasmuch as this natural disproportionation subverts the effort to supply external hydrogen via H₂, catalyst, and donor solvent, it is of course unwanted.

Table 4
Relative Intensities of Prominant Ions

M/Z (Da)	CONSOL SAMPLE NUMBER/TYPE/INITIAL TEMPERATURE																	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
	PFL	PFC	INT	SOH	PFL	PFC	INT	SOH	PFL	PFC	INT	SOH	PFL	PFC	SOH	PFL	PFC	SOH
	-62	+30	-64	NA	-62	+30	-66	NA	-65	+30	-16	NA	-66	-64	NA	-66	+30	NA
168	471	632	678	1230	533	182	450	2230	342	127	24	1747	163	115	1272	177	34	1623
172	576	79	385	1840	481	156	161	3000	259	122	27	2291	199	132	1653	124	23	1725
202	1293	832	1344	1800	968	943	1235	1050	1010	792	987	1993	1021	982	1949	1415	1118	2181
208	894	704	750	1050	742	632	801	1231	886	614	542	1145	994	915	1550	881	460	1993
242	1082	982	785	460	687	845	816	482	814	790	780	532	1302	1275	1399	1352	1150	1617
276	664	658	542	100	498	756	597	142	600	690	591	146	775	776	187	875	1033	322
300	337	384	290	0	291	340	295	0	312	421	302	72	401	383	44	300	536	60
316	377	467	344	0	347	387	383	0	358	501	333	0	516	538	0	667	682	0

- a. Intensities are given here in the same units as in the pattern tables, that is, normalized to 100,000 counts as the sum of all ion intensities, after ^{13}C correction. Thus an intensity of 1000 corresponds to 1% of the total of all ions produced by that sample.

Table 2 above lists a pair of m/z values that were not observed in our analyses of the Wilsonville 850°F+ resids, namely those at 168 and 172 Da. The ion at 168 Da is expected to have contributions from dibenzofuran and benzindans, but could as well have significant contribution as well from by the analog of 242 Da, namely, dihydroperinaphthene or dihydrophenalene, at 168 Da. The latter is the base compound in the series of odd-carbon aromatics discussed below. The intensities of the peaks at 168 and 172 seem to fluctuate together, on a sample-to-sample basis, but as discussed in the following paragraph, this correlation is as much a matter of similar vaporization behavior as it is of similar chemical origin.

As Table 4 shows, the peaks at 168 and 172 Da (and at other low masses) are strikingly less abundant in some particular analyses of PFC and INT samples. Inspection of the spectra or pattern tables in the appendix show that this in most cases this is because for the less volatile (PFC) samples, the probe was pumped down and the analysis begun at room temperature rather than at $\sim 60^\circ\text{C}$, as had been done with the PFL and INT samples. This choice was made because the PFC samples were felt to be less volatile than the PFL and INT samples; we were not at the time fully aware of the impact of what turns out to be more than a trace of low molecular-weight wash oil in the "dry" filter cakes. [The presence of the low-molecular weight fraction can be seen in the tetrahydrophenanthrene spectra shown in the Appendix (A14006.000 to A14006.004).] Having recognized these general differences due to different heating profiles, it is possible to make additional comments on the basis of chemical and vapor pressure differences.

At 172 Da, both hexahydrophenalene and tetrahydrodibenzofuran would seem to have rather high degrees of hydrogenation for such an abundant product, so *on this basis* the most likely candidates for the bulk of the 172-Da intensity would seem to be tetrahydrobenzindans (see Table 2). On the other hand, assignment of the bulk of the 168 Da peak to ring contraction of tetrahydrophenanthrene (182 Da) to benzindan would lead one to expect a 168/172 ratio that is at least roughly similar to that at 132/118 (tetralin/indan) where a similar ring contraction is possible, but where there is no possible analog to the dihydrophenalene. What we see however, are quite different ratios at these two pairs, for example, in SOH-ASOH Sample No. 8, $I_{168}/I_{172} = 0.93$, but $I_{118}/I_{132} = 0.13$. The much lower ratio of ring-contraction product to tetrahydro- PAH parent seen with indan and tetralin suggests that ring-contraction from tetrahydro-phenanthrene is, after all, not a good explanation for the abundance of the peak at 168 Da.

In the original work of Fetzer et al.¹⁰ on the basis of which we speculatively identified the peak at 242 Da as the hexahydro-phenalene analog, the data did not allow a definitive choice between ring-contraction to a system having a five-membered ring fused to the six-membered PAH system, or a ring-growth process to produce the phenalene analogs. However, the authors seemed

to prefer the ring-growth option, presumably partly on the intuitive judgment that tends to assign products that accumulate during growth toward coke to ring-growth, rather than to ring breakdown processes. This intuition is supported by recent preliminary studies performed at SRI to examine the heavy products of long-chain alkyl pyrenes and other alkyl-PAH. In that work,^{25,26} we have found m/z 242 to be a significant component of the high-molecular weight "incipient coke" that accompanies alkyl side-chain cleavage. Thus, in the present case, we consider it very probable, but not conclusive, that dihydrophenalene and other six-membered-ring odd-carbon structures are major components of the peaks at 168, 242, 316 Da, etc.

If we examine more closely the question of relative abundance of 168, 178, and 202 in the lighter (SOH-ASOH) and in the heavier (PFL) fractions, the questions about the origin of m/z 168 become still more intriguing. The peaks at 168 and 172 Da are generally two to five times as abundant as phenanthrene (m/z 178) in the PFL samples, even though as two- and one-ring aromatics of 13 carbons they should both be significantly more volatile than phenanthrene, a three-ring aromatic of 14 carbons. Table 5 shows further how the intensity ratios for 168/178 and 178/202 change in going from each of the five PFL to the corresponding ASOH-SOH samples.

Table 5
Intensity Ratios for Low Molecular-Weight Peaks in PFL and ASOH-SOH Samples^a

M/Z Values	SAMPLE NUMBERS AND INTENSITY RATIOS									
PFL	1		5		9		13		16	
SOH-ASOH		4		8		12		15		18
168/178	4.44	2.41	3.25	0.74	4.38	2.68	2.55	2.31	4.53	3.12
178/202	0.082	0.28	0.17	2.18	0.077	0.33	0.063	0.28	0.028	0.24

^aData taken from pattern tables in the Appendix

These values illustrate the peculiar fact that whereas the 178 peak is enhanced (relative to the 202 peak) in each of the ASOH samples, as compared to the respective PFL samples, the opposite is true for the 168/178 ratio. That is, the lower molecular weight and less condensed aromatic (178) is relatively concentrated, as it should be (compared to 202), in the lower boiling fraction. However, the 168/178 ratio does *not* go up from PFL to the respective ASOH sample, but instead generally goes down. For some reason, the material at 168 Da is *not* concentrated in the lower boiling fraction as a lower molecular weight and less aromatic material should be.

The contrast between the temperature behavior of peaks 168, 172, 178, and 208 even raises the question of whether the components of masses 168 and 172 Da were actually present as such during the atmospheric distillation. Kim et. al.,²⁷ in discussing electron spin resonance data of coal pyrolysis liquids, report that phenalenyl-like radicals were present at concentrations up to 10^{-4} molar *at room temperature*, until the samples were exposed to oxygen. Perhaps the material appearing at 168 Da is not fully removed in the ASOH precisely because it is partly present as some higher boiling derivative. This might be the fully aromatic phenalenyl radical ($C_{13}H_9^{\bullet}$, m/z 165), which as an aromatic three-ring system would be somewhat less volatile than the bridged two-ring aromatic dihydrophenalene. When the samples examined here were further cooled and/or exposed to oxygen, the phenalenyl radicals would be quenched either by hydrogen transfer or by oxidation. The most obvious oxidation product of the phenalenyl radical would be phenaleneone, 180 Da. The pattern tables reveal that 180 Da also has a high intensity.**

The inability, from the present data alone, to eliminate the remaining uncertainty as to the major contributors to peaks at 168 and 172 does nothing to lessen our interest in the implications of the odd-carbon analogs at 242 and 316 Da. Phenalenyl radical (along with its analogs) is one of the most stable of all π -radicals and has been shown by ESR to be essentially ubiquitous *at room temperature* in thermally treated fossil fuel samples.^{27,28} However, it has never been clear whether it was a key intermediate in large PAH and coke formation, or whether it was simply in a "side alley," that is, present in high concentrations because of its unusual stability. The possible presence of some closed-shell relatives of phenalenyl radical has often been obscured in GC-MS analyses because phenalene itself (166 Da) will be readily oxidized (presumably to phenaleneone) and can furthermore be confused with its much more stable isomers, fluorene and methyl-acenaphthylenes.²⁹ The product seen here (dihydrophenalene, 168 Da) may be confused in GC-MS analyses with a methyl acenaphthene. In the present case, it is unlikely that any significant portion of the 168 Da peak is due to methylacenaphthenes, since intensity at 154 Da, where the parent acenaphthene would appear, is very low.

The identification of mass 168 as yet another member of the odd-carbon fused-ring systems present in high concentrations (along with those at 242 and 316 Da) in these coal liquids (as well as in petroleum-derived resid streams) only increases our suspicion that they could be playing a key role in the formation of refractory resids and carbon buildup. However, the evidence at this point is still primarily circumstantial: higher concentrations of these materials are present in samples

**The peak at 180 Da will also have contributions from dihydrophenanthrene, but this contribution is probably minor, since the intensity at 180 is typically twice that at 178, whereas that at 204 for dihydropyrene is only 1/3 that for pyrene.

obtained under conditions where process performance was poorer (lower non-distillables conversion, etc.) or from streams having more insolubles content (i.e., more potential for the phase separation known to aggravate coke formation). We believe that experiments are now warranted to determine directly how much of a role these odd-carbon PAH have in coke formation during resid hydroprocessing. These experiments could be done by doping process-stream samples with isotopically labeled precursor suspects and then following their evolution in the reaction mixtures.

Notwithstanding the prominence of the projected hydrocarbon coke precursors in the HRI samples, a very substantial portion of the insoluble matter in these heteroatom-rich coal-derived streams will contain oxygen and nitrogen and not consist simply of pure hydrocarbon structures. This is made evident by the higher nitrogen contents and odd/even ratios of the PFC samples, as discussed above. At this time we cannot judge which class of solids-forming structures is more important. It could be, for instance, that the heteroatom-free solids require "mistreatment" (i.e., excessive temperatures, H-donor shortage, acidic surfaces) to be produced in substantial amounts, whereas heteroatom-containing retrograde products can form more on their own. If this were the case, the former class of retrograde materials would be the ones most readily affected by improved processing techniques. Thus they could be of critical process importance not only in relatively heteroatom-free petroleum streams, but also in more heteroatom-rich coal-derived streams.

Other Prominent Components. While the low-solubility and higher molecular weight condensed aromatics discussed above can be associated with solids formation, certain other condensed aromatics, such as pyrene and hydropyrenes, are well known as very beneficial components of liquefaction solvents. The intensities at 202 and 208 Da are very high in all the samples, particularly the filtered liquids. They are also higher in the run periods where the distillate yields were higher (Period 8 for Run 15 and Period 13 for Run 16). Their prominence is commonly noted in GC-MS analyses of liquefaction products and recycle solvents.

The peaks at 208 Da, presumably derived from hexahydropyrenes, are more intense than those at either 204 or 206 Da, as expected from the relative stability of the di-, tetra-, and hexahydropyrenes. The peak at 208 Da is invariably lower in the PFC samples than in the PFLs. No consistent trend is identifiable in the three INT samples.

Trends with Changes in Processing Conditions

In this set of 18 samples, there are only two "all-other-things-being-equal" changes in processing conditions from which to make product comparisons. The first is in Run CC-15, going from Period 8 to 11 to 14. In period 11, the impregnated hydrated iron oxide catalyst use in Period 8 was eliminated, and restored in Period 14 (Conditions 2, 3, and 4, respectively). Except for this

change (and for continuously increasing second stage catalyst age), the run conditions were identical during these three periods. In Run CC-16 with Illinois No. 6 coal, Period 13 was operated with Stage 1 and 2 temperatures increased from 750 and 800°F to 775 and 810°F, respectively, and solvent/coal ratio decreased from 1.5/1 to 1.1/1.

Effect of Iron Oxide Removal. Following the discussion of changes in run conditions in the documentation provided by CONSOL Inc. along with the samples,¹¹ we will focus on the Interstage samples from the three periods of Run CC-15, because they show the minimum "leveling" effect from the second stage supported catalyst, which was present in all cases. As noted by CONSOL Inc.,¹¹ Condition 3, without any iron catalyst, resulted in the highest condensed aromatic, the lowest solvent quality, somewhat as expected, but also resulted in the lowest phenolic -OH and the lowest average molecular weight ($\bar{M}_w$, by FIMS). The question is, are these observations consistent with other FIMS parameters, and can a plausible explanation be given. We believe the answer to both questions is yes. First, with respect to the average molecular weights, the HRI process data¹¹ show that although the distillate yield in Condition 3 is lower, the distillate is lighter than in either Condition 2 or 4. (The 650 to 975°F+ portion goes from 17.6 to 16.3 to 23.1 % of the total distillate.¹¹) We suggest that these changes might correlate with the phenolic OH and the condensed aromatics in the following way. Iron oxide/sulfide catalysts are known to promote initial coal conversion (cracking?) more effectively than they promote upgrading (deoxygenation?). When the iron is present, the large structures containing phenolic -OH are preferentially cracked into smaller OH-containing structures that report to the distillate. When iron is not present, those original OH-containing structures tend to undergo thermal retrograde and disproportionation reactions in which most of the structure (including the OH) sinks into heavy residual material with *some* lighter materials produced in the disproportionation (note that C₄ to C₇ gas actually goes up slightly in Condition 3.¹¹) The net result is thus that there is less heavy material in the distillate: The material that the iron would have cracked to distillate has gone instead to non-volatile (and/or non-soluble) retrograde products, and has taken the oxygen with it.

The pronounced increase in condensed aromatics observed under Condition 3 is the natural result of the increased retrograde and disproportionation reactions. However, we can ask what these condensed aromatics were and why they were not accompanied (in the presence of the second stage catalyst) by an increase in cyclic α and cyclic β protons and an increase in solvent quality. In Table 4, where we show the relative intensities of some prominent ions in the spectra of the eighteen samples, one can see that in fact the intensity of the condensed aromatic most often associated with high solvent quality, namely, pyrene (and fluoranthene) at m/z 202, does *not* go up as we progress from the interstage sample from Condition 2 to that for Condition 3. Furthermore,

when we sum the intensities of m/z 202, 178, 168, 300, and other prominent PAH of intermediate molecular weight (along with their C₁, C₂, and C₃ derivatives, for a total of 27 peaks), we find that these solvent- and near-solvent range PAH go from 14.9 to 15.5 to 10.2 % of the total ion intensity for the interstage samples from Conditions 2, 3, and 4, respectively. The increase from 14.9 to 15.5 is considerably smaller than the increase in NMR-determined¹¹ condensed aromatics content from 13.2 to 20.5. In other words, there is little increase in the PAH or hydro-PAH for some of the species most associated with high solvent quality, and therefore the significant increase in "condensed aromatics" for Condition 3 must come in still higher molecular weight and/or oxygenated PAH (i.e., more retrograde products). This observation is a plausible reconciliation of the coincidence of higher PAH and *lower* solvent quality. [We note that the sum of the four principal suspected coke precursors (m/z 242, 276, 300, 316, and their C₁ and C₂ derivatives) increases by 14% on going from Condition 2 to Condition 3, whereas the sum of 27 PAH had increased by only 4% and the NMR condensed aromatics increased by 55%.] Evidently, the differences between the NMR condensed aromatics content and the solvent quality values are reflecting the difference between "good" and "bad" PAH, and the FIMS data are at least beginning to help us understand the distinction between the two categories.

If we examine the changes in intensity of ions corresponding to the types of phenols expected to be most resistant to hydrodeoxygenation, namely those in which the phenolic -OH group is attached to a single aromatic ring, or at most to a naphthalene ring system (cresols, hydroxy biphenyls, hydroxy phenylnaphthyls), we see that they go down significantly from Condition 2 to 3. (However, they do not rise again in going to Condition 4, as we would expect if they were to exactly parallel the FTIR-based OH measurements.)

Effect of Increasing Temperature in Run CC-16. The general correlation between increasing distillate yield and decreasing PFL average molecular weight (M_w) noted above also holds for the two Run 16 run periods. A further consistency exists in that the distillate for Period 13 is also lighter than that for Period 5. Similarly, the increasing Nitrogen Wt % is mirrored in the increasing odd/even ratio from the FIMS data.(Table 1) In terms of the prominent individual peaks, anticipated solvent quality, and coking tendency, comparison of PFL Samples 13 and 16 reveals that the higher temperature condition (as well as the lower solvent/coal ratio and the higher catalyst age) increases the m/z 202 intensity by about 40%, but decreases the m/z 208 intensity by about 10%. This would appear to be consistent with the change in solvent quality anticipated from very significant decreases in cyclic α and cyclic β protons. Increases in all of the suspected coke precursors (except coronene at m/z 300) were observed in going from Sample 13 to Sample 16. The decrease in m/z 300 intensity in the PFL sample is in part a reflection of the low solubility of this PAH, since this decrease in the PFL sample is more than compensated for by an observed m/z

300 increase in the PFC samples (Sample 17 vs. 14, Table 3). Thus the FIMS data help to elaborate on and to better explain the trend towards generating higher distillate yield but more refractory resid with higher temperature and catalyst age and lower solvent to coal ratio.

Recommendations

As stated above, we believe that experiments are now warranted to determine directly how much of a role these odd-carbon PAH and the other suspected coke precursors actually have in coke formation during resid hydroprocessing, and moreover to determine how changes in reaction conditions might (or might not) serve to limit this coke formation. Reaching of these objectives is important to optimal achievement of one of the stated goals of the "Proof of Concept" program now underway at HRI: the achievement of full resid extinction (without costly reliance on rapid catalyst replacement, long residence times, and high H₂ pressures) may depend either on (1) change of reaction conditions to limit buildup of increasingly refractory resid components as true steady state is approached in long term heavy-recycle operation, (2) optimization of anti-solvent de-ashing to increase the removal of coke precursors, and/or (3) coking/gasification/combustion of a stream enriched in these materials.

We suggest that determination of the actual roles of particular suspected precursors in coke formation and of the factors affecting these roles is best achieved by a coordinated effort to track suspected coke precursors in actual product streams, coupled with a focused effort to elucidate the chemistry of selected individual precursors and precursor classes. Notwithstanding the disfavor that "model compound" studies have in some circles, the opportunity to examine the reaction of selected precursors can reduce the analytical problem to one of seeing the target products in the midst of only 20 to 100 other products (rather than the 100,000 or more other products as are present in a real resid). We believe that a very good basis for a suitably focused effort to elucidate this chemistry is constituted by the present analytical effort, together with the work of Savage and coworkers over the last five years³⁰ to examine the light products of the pyrolysis of long chain alkyl-PAH, and with our recent efforts^{25,26} to examine the heavy products (i.e., the coke precursors) in these prototypical distillate-forming reactions.

We believe that a useful understanding of the factors controlling coke formation will come from a hybrid study that attempts to bridge the gap between the chemical details available from model compound work and the relevance of changes in the actual process streams. Thus, the analysis of real liquefaction products should involve not only liquid product streams and filter cake, but also recovered catalyst samples, and perhaps reactor deposits. It should involve not only analysis of these normal process samples but should be connected to the selected precursor studies by experiments in which product stream samples are doped with suspected precursors (either pure

compounds or fossil fuel products very rich in particular suspects), allowed to react in suitable microreactors, and analyzed to determine whether and under what conditions added precursor suspects actually result in increased levels of high molecular weight PAH and/or increased coke. A desirable microreactor might be one in which a small sample of a recycle stream is exposed, either in a static cell or flowing in a closed loop over one or a few catalyst pellets. FIMS would certainly be a useful and reliable tool for the required analyses, but other techniques (such as laser desorption mass spectrometry for molecular weight species above 1000 Daltons) would be useful complements. In specific cases it might be worthwhile to dope process-stream samples with isotopically labeled (either ^{13}C or ^{14}C) precursor suspects and then following their evolution in the reaction mixtures.

SUMMARY

As with the Wilsonville samples analyzed earlier, FIMS analysis again reveals molecular weight distributions and individual component concentrations that correlate with run conditions and process performance. Some of these observations and correlations can be made and have been made without benefit of FIMS analysis. However some of them (e.g., the abundance of moderate molecular weight coke precursors of molecular weights exceeding 300) could not have been made as readily, if at all, by GC-MS or any other technique (except for other relatively nonfragmenting MS techniques). For these full-boiling-range materials, the clearly bimodal molecular weight distributions that we saw for the Wilsonville 850°C+ resid samples^{8,9} were not so pronounced, but the molecular weight distributions shifted with sampling location and process performance in a similar fashion. The two-component fitting of the molecular weight distributions that we did for the earlier samples could have been performed here (with perhaps not quite as good a fit), but once again the set of samples and number of all-other-things-being-equal comparisons was really too small to expect any correlations that were not already apparent from the normal process performance criteria.

We believe that the greatest potential for use of FIMS in this context comes from the ability to identify and track through many feed and process conditions the nitrogen-containing heavy materials and certain hydrocarbon coke precursors. These should be tracked not only in the normal process stream samples, but also in recovered catalyst samples and in other reactor deposits that may appear to determine (1) if these suspected coke precursors are in fact important in the generation of refractory liquids and solids and (2) if so, what changes in process conditions could most usefully limit their formation and subsequent generation of coke.

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APPENDIX

SPECTRA, VACUUM EVAPORATION CURVES, AND PATTERN TABLES

SUM SPECTRA OF SAMPLES 1-18

A14003.SUM -64 to 494°C No. Av. MW = 407. Wt. Av. MW = 528.
REF NO. 3 (CONSOL) ¹³C-Corrected

B14004.SUM 1 to 1°C No. Av. MW = 147. Wt. Av. MW = 170.
REF #4 SOH-ASOH ¹³C-Corrected

A14005.SUM -62 to 501°C No. Av. MW = 429. Wt. Av. MW = 531.
REF NO. 5 (CONSOL) ¹³C-Corrected

A14006.SUM 30 to 501°C No. Av. MW = 401. Wt. Av. MW = 473.
REF NO. 6(CONSOL) ¹³C-Corrected

B14006.SUM 31 to 502°C No. Av. MW = 438. Wt. Av. MW = 501.
REPEAT REF #6 PFC (CONSOL) ¹³C-Corrected

C14006.SUM 29 to 501°C No. Av. MW = 444. Wt. Av. MW = 509.
REPEAT REF. NO 6 PFC 11A ¹³C-Corrected

B14007.SUM -66 to 501°C No. Av. MW = 408. Wt. Av. MW = 503.
REF NO. 7 (CONSOL) ¹³C-Corrected

A14008.SUM 1 to 1°C No. Av. MW = 161. Wt. Av. MW = 179.
REF #8 SOH-ASOH (CONSOL) ¹³C-Corrected

43

A14009.SUM -65 to 501°C No. Av. MW = 422. Wt. Av. MW = 526.
REF NO. 9 (CONSOL) ¹³C-Corrected

A14010.SUM 30 to 501°C No. Av. MW = 398. Wt. Av. MW = 465.
REF NO. 10 (CONSOL) ¹³C-Corrected

A14011.SUM -16 to 501°C No. Av. MW = 464. Wt. Av. MW = 567.
REF NO. 11 (CONSOL) ¹³C-Corrected

B14011.SUM -67 to 498°C No. Av. MW = 451. Wt. Av. MW = 555.
REPEAT REF #11 INT (CONSOL) ¹³C-Corrected

A14012.SUM 0 to 0°C No. Av. MW = 167. Wt. Av. MW = 181.
REF #12 SOH-ASOH (CONSOL) ¹³C-Corrected

A14013.SUM -66 to 501°C No. Av. MW = 435. Wt. Av. MW = 557.
REF NO. 13 (CONSOL) ¹³C-Corrected

A14014.SUM -64 to 501°C No. Av. MW = 435. Wt. Av. MW = 546.
REF NO. 14 (CONSOL) ¹³C-Corrected

A14016.SUM -66 to 501°C No. Av. MW = 431. Wt. Av. MW = 537.
REF NO. 16 (CONSOL) ¹³C-Corrected

A14017.SUM 30 to 500°C No. Av. MW = 436. Wt. Av. MW = 522.
REF NO. 17 (CONSOL) ¹³C-Corrected

A14018.SUM 2 to 0°C No. Av. MW = 174. Wt. Av. MW = 195.
REF #18 SOH-ASOH (CONSOL) ¹³C-Corrected

VACUUM EVAPORATION CURVES FOR PFL, PFC, AND INT SAMPLES

B14001 FIMS VACUUM EVAPORATION CURVE

REF NO. 1 (CONSOL)

0-14

A14002 FIMS VACUUM EVAPORATION CURVE

REF NO. 2 (CONSOL)

A14003 FIMS VACUUM EVAPORATION CURVE

REF NO. 3 (CONSOL)

0-11

A14005 FIMS VACUUM EVAPORATION CURVE

REF NO. 5 (CONSOL)

0-12

A14006 FIMS VACUUM EVAPORATION CURVE

REF NO. 6 (CONSOL)

0-11

B14006 FIMS VACUUM EVAPORATION CURVE

REPEAT REF #6 PFC (CONSOL)

0-8

C14006 FIMS VACUUM EVAPORATION CURVE

REPEAT REF. NO 6 PFC 11A

0 - 9

B14007 FIMS VACUUM EVAPORATION CURVE

REF NO. 7 (CONSOL)

0-8

A14009 FIMS VACUUM EVAPORATION CURVE

REF NO. 9 (CONSOL)

0-10

A14010 FIMS VACUUM EVAPORATION CURVE

REF NO. 10 (CONSOL)

0- 9

59

A14011 FIMS VACUUM EVAPORATION CURVE

REF NO. 11 (CONSOL.)

0-9

B14011 FIMS VACUUM EVAPORATION CURVE

REPEAT REF #11 INT (CONSOL)

0- 9

A14013 FIMS VACUUM EVAPORATION CURVE

REF NO. 13 (CONSOL)

0-11

A14014 FIMS VACUUM EVAPORATION CURVE

REF NO. 14 (CONSOL)

0-10

A14016 FIMS VACUUM EVAPORATION CURVE

REF NO. 16 (CONSOL)

0-9

SUM SPECTRA PATTERN TABLES FOR SAMPLES 1-18

B14001.SUM 1237 PKS W MIN. 1 CNTS. 08-JUN-93 12:01:02 SUM I: 0.1799E+05
 REF NO. 1 (CONSOL) 0-14 N AV MW: 395.9
 ACQUIRED 5-26-93 17:31:03 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 505.7
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.0 °C PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2					RH		ROH	
48>	0	0	0	0	0	0	0	41: 56>	54	75	50	0	0	0	
62>	0	0	0	0	0	0	30	0: 70>	36	25	0	38	0	0	
76>	0	0	0	0	0	0	0	29: 84>	0	27	0	0	0	0	
90>	0	0	30	0	27	0	0	0: 98>	21	21	0	0	0	21	
104>	0	22	0	0	29	0	18	18: 112>	0	0	0	0	0	0	
118>	0	0	0	25	31	0	0	26: 126>	25	0	28	26	20	27	
132>	56	19	23	23	41	12	0	19: 140>	0	0	45	0	0	61	
146>	177	32	37	56	35	25	32	21: 154>	47	0	91	32	76	49	
160>	293	80	58	45	42	0	74	18: 168>	471	50	145	74	576	73	
174>	352	107	61	40	106	19	237	65: 182>	909	33	190	99	1143	107	
188>	513	95	96	36	185	29	366	103: 196>	733	52	264	125	1084	158	
202>	1293	103	429	52	336	75	894	108: 210>	633	88	467	102	901	118	
216>	1138	95	601	45	549	121	1030	106: 224>	616	100	618	114	805	105	
230>	625	75	548	64	712	138	918	122: 238>	533	103	557	111	1082	88	
244>	570	95	523	76	642	140	680	124: 252>	384	74	410	105	742	107	
258>	605	80	481	80	582	101	503	108: 266>	376	54	389	76	507	79	
272>	489	62	400	125	664	109	480	95: 280>	302	93	512	108	389	113	
286>	377	64	334	112	510	103	347	71: 294>	262	69	460	108	429	95	
300>	337	83	314	77	352	90	294	89: 308>	267	71	361	102	327	99	
314>	289	108	377	86	310	107	232	65: 322>	296	68	311	85	287	103	
328>	269	75	331	96	297	66	226	77: 336>	241	79	290	84	288	87	
342>	214	75	251	101	260	79	206	67: 350>	281	88	282	78	268	95	
356>	244	88	224	99	213	72	197	82: 364>	250	86	260	72	196	76	
370>	245	98	213	94	213	93	193	81: 378>	221	74	240	84	200	64	
384>	214	95	215	87	169	97	229	92: 392>	206	94	179	92	191	84	
398>	188	89	171	97	164	103	186	72: 406>	177	107	165	86	180	74	
412>	187	88	196	88	159	86	162	85: 420>	194	81	175	77	196	79	
426>	175	100	157	103	169	79	160	75: 434>	163	73	153	82	179	89	
440>	171	80	143	93	156	80	145	90: 448>	165	84	148	78	170	87	
454>	168	82	157	76	139	77	127	72: 462>	163	80	155	63	152	91	
468>	141	78	143	84	143	78	142	81: 476>	141	101	132	80	136	92	
482>	128	84	123	85	137	80	161	77: 490>	124	72	126	77	135	77	
496>	127	83	135	89	116	74	132	72: 504>	135	69	121	80	119	66	
510>	129	79	136	86	126	80	120	76: 518>	119	86	101	80	145	92	
524>	110	78	126	79	122	74	120	66: 532>	121	66	115	72	128	76	
538>	126	81	105	62	123	79	115	73: 546>	126	69	106	63	131	61	
552>	113	82	104	73	111	61	106	73: 560>	117	79	114	81	103	67	
566>	117	74	116	63	107	68	117	70: 574>	114	66	107	70	114	65	
580>	94	72	105	60	112	53	113	75: 588>	93	76	98	84	99	69	
594>	101	69	99	65	92	61	126	56: 602>	103	62	107	66	111	53	
608>	97	72	73	71	83	71	90	72: 616>	106	65	92	75	86	71	
622>	95	62	98	62	84	61	98	58: 630>	82	56	72	74	82	63	
636>	92	55	80	75	82	62	90	68: 644>	78	64	77	56	75	66	
650>	81	61	77	64	78	65	66	59: 658>	80	58	76	57	73	56	
664>	88	48	80	51	72	65	58	61: 672>	64	58	67	54	74	58	
678>	68	60	65	68	63	45	74	48: 686>	69	52	61	58	60	42	
692>	74	49	70	45	60	48	56	50: 700>	67	48	61	37	54	52	
706>	60	44	58	43	72	39	53	45: 714>	59	41	50	51	47	50	
720>	43	57	38	55	43	53	49	42: 728>	43	44	49	52	42	41	
734>	49	47	46	54	37	52	38	51: 742>	35	45	51	37	51	39	
748>	39	44	37	46	36	37	40	41: 756>	34	41	40	41	33	50	
762>	26	40	37	44	33	41	31	39: 770>	42	32	31	39	28	41	

B14001.SUM 1237 PKS W MIN. 1 CNTS. 08-JUN-93 12:01:45 SUM 1: 0.1799E+05
 REF NO. 1 (CONSOL) 0-14 N AV MW: 395.9
 ACQUIRED 5-26-93 17:31:03 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 505.7
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
776>	29	39	30	30	39	34	34	38	784>	34	35	27	39	26	39
790>	25	41	24	35	31	34	33	31	798>	31	25	36	30	26	27
804>	29	41	22	38	19	34	0	46	812>	23	30	24	26	38	20
818>	38	24	28	29	25	34	21	26	826>	17	28	25	26	24	32
832>	20	23	22	29	22	22	23	22	840>	29	23	29	17	31	18
846>	30	16	25	23	18	23	26	11	854>	23	29	14	25	22	24
860>	17	23	22	19	26	18	14	27	868>	16	20	24	15	19	25
874>	21	17	18	22	10	20	15	19	882>	16	19	15	17	24	11
888>	21	17	12	22	17	13	20	17	896>	19	15	22	11	16	17
902>	19	16	14	22	10	18	12	14	910>	16	13	19	6	22	12
916>	19	12	11	12	14	12	13	11	924>	19	7	14	18	6	22
930>	10	18	10	13	12	7	16	11	938>	17	7	14	11	13	12
944>	18	10	14	10	15	9	9	14	952>	12	12	13	13	8	11
958>	13	12	13	12	11	9	12	12	966>	10	13	9	14	6	12
972>	6	16	4	12	5	15	8	9	980>	11	7	11	11	8	10
986>	8	11	4	0	18	6	14	2	994>	14	4	11	10	5	9
1000>	10	7	10	5	9	7	10	6	1008>	10	4	9	8	9	6
1014>	8	6	9	7	6	5	12	8	1022>	4	10	11	0	12	7
1028>	4	7	7	8	9	6	5	8	1036>	7	5	8	6	8	5
1042>	8	5	8	5	3	6	10	4	1050>	6	5	4	7	8	0
1056>	11	1	9	5	6	7	3	10	1064>	6	4	3	11	4	6
1070>	3	8	1	14	0	8	5	5	1078>	8	3	5	6	7	3
1084>	7	6	5	6	5	8	3	5	1092>	9	1	6	2	5	8
1098>	2	4	3	7	3	7	4	3	1106>	8	1	4	4	5	6
1112>	2	7	4	5	4	5	5	4	1120>	0	7	4	7	1	3
1126>	4	3	4	6	4	3	5	5	1134>	2	2	6	1	6	2
1140>	4	3	3	5	4	4	6	3	1148>	2	6	5	4	2	6
1154>	0	5	3	4	4	3	4	5	1162>	3	5	3	5	3	5
1168>	1	6	3	5	2	7	0	4	1176>	3	3	3	1	5	2
1182>	3	3	4	0	5	2	4	3	1190>	2	4	7	3	6	0
1196>	5	4	3	3	0	5	1	3	1204>	6	0	6	6	0	0
1210>	3	6	0	8	0	0	5	3	1218>	0	0	7	0	0	6
1224>	1	2	19	0	0	3	0	6	1232>	1	3	0	3	5	3
1238>	3	2	0	1	3	3	0	3	1246>	0	6	0	6	0	0
1252>	0	0	9	0	6	0	4	1	1260>	0	5	1	3	6	0
1266>	0	0	5	0	4	3	1	2	1274>	0	3	0	5	0	0
1280>	0	0	0	0	7	5	0	0	1288>	0	0	0	0	6	0
1294>	0	3	0	0	5	1	0	0	1302>	0	6	0	2	0	6
1308>	0	0	5	0	0	0	0	6	1316>	0	5	0	4	0	0
1322>	4	0	3	4	0	1	0	5	1330>	0	0	0	0	7	0
1336>	1	0	0	0	0	9	0	0	1344>	0	0	0	4	0	0
1350>	0	4	0	0	0	0	0	0	1358>	0	7	0	0	0	0
1364>	0	0	0	0	5	4	0	0	1372>	0	0	0	6	0	0
1378>	0	0	0	0	0	0	0	0	1386>	4	0	0	0	1	0
1392>	0	2	0	2	0	0	0	0	1400>	0	0	0	0	0	0

SUM ODD 3846.4 3746.3 3664.6 3774.9 3553.8 3869.1 3951.1
 EV 11597.4 8696.9 9403.6 10327.3 10391.3 9210.9 12705.4
 RATIO 0.33166 0.43076 0.38971 0.36553 0.34200 0.42006 0.31098
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.365066

A14002.SUM 816 PKS W MIN. 1 CNTS. 08-JUN-93 13:29:54 SUM I: 0.9972E+04
 REF NO. 2 (CONSOL) 0- 8 N AV MW: 391.3
 ACQUIRED 6- 4-93 12:45:28 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 391.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF- .
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2				U1		RH		ROH
48>	0	0	0	0	0	0	0	0	56>	56	63	0	0	0	0
62>	0	0	0	0	0	0	0	0	70>	75	31	0	0	0	0
76>	0	0	38	0	45	0	47	0	84>	48	0	0	0	0	0
90>	0	0	0	0	48	0	0	0	98>	37	0	0	0	0	0
104>	0	0	0	0	75	21	0	0	112>	0	0	0	0	0	0
118>	0	0	0	38	70	45	0	28	126>	0	0	22	0	0	37
132>	41	0	33	26	0	0	0	0	140>	0	0	0	0	33	49
146>	48	25	32	28	40	0	23	0	154>	0	0	56	0	22	50
160>	33	44	32	0	33	32	22	34	168>	63	13	50	33	79	43
174>	62	53	40	29	67	0	88	79	182>	295	43	66	0	197	127
188>	52	42	126	26	90	29	220	109	196>	409	99	101	117	236	123
202>	832	124	374	54	190	108	704	122	210>	402	142	254	143	340	133
216>	655	0	409	84	307	162	800	164	224>	495	139	450	145	430	134
230>	430	174	417	112	441	173	712	185	238>	361	148	410	125	922	156
244>	491	161	389	125	437	150	528	141	252>	325	102	326	128	731	188
258>	537	141	414	123	470	160	384	136	266>	284	91	316	122	474	175
272>	450	133	387	169	658	226	437	110	280>	260	95	524	186	360	145
286>	404	150	328	199	480	167	334	115	294>	234	128	451	223	389	145
300>	384	141	313	142	358	141	311	131	308>	264	136	310	173	360	188
314>	270	164	467	197	311	150	257	159	322>	256	154	291	196	296	176
328>	257	172	422	179	307	188	232	151	336>	252	163	267	221	353	204
342>	245	152	295	155	278	192	223	170	350>	383	190	260	196	352	212
356>	308	188	274	176	236	164	253	150	364>	312	208	292	173	251	165
370>	271	203	267	177	327	188	203	0	378>	316	218	291	197	258	0
384>	301	140	257	165	263	179	340	175	392>	248	191	225	183	290	141
398>	311	181	266	195	239	181	298	143	406>	277	172	272	154	225	152
412>	255	175	358	178	259	173	232	139	420>	252	170	229	150	333	155
426>	251	168	287	135	267	148	241	170	434>	233	132	223	147	334	159
440>	265	162	262	171	253	125	232	140	448>	310	145	236	135	267	188
454>	259	124	237	142	214	134	253	140	462>	272	185	266	134	263	144
468>	239	153	188	143	276	127	248	160	476>	222	142	241	155	206	153
482>	185	137	205	122	241	165	250	135	490>	220	141	225	127	220	131
496>	189	139	246	131	195	143	215	154	504>	209	151	194	135	172	128
510>	183	142	205	156	195	130	197	126	518>	186	142	157	102	223	130
524>	194	124	187	144	195	91	176	141	532>	158	120	171	103	182	139
538>	175	121	152	122	176	109	176	102	546>	184	89	169	112	160	116
552>	163	97	187	106	148	77	145	112	560>	155	91	149	94	161	98
566>	131	89	119	104	127	91	141	76	574>	142	83	122	94	135	85
580>	133	98	111	87	114	79	118	85	588>	0	133	118	78	129	63
594>	113	73	78	101	90	78	111	70	602>	116	70	97	82	101	72
608>	106	63	82	64	97	65	85	68	616>	94	60	99	58	88	52
622>	80	62	71	59	86	64	87	73	630>	78	57	73	47	77	0
636>	79	59	79	52	78	49	71	56	644>	69	36	79	47	74	51
650>	59	49	61	62	63	36	75	31	658>	69	45	66	30	79	30
664>	61	37	65	22	66	36	37	33	672>	54	32	51	36	55	38
678>	50	45	41	38	41	34	38	50	686>	34	35	55	36	43	35
692>	46	27	44	33	40	48	27	43	700>	24	24	49	28	47	17
706>	33	44	27	33	35	19	45	26	714>	28	27	33	29	38	18
720>	40	33	25	32	26	30	27	37	728>	18	31	28	22	33	17
734>	28	32	21	0	42	17	30	26	742>	28	23	30	17	26	12
748>	26	27	13	29	15	24	24	21	756>	22	19	24	16	20	16
762>	29	17	19	17	24	18	17	20	770>	21	9	30	11	18	16

A14002.SUM 816 PKS W MIN. 1 CNTS. 08-JUN-93 13:30:36 SUM I: 0.9972E+04
 REF NO. 2 (CONSOL) 0- 8 N AV MW: 391.3
 ACQUIRED 6- 4-93 12:45:28 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 450.5
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% C PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	U1	12	19	13	17
776>	20	15	23	3	28	0	32	17:	784>	15	12	19	13	17
790>	12	21	20	19	14	10	21	11:	798>	12	16	5	14	20
804>	16	21	15	8	14	14	18	14:	812>	17	6	18	10	15
818>	20	3	13	16	10	11	14	6:	826>	14	4	10	10	14
832>	14	4	16	9	11	12	8	16:	840>	7	11	11	4	16
846>	18	6	13	10	11	8	13	6:	854>	7	0	13	11	0
860>	0	11	0	0	16	7	9	5:	868>	0	16	2	0	17
874>	12	6	5	10	9	7	7	8:	882>	4	9	5	7	7
888>	9	9	0	13	3	0	12	2:	896>	8	7	0	13	0
902>	13	0	7	9	3	5	6	11:	910>	4	7	8	5	0
916>	15	3	0	13	2	7	3	7:	924>	0	10	0	0	0
930>	0	0	11	6	8	0	0	0:	938>	0	11	2	0	0
944>	7	0	0	12	0	0	0	0:	952>	0	0	0	0	0
958>	0	0	0	9	5	0	11	0:	966>	6	0	0	9	0
972>	0	0	0	0	11	0	0	0:	980>	0	0	0	0	0
986>	0	0	0	0	0	0	0	0:	994>	0	0	0	0	0
1000>	0	0	0	0	0	0	0	0:	1008>	0	0	8	0	9
1014>	0	0	0	0	0	0	0	0:	1022>	0	0	0	0	8
1028>	0	0	0	0	0	0	0	0:	1036>	0	0	0	0	0
1042>	0	0	0	0	0	0	0	0:	1050>	0	0	6	0	0
1056>	0	0	0	0	0	0	0	0:	1064>	0	0	0	0	0
1070>	0	0	0	0	0	0	0	0:	1078>	0	0	0	0	0
1084>	0	0	0	0	0	0	0	0:	1092>	0	0	0	0	0
1098>	0	0	0	0	0	0	0	0:	1106>	0	7	0	0	7

SUM ODD 4777.4 4821.3 4865.8 4634.0 4837.7 4835.7 4922.0
 EV 9911.6 9076.3 9281.0 9863.5 8946.7 8554.0 10208.0
 RATIO 0.48200 0.53119 0.52427 0.46982 0.54073 0.56531 0.48217
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.511745

A14003.SUM 1293 PKS W MIN. 1 CNTS. 11-JUN-93 09:30:14 SUM I: 0.2016E+05
 REF NO. 3 (CONSOL) 0-11 N AV MW: 407.8
 ACQUIRED 5-27-93 12:12:04 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 528.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -64 TO 494 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2					RH		ROH	
48>	0	0	0	0	0	0	0	43:	56>	44	58	0	0	0	0
62>	0	0	0	0	0	0	0	33:	70>	18	38	0	0	0	0
76>	0	0	0	0	27	27	0	0:	84>	29	24	0	0	0	0
90>	0	20	0	0	61	31	19	19:	98>	33	28	0	0	0	0
104>	0	0	0	0	139	24	31	0:	112>	27	34	26	20	0	18
118>	0	16	0	21	173	20	25	12:	126>	38	17	41	0	0	49
132>	90	35	115	44	152	18	55	18:	140>	27	13	143	26	33	75
146>	228	83	204	60	119	27	42	24:	154>	52	15	266	73	75	74
160>	294	115	235	49	99	15	95	51:	168>	678	55	330	98	385	81
174>	379	119	202	44	180	25	211	93:	182>	1156	93	352	125	798	107
188>	507	87	154	52	278	41	422	103:	196>	944	90	380	126	751	107
202>	1344	84	355	59	370	76	750	109:	210>	719	77	434	91	678	101
216>	1055	89	505	59	464	106	834	112:	224>	654	82	514	80	557	64
230>	562	116	483	75	551	128	684	115:	238>	506	81	405	89	785	94
244>	537	101	420	108	433	118	475	99:	252>	361	69	311	83	574	110
258>	510	94	395	109	408	88	362	83:	266>	297	70	329	72	414	124
272>	400	93	313	118	542	115	320	80:	280>	262	101	372	92	332	124
286>	313	92	278	101	392	103	293	82:	294>	248	69	314	110	332	122
300>	290	119	245	75	303	99	248	82:	308>	236	97	263	111	248	116
314>	233	97	344	89	274	108	231	93:	322>	216	116	230	115	240	101
328>	205	92	292	113	251	100	195	103:	336>	203	113	222	119	242	108
342>	193	87	208	118	228	104	199	107:	350>	238	114	203	111	235	104
356>	232	76	230	98	215	103	182	108:	364>	233	104	211	95	166	107
370>	178	96	221	91	216	99	184	88:	378>	191	102	189	98	174	95
384>	190	84	190	93	184	97	188	106:	392>	177	98	163	91	167	90
398>	175	97	179	104	150	106	165	94:	406>	167	92	154	98	151	87
412>	146	87	180	117	147	98	155	87:	420>	155	80	148	106	167	88
426>	135	93	159	96	159	0	172	86:	434>	124	103	131	0	190	98
440>	153	83	148	95	160	84	144	90:	448>	177	101	143	91	129	95
454>	148	99	161	83	134	92	120	80:	462>	149	95	151	96	132	79
468>	151	82	132	82	154	82	149	80:	476>	134	99	124	95	127	84
482>	130	92	125	91	131	90	157	89:	490>	145	86	136	91	120	103
496>	123	80	150	86	111	104	139	92:	504>	121	91	112	87	114	86
510>	125	89	153	89	131	100	112	108:	518>	127	92	119	93	125	91
524>	137	83	136	90	140	89	134	84:	532>	118	98	108	89	131	94
538>	133	95	128	89	131	84	130	73:	546>	126	81	118	90	138	83
552>	129	95	113	89	124	87	109	98:	560>	129	76	125	91	120	91
566>	114	86	122	91	118	83	118	78:	574>	118	75	123	85	130	86
580>	113	101	103	84	109	89	117	88:	588>	112	93	125	79	114	92
594>	115	88	114	70	114	91	112	82:	602>	120	80	111	82	109	86
608>	108	82	118	67	100	90	89	101:	616>	97	84	96	82	97	87
622>	103	79	103	87	101	70	113	74:	630>	97	86	92	81	100	77
636>	95	67	94	74	83	73	77	81:	644>	85	87	80	72	100	60
650>	88	82	77	63	89	71	91	73:	658>	88	69	74	69	78	56
664>	69	61	93	62	82	68	75	66:	672>	67	57	75	64	82	61
678>	85	61	83	55	84	57	69	65:	686>	76	58	69	61	69	59
692>	69	63	69	55	68	47	74	61:	700>	62	69	51	68	59	54
706>	68	52	65	55	56	53	57	59:	714>	50	57	61	49	64	54
720>	65	52	56	53	63	57	53	45:	728>	66	47	55	54	48	57
734>	51	50	53	49	58	37	62	46:	742>	54	37	46	46	59	39
748>	53	44	44	41	56	46	47	49:	756>	39	51	41	47	41	48
762>	52	31	53	44	44	53	33	37:	770>	47	39	40	43	41	35

A14003.SUM 1293 PKS W MIN. 1 CNTS. 11-JUN-93 09:30:57 SUM I: 0.2016E+05
 REF NO. 3 (CONSOL) 0-11 N AV MW: 407.8
 ACQUIRED 5-27-93 12:12:04 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 528.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -64 TO 494 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2					RH		ROH	
776>	44	36	49	30	38	36	49	32: 784>	41	34	45	33	40	36	
790>	40	31	43	35	41	31	43	34: 798>	37	37	42	29	38	31	
804>	45	24	43	25	38	28	30	34: 812>	40	31	36	26	33	39	
818>	32	30	25	35	22	31	36	23: 826>	34	27	32	24	28	28	
832>	28	32	29	29	27	26	36	25: 840>	28	20	31	30	27	26	
846>	23	35	21	22	32	23	25	33: 854>	19	33	15	33	16	28	
860>	26	25	26	22	20	26	28	18: 868>	22	24	21	16	29	21	
874>	24	23	17	28	17	17	31	18: 882>	19	21	21	19	21	26	
888>	18	17	23	17	24	13	19	27: 896>	15	21	24	20	15	22	
902>	19	20	12	19	19	17	15	18: 910>	16	23	12	22	12	23	
916>	12	22	15	20	14	15	20	20: 924>	19	10	27	7	16	22	
930>	10	21	15	16	14	16	17	17: 938>	12	22	11	18	13	17	
944>	16	18	13	10	22	4	24	13: 952>	17	11	13	15	12	16	
958>	15	14	17	8	18	13	12	16: 966>	12	14	10	18	15	15	
972>	0	24	4	20	14	11	11	10: 980>	16	10	15	11	11	16	
986>	6	12	16	10	6	11	13	13: 994>	3	17	9	11	9	12	
1000>	12	6	15	15	7	15	7	15: 1008>	8	13	11	12	10	11	
1014>	7	7	9	15	6	13	8	10: 1022>	12	8	8	11	9	10	
1028>	10	11	6	13	9	8	7	11: 1036>	8	8	10	10	6	7	
1042>	10	16	3	12	8	6	12	7: 1050>	6	12	6	9	10	5	
1056>	9	7	5	8	9	6	5	14: 1064>	3	10	7	7	5	9	
1070>	7	6	8	6	3	12	6	6: 1078>	8	5	10	2	9	10	
1084>	4	9	8	5	4	9	7	5: 1092>	6	8	6	5	7	0	
1098>	12	4	9	2	8	4	6	5: 1106>	6	5	8	4	2	9	
1112>	2	10	0	11	2	7	6	1: 1120>	6	4	5	4	9	3	
1126>	9	5	6	3	4	7	4	3: 1134>	5	4	8	2	6	5	
1140>	7	5	2	6	7	2	6	4: 1148>	3	8	0	7	2	4	
1154>	4	6	3	7	0	7	5	3: 1162>	5	5	1	9	4	6	
1168>	4	2	4	7	2	4	3	7: 1176>	4	3	1	6	2	6	
1182>	4	6	2	9	3	0	4	4: 1190>	5	3	5	2	3	7	
1196>	0	4	4	4	3	6	1	5: 1204>	4	4	4	0	5	5	
1210>	2	4	4	5	1	8	2	5: 1218>	3	4	2	3	1	6	
1224>	4	1	6	0	4	4	4	1: 1232>	0	6	2	5	3	1	
1238>	4	0	3	7	2	2	0	7: 1246>	4	2	4	1	4	0	
1252>	6	1	5	1	4	2	5	1: 1260>	0	5	1	7	0	5	
1266>	1	2	2	0	6	0	5	0: 1274>	3	4	2	2	2	3	
1280>	0	4	2	2	1	4	1	2: 1288>	0	6	0	0	4	3	
1294>	2	0	7	0	3	0	0	9: 1302>	0	2	2	5	0	3	
1308>	0	5	0	4	0	7	0	4: 1316>	0	0	0	6	0	3	
1322>	3	0	5	0	3	0	5	0: 1330>	6	0	0	0	5	0	
1336>	4	0	0	0	7	0	0	4: 1344>	0	0	4	0	4	0	
1350>	0	3	3	1	0	0	0	6: 1358>	0	0	3	0	0	6	
1364>	0	0	0	5	1	3	3	0: 1372>	5	0	0	5	0	2	
1378>	0	0	4	0	3	0	0	0: 1386>	0	5	0	1	0	0	
1392>	0	2	0	0	1	0	0	0: 1400>	0	0	0	0	0	0	

SUM ODD 4378.7 4123.2 4118.9 4308.6 4324.8 4288.4 4522.8
 EV 11160.9 8892.1 9441.3 9448.9 10925.1 8879.6 10480.6
 RATIO 0.39233 0.46369 0.43626 0.45599 0.39586 0.48295 0.43154
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.434291

B14004.SUM 212 PKS W MIN. 1 CNTS. 18-JUN-93 17:42:35 SUM I: 0.6173E+04
 REF #4 SOH-ASOH 1- 7 N AV MW: 147.2
 ACQUIRED 6-18-93 17:39:25 CHAN.#5 0- 4095; 6 MS/CHAN. WT AV MW: 170.7
 MAG. RET. TIME: 9999 MS, 8 SCANS/SPECTRM. 1 TO 1 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 10000. C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	21	0:	56>	18	19	1451	105	0	0
62>	0	7	0	0	7	0	0	0:	70>	14	8	16	0	0	0
76>	0	0	22	0	0	0	0	21:	84>	196	10	42	8	0	0
90>	0	0	395	14	22	6	13	20:	98>	247	1	51	7	0	0
104>	0	0	72	41	33	0	11	11:	112>	197	6	38	5	0	9
118>	29	4	103	44	47	5	68	12:	126>	149	6	44	4	0	16
132>	197	20	92	48	47	6	120	13:	140>	115	3	66	3	0	22
146>	352	40	63	39	36	5	102	7:	154>	77	5	72	5	42	19
160>	324	43	60	28	35	7	104	6:	168>	123	4	63	8	184	19
174>	266	26	54	19	51	7	110	9:	182>	136	0	54	8	250	8
188>	248	22	51	10	66	6	97	7:	196>	95	3	45	5	168	9
202>	160	7	41	9	66	3	105	4:	210>	67	4	45	7	103	4
216>	86	8	39	5	49	3	74	4:	224>	52	2	55	4	72	6
230>	45	3	35	0	43	2	50	1:	238>	32	3	33	5	46	3
244>	23	6	23	2	26	0	29	4:	252>	20	1	22	2	22	2
258>	14	3	12	1	15	2	16	1:	266>	13	0	18	2	10	1
272>	9	0	9	0	10	1	11	0:	280>	9	0	11	0	7	0
286>	3	0	4	0	7	0	5	0:	294>	6	0	5	0	4	0
300>	0	0	3	0	0	0	0	0:	308>	4	0	5	0	3	0
314>	0	0	0	0	2	0	0	0:	322>	0	0	3	0	0	0
328>	0	0	0	0	0	0	0	0:	336>	0	0	0	0	0	0
342>	0	0	0	0	0	0	0	0:	350>	0	0	0	0	11	0
356>	0	0	0	0	0	0	0	0:	364>	0	0	0	0	0	0
370>	0	0	0	0	0	0	0	0:	378>	0	0	0	0	0	0
384>	0	0	0	0	0	0	0	0:	392>	0	0	0	0	0	0
398>	0	0	0	0	0	0	0	0:	406>	0	0	0	0	0	0
412>	0	0	0	0	0	0	0	0:	420>	0	0	0	0	0	0
426>	0	0	0	0	0	0	0	0:	434>	0	0	0	0	0	0
440>	0	0	0	0	0	0	0	0:	448>	0	0	0	0	0	0
454>	0	0	0	0	0	0	0	0:	462>	0	0	0	0	0	0
468>	0	1	0	0	0	0	0	0:	476>	0	0	0	0	0	0

SUM ODD 188.7 259.7 53.8 121.4 76.7 177.8 118.1
 EV 1776.9 1097.9 561.7 937.2 1568.2 2141.3 920.6
 RATIO 0.10620 0.23653 0.09575 0.12956 0.04892 0.08302 0.12824
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.110638

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C14004.SUM 171 PKS W MIN. 1 CNTS. 21-JUN-93 19:52:38 SUM I: 0.2577E+04
 REPEAT REF #4 (CONSOL) 0- 4 N AV MW: 153.0
 ACQUIRED 6-21-93 19:49:25 CHAN.#5 0- 4095; 6 MS/CHAN. WT AV MW: 175.9
 MAG. RET. TIME: 9999 MS, 8 SCANS/SPECTRM. 1 TO 0 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 10000. C13XN, 86.00% C PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	0	0:	56>	0	0	1626	93	0	0
62>	0	0	0	0	0	0	0	0:	70>	0	0	16	0	0	0
76>	0	0	11	0	0	0	0	0:	84>	157	11	55	0	12	0
90>	0	0	34	0	17	0	13	0:	98>	158	3	41	0	0	0
104>	0	0	80	34	50	0	14	0:	112>	145	12	32	0	0	0
118>	26	0	97	58	58	0	55	7:	126>	126	3	46	0	0	18
132>	212	16	102	70	64	8	120	6:	140>	72	15	55	6	0	26
146>	355	35	82	59	41	6	107	1:	154>	70	6	72	2	41	27
160>	330	50	85	35	39	0	101	5:	168>	144	1	64	11	186	23
174>	278	29	60	22	49	11	95	12:	182>	156	4	48	10	275	15
188>	289	29	53	17	62	10	95	10:	196>	110	4	52	11	184	20
202>	197	28	38	13	59	6	114	8:	210>	73	4	62	6	126	20
216>	97	13	47	3	51	5	99	0:	224>	55	12	69	5	85	8
230>	53	3	36	3	45	5	49	6:	238>	40	5	40	4	53	8
244>	45	4	23	0	26	0	39	0:	252>	22	0	30	0	27	5
258>	22	0	15	0	20	0	18	5:	266>	14	0	21	3	15	0
272>	14	0	10	0	10	0	12	7:	280>	12	0	12	0	10	0
286>	7	0	0	0	0	0	0	0:	294>	8	0	8	0	0	0
300>	0	0	0	0	0	0	0	0:	308>	0	0	0	0	0	0
314>	0	0	0	0	0	0	0	0:	322>	0	0	0	0	0	0
328>	0	0	0	0	0	0	0	0:	336>	0	0	0	0	0	0
342>	0	0	0	0	0	0	0	0:	350>	0	0	0	0	12	0

SUM ODD 207.5 314.2 49.4 67.5 78.8 152.6 169.5
 EV 1924.1 775.6 592.0 931.8 1363.1 2348.7 1025.2
 RATIO 0.10782 0.40510 0.08348 0.07243 0.05781 0.06499 0.16537
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.116015
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A14005.SUM 1289 FKS W MIN. 1 CNTS. 08-JUN-93 14:05:28 SUM I: 0.3512E+05
 REF NO. 5 (CONSOL) 0-12 N AV MW: 429.2
 ACQUIRED 5-28-93 14:13:58 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 531.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO 501 IEFG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	0	23:	56>	34	59	0	0	0	0
62>	0	0	0	0	0	0	0	22:	70>	0	24	0	19	10	13
76>	0	0	0	0	0	0	14	15:	84>	17	17	0	0	0	0
90>	0	0	0	0	21	0	16	13:	98>	0	18	0	0	0	0
104>	13	13	12	11	16	0	15	13:	112>	13	0	0	0	0	0
118>	11	0	0	10	16	11	0	0:	126>	15	9	10	11	12	20
132>	36	13	15	14	35	8	10	0:	140>	12	0	62	19	0	39
146>	143	28	36	34	35	8	15	0:	154>	42	10	157	21	64	43
160>	255	47	47	18	34	10	81	37:	168>	533	14	194	51	481	59
174>	331	62	69	23	164	14	298	79:	182>	1031	38	246	71	1027	76
188>	464	69	77	20	244	21	459	83:	196>	807	63	301	63	872	89
202>	968	59	328	23	355	47	742	90:	210>	557	68	381	50	686	71
216>	772	85	449	36	489	90	761	106:	224>	452	53	414	48	523	51
230>	487	64	442	54	505	114	611	87:	238>	327	50	321	75	687	93
244>	411	85	377	69	413	83	388	72:	252>	249	51	251	61	533	77
258>	420	80	322	91	357	112	295	75:	266>	214	45	240	84	352	106
272>	392	78	296	94	498	84	241	83:	280>	198	53	396	72	315	107
286>	275	105	237	99	393	86	259	68:	294>	182	83	359	99	312	95
300>	291	78	220	75	271	94	264	65:	308>	239	70	300	108	269	90
314>	227	87	347	102	268	88	242	87:	322>	257	81	255	111	263	95
328>	186	94	312	99	289	96	235	85:	336>	265	88	249	90	282	96
342>	203	80	271	98	268	88	224	99:	350>	296	109	247	100	247	79
356>	279	81	279	97	248	91	236	86:	364>	271	100	238	94	182	94
370>	249	103	243	97	270	100	223	88:	378>	239	87	253	98	226	73
384>	239	92	240	92	242	95	228	99:	392>	206	100	215	88	221	82
398>	247	83	227	100	199	94	228	84:	406>	238	87	205	96	194	85
412>	207	98	244	94	211	84	200	87:	420>	218	83	191	78	226	82
426>	198	95	225	88	200	88	192	86:	434>	181	98	177	84	204	99
440>	191	94	204	85	180	100	184	91:	448>	210	74	183	89	190	89
454>	198	87	204	78	190	80	171	88:	462>	182	96	199	73	175	89
468>	184	88	181	90	185	82	193	84:	476>	179	86	199	89	189	80
482>	183	84	167	84	179	89	206	97:	490>	183	88	171	93	177	94
496>	179	87	176	84	168	76	187	98:	504>	192	83	179	89	173	84
510>	162	95	200	86	188	87	176	97:	518>	162	83	169	80	169	100
524>	163	86	181	94	185	82	187	88:	532>	141	94	150	84	183	111
538>	168	98	162	93	168	99	168	91:	546>	164	90	156	99	162	97
552>	171	114	179	90	159	95	169	87:	560>	165	91	174	90	163	96
566>	172	97	168	90	162	95	157	84:	574>	154	90	158	102	167	97
580>	173	84	152	102	162	85	153	95:	588>	152	87	174	91	170	94
594>	159	102	152	86	154	90	144	86:	602>	154	91	151	105	151	87
608>	155	87	140	95	130	88	141	82:	616>	143	95	133	105	154	75
622>	151	81	144	74	143	74	138	92:	630>	138	89	141	86	121	100
636>	123	84	121	87	113	89	136	61:	644>	148	70	133	81	116	77
650>	114	78	115	93	114	80	120	84:	658>	122	77	108	76	114	80
664>	110	79	99	77	115	64	112	69:	672>	100	76	105	71	106	65
678>	103	72	96	68	100	66	105	64:	686>	109	61	99	64	97	69
692>	98	60	101	64	90	64	92	63:	700>	87	67	80	71	85	71
706>	84	60	93	58	79	60	75	63:	714>	81	54	81	56	69	58
720>	83	51	76	56	74	50	79	53:	728>	73	50	77	55	69	49
734>	66	56	64	55	75	49	65	45:	742>	63	48	63	51	64	43
748>	62	48	64	42	68	40	55	46:	756>	58	38	60	38	58	43
762>	55	48	48	51	48	38	56	40:	770>	58	40	55	39	55	39

A14005.SUM 1289 PKS W MIN. 1 CNTS. 08-JUN-93 14:06:12 SUM I: 0.3512E+05
 REF NO. 5 (CONSOL) 0-12 N AV MW: 429.2
 ACQUIRED 5-28-93 14:13:58 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 531.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2	MASS>	U1		RH		ROH		
776>	59	41	52	39	51	40	39	42: 784>	48	35	47	35	51	33	
790>	51	30	41	43	40	36	52	35: 798>	35	38	43	31	43	29	
804>	43	32	43	30	41	34	36	32: 812>	35	38	37	33	35	27	
818>	38	31	35	28	37	26	38	28: 826>	38	23	40	25	29	28	
832>	33	32	32	24	34	28	30	29: 840>	28	25	29	32	27	21	
846>	28	31	26	26	26	25	24	24: 854>	26	25	29	19	33	22	
860>	25	25	21	26	27	21	29	19: 868>	24	21	28	22	24	16	
874>	26	23	27	17	29	14	26	17: 882>	21	19	22	20	21	21	
888>	20	20	15	25	17	19	20	21: 896>	19	18	20	16	14	24	
902>	17	20	14	19	19	14	23	14: 910>	17	15	21	13	20	14	
916>	17	15	19	16	17	17	18	13: 924>	16	14	16	15	14	8	
930>	21	15	14	12	18	13	14	12: 938>	16	9	15	11	15	14	
944>	12	14	11	18	10	13	14	11: 952>	10	18	9	13	14	13	
958>	14	10	14	12	11	16	8	14: 966>	11	13	12	13	10	12	
972>	10	11	11	8	11	11	9	13: 980>	9	9	10	11	7	14	
986>	8	10	8	7	12	9	9	9: 994>	12	6	11	6	15	6	
1000>	9	10	9	10	8	4	12	6: 1008>	9	7	10	9	4	15	
1014>	1	13	6	7	8	6	9	8: 1022>	7	8	5	13	2	12	
1028>	5	11	6	8	7	7	6	9: 1036>	8	5	7	7	9	6	
1042>	6	8	3	9	8	5	6	9: 1050>	4	8	3	8	6	3	
1056>	11	3	6	6	8	2	8	5: 1064>	4	7	5	8	6	4	
1070>	7	2	9	2	7	5	5	6: 1078>	4	6	5	6	3	5	
1084>	7	5	5	7	2	5	6	4: 1092>	4	6	0	9	2	6	
1098>	4	4	7	1	8	1	7	4: 1106>	5	3	4	3	4	4	
1112>	5	2	6	4	5	4	4	4: 1120>	2	7	4	3	3	5	
1126>	3	5	1	7	2	2	7	0: 1134>	8	1	5	4	2	5	
1140>	0	5	3	4	2	5	4	2: 1148>	5	1	6	2	5	1	
1154>	4	2	5	2	4	4	1	3: 1162>	1	6	0	7	3	4	
1168>	2	5	3	3	2	4	4	2: 1176>	2	4	2	4	2	5	
1182>	0	4	1	4	1	5	0	4: 1190>	1	2	3	1	3	2	
1196>	3	2	2	5	0	4	0	3: 1204>	4	0	3	2	1	3	
1210>	0	3	4	0	3	2	2	4: 1218>	0	4	2	3	2	3	
1224>	2	0	3	1	2	3	2	2: 1232>	2	2	2	3	0	2	
1238>	4	2	2	1	4	3	0	6: 1246>	0	3	2	1	2	3	
1252>	1	3	0	3	2	2	1	4: 1260>	0	2	1	2	3	2	
1266>	0	2	3	0	2	2	0	2: 1274>	2	0	3	1	1	2	
1280>	2	1	3	0	2	1	2	0: 1288>	3	1	1	2	2	0	
1294>	3	1	0	0	5	0	0	0: 1302>	0	4	0	2	0	4	
1308>	1	2	0	0	3	1	0	3: 1316>	1	1	1	2	1	1	
1322>	1	0	3	0	2	1	1	2: 1330>	0	2	0	3	0	1	
1336>	0	0	3	0	2	0	2	2: 1344>	1	2	0	2	0	0	
1350>	0	4	0	1	0	3	0	0: 1358>	2	1	0	0	0	0	
1364>	3	0	1	0	2	0	2	1: 1372>	0	0	0	3	1	0	
1378>	0	0	3	0	1	0	3	0: 1386>	1	0	0	3	0	0	
1392>	0	1	0	1	0	1	1	0: 1400>	0	0	0	0	0	0	

SUM ODD 4058.3 3863.7 3843.7 4007.7 3797.6 3998.8 4102.1
 EV 11110.7 9083.4 9771.8 10227.4 10754.5 9322.7 11800.3
 RATIO 0.36526 0.42536 0.39334 0.39186 0.35312 0.42893 0.34762
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.383952

A14006.SUM 1166 PKS W MIN. 1 CNTS. 14-JUN-93 10:56:20 SUM I: 0.4281E+05
 REF NO. 6(CONSOL) 0-11 N AV MW: 401.6
 ACQUIRED 6- 4-93 16:09:13 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 473.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% C PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	16	0	0	0	14:	56>	58	49	20	0	0	0
62>	0	0	0	0	0	0	25	24:	70>	41	25	0	0	0	0
76>	0	0	0	0	16	0	29	27:	84>	39	21	19	0	0	23
90>	12	0	13	0	31	0	30	15:	98>	28	14	9	8	0	0
104>	0	0	12	12	48	8	24	7:	112>	17	13	11	0	0	10
118>	11	6	17	18	56	11	17	11:	126>	18	17	17	0	14	18
132>	22	15	27	12	40	11	12	11:	140>	7	12	32	10	22	23
146>	66	23	39	19	32	11	20	15:	154>	19	13	46	18	39	34
160>	85	37	40	22	35	12	39	34:	168>	182	24	65	40	156	53
174>	103	47	69	18	104	16	150	91:	182>	499	40	111	79	384	77
188>	148	42	104	22	191	29	286	119:	196>	487	70	167	64	398	88
202>	943	71	370	42	272	67	632	126:	210>	433	71	284	64	338	81
216>	888	101	523	67	424	170	728	143:	224>	421	72	338	66	387	60
230>	506	129	543	91	601	171	713	131:	238>	348	75	296	115	845	120
244>	571	114	461	95	473	163	463	129:	252>	315	60	304	103	612	188
258>	494	151	426	132	454	122	376	101:	266>	313	66	335	109	504	143
272>	473	113	386	0	756	133	381	92:	280>	286	93	485	149	433	143
286>	401	91	323	126	465	154	280	110:	294>	264	101	435	125	410	140
300>	340	116	289	128	348	132	294	117:	308>	289	112	390	134	362	112
314>	240	117	387	140	341	121	281	117:	322>	283	124	337	130	345	115
328>	262	98	356	156	332	120	269	124:	336>	271	114	253	0	344	174
342>	213	0	299	144	291	127	253	115:	350>	363	141	250	156	244	122
356>	298	125	274	140	250	133	215	115:	364>	325	136	249	182	169	0
370>	314	128	260	149	281	137	211	112:	378>	252	177	272	144	204	178
384>	155	134	234	173	203	168	244	205:	392>	183	179	217	191	200	154
398>	231	147	211	207	172	185	240	176:	406>	215	143	197	170	175	162
412>	174	181	216	229	174	180	169	189:	420>	194	173	168	166	228	196
426>	161	185	194	201	183	197	170	169:	434>	186	170	152	171	220	197
440>	182	179	189	156	199	151	182	160:	448>	229	186	175	142	201	190
454>	193	181	178	174	161	161	156	176:	462>	186	202	208	185	176	169
468>	192	171	173	159	176	172	189	182:	476>	183	168	189	190	187	170
482>	174	171	150	158	157	160	204	183:	490>	182	167	169	172	161	164
496>	174	152	190	160	171	151	175	183:	504>	178	181	152	158	159	144
510>	153	154	186	172	169	164	161	173:	518>	153	152	149	146	163	149
524>	157	145	160	171	176	150	161	158:	532>	171	150	133	131	165	136
538>	166	156	164	134	155	157	154	143:	546>	147	129	153	140	140	151
552>	153	155	154	142	145	128	129	135:	560>	128	131	136	136	142	141
566>	137	140	142	132	128	122	124	119:	574>	126	114	138	130	133	134
580>	136	124	126	117	116	120	118	113:	588>	122	106	123	116	122	120
594>	118	121	114	111	101	100	110	100:	602>	109	106	112	106	112	104
608>	111	100	107	86	101	90	106	98:	616>	101	95	96	91	96	89
622>	95	80	94	77	87	89	87	90:	630>	85	95	87	86	87	81
636>	87	76	70	78	77	81	77	87:	644>	73	91	74	63	75	71
650>	77	69	67	67	69	74	66	66:	658>	69	67	68	67	65	62
664>	70	63	63	65	62	57	65	63:	672>	57	55	62	54	53	58
678>	53	54	50	62	50	62	42	50:	686>	59	44	49	51	51	51
692>	46	48	55	46	50	44	49	45:	700>	45	43	43	49	34	45
706>	43	42	43	46	39	40	34	41:	714>	38	38	40	36	37	41
720>	36	36	41	37	36	34	40	27:	728>	38	33	34	29	35	30
734>	35	29	30	40	26	33	27	29:	742>	30	30	31	31	28	25
748>	35	20	32	24	27	28	24	26:	756>	26	31	26	23	23	24
762>	26	23	26	20	28	22	21	25:	770>	22	24	22	23	36	38

A14006.SUM 1166 PKS W MIN. 1 CNTS. 14-JUN-93 10:57:02 SUM I: 0.4281E+05
 REF NO. 6(CONSOL) 0-11 N AV MW: 401.6
 ACQUIRED 6- 4-93 16:09:13 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 473.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
776>	52	11	25	19	22	19	20	22	784>	16	22	13	23	17	19
790>	21	17	21	15	21	18	16	20	798>	17	18	18	13	18	14
804>	18	15	16	14	19	13	16	15	812>	12	16	13	16	15	13
818>	15	14	14	15	15	14	11	15	826>	13	11	13	12	11	15
832>	15	10	14	14	12	12	12	9	840>	13	11	13	9	12	11
846>	11	10	11	10	11	9	13	9	854>	12	7	12	8	11	8
860>	9	14	5	14	5	11	7	9	868>	7	14	6	11	9	9
874>	8	8	8	9	10	7	10	7	882>	7	9	9	5	8	7
888>	8	7	8	5	8	10	4	9	896>	6	8	9	6	7	6
902>	8	5	6	8	4	10	5	7	910>	7	6	7	6	5	7
916>	5	6	7	7	6	3	8	3	924>	7	5	5	6	4	5
930>	7	5	5	6	6	3	4	3	938>	6	4	2	6	5	4
944>	4	5	7	3	8	4	4	6	952>	4	6	3	4	6	1
958>	6	5	3	5	5	3	6	5	966>	3	4	4	5	3	5
972>	3	5	2	6	3	4	4	5	980>	3	5	2	5	3	3
986>	4	3	3	4	2	2	5	3	994>	4	2	5	3	2	5
1000>	2	4	4	3	2	5	3	2	1008>	4	2	4	2	4	2
1014>	0	4	1	5	2	2	2	4	1022>	2	2	4	4	2	4
1028>	2	3	2	3	2	3	3	2	1036>	4	1	3	1	4	2
1042>	2	0	7	1	3	1	3	3	1050>	2	3	1	2	2	3
1056>	1	3	1	3	1	3	1	4	1064>	0	3	2	1	3	2
1070>	2	2	3	0	3	2	1	2	1078>	3	1	3	1	2	2
1084>	1	3	1	2	1	0	3	0	1092>	3	1	0	3	1	2
1098>	2	2	2	0	2	1	3	0	1106>	4	1	1	2	2	1
1112>	1	3	0	3	1	2	2	0	1120>	3	1	1	0	0	4
1126>	1	1	0	3	2	0	1	3	1134>	0	3	2	2	1	0
1140>	3	0	0	2	1	1	1	0	1148>	2	1	2	2	1	0
1154>	3	0	2	1	2	0	3	0	1162>	0	4	0	2	0	2
1168>	1	0	2	0	2	0	1	1	1176>	2	0	2	1	1	0
1182>	1	0	0	0	2	1	0	0	1190>	2	1	2	1	0	0
1196>	2	0	0	2	0	2	1	0	1204>	0	0	0	0	3	1
1210>	0	2	0	0	0	0	0	0	1218>	0	2	0	0	0	3
1224>	0	0	2	1	0	1	0	1	1232>	0	0	2	2	0	0
1238>	0	0	2	0	1	0	3	0	1246>	1	0	1	1	0	0
1252>	2	0	0	0	2	0	1	0	1260>	0	2	0	0	2	0
1266>	0	0	0	0	0	0	0	0	1274>	0	2	0	0	0	0
1280>	2	0	1	0	0	0	0	2	1288>	0	0	0	0	2	0
1294>	1	0	0	0	0	0	0	0	1302>	2	0	1	0	0	0
1308>	0	0	2	0	0	0	0	0	1316>	0	0	0	0	0	0
1322>	0	0	0	0	0	0	0	0	1330>	0	0	0	0	2	0
1336>	0	0	0	0	0	0	0	0	1344>	0	0	0	0	2	0
1350>	0	0	0	0	0	0	0	0	1358>	0	0	0	0	0	0
1364>	0	0	1	0	0	0	0	0	1372>	0	0	0	0	0	0

SUM ODD 4829.6 4974.6 5132.9 5286.3 4918.8 4913.7 5156.9
 EV 9980.7 8864.5 9266.9 9226.7 9064.5 8093.5 9684.3
 RATIO 0.48390 0.56118 0.55390 0.57294 0.54265 0.60711 0.53251
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.548650

B14006.SUM 1037 PKS W MIN. 1 CNTS. 17-JUN-93 14:21:03 SUM I: 0.2588E+05
 REPEAT REF #6 PFC (CONSOL) 0- 6 N AV MW: 438.6
 ACQUIRED 6-17-93 13:57:18 CHAN.#5 0- 81911 6 MS/CHAN. WT AV MW: 501.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 31 TO 502 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
	AR			U3		U2				U1	RH		ROH		
48>	0	0	0	0	0	0	0	17: 56>	52	61	25	0	16	52	
62>	0	0	0	0	0	0	13	23: 70>	31	31	0	0	0	0	
76>	0	0	0	0	22	0	18	0: 84>	14	0	0	0	0	0	
90>	0	0	0	0	48	15	26	13: 98>	22	15	0	0	0	0	
104>	102	10	0	11	26	0	17	0: 112>	19	0	7	0	0	0	
118>	21	9	15	6	44	0	14	0: 126>	22	10	0	13	0	0	
132>	21	8	18	11	21	0	15	0: 140>	0	0	0	0	22	16	
146>	16	21	24	19	19	0	0	0: 154>	0	0	12	10	20	16	
160>	28	25	24	19	15	7	21	25: 168>	46	15	34	25	48	29	
174>	33	29	27	17	47	14	73	66: 182>	209	28	36	54	134	52	
188>	37	26	63	15	91	24	166	71: 196>	277	37	101	60	132	64	
202>	456	64	196	39	134	55	383	80: 210>	281	53	162	42	156	52	
216>	482	78	278	36	233	85	473	79: 224>	260	52	195	52	214	43	
230>	343	73	296	71	317	118	391	98: 238>	200	61	183	70	583	88	
244>	355	102	299	81	314	107	282	82: 252>	200	47	173	67	524	121	
258>	443	76	284	102	329	96	248	87: 266>	194	69	215	91	398	141	
272>	412	79	303	102	624	108	278	65: 280>	235	84	452	106	343	141	
286>	327	100	251	112	477	119	293	74: 294>	222	91	411	117	399	120	
300>	330	103	268	93	345	117	321	84: 308>	274	104	352	140	318	114	
314>	268	116	434	130	347	118	297	100: 322>	309	116	312	145	332	121	
328>	268	93	429	107	350	121	284	117: 336>	305	118	281	133	356	136	
342>	257	106	365	147	337	118	280	122: 350>	422	136	313	126	319	130	
356>	341	120	329	134	290	139	253	108: 364>	393	136	324	112	290	112	
370>	314	129	343	133	352	139	281	109: 378>	293	147	311	146	281	121	
384>	299	144	289	113	274	142	340	131: 392>	290	143	322	108	299	117	
398>	330	105	327	137	276	139	324	132: 406>	309	130	273	139	253	116	
412>	270	157	332	165	283	125	281	137: 420>	300	134	265	113	362	133	
426>	266	127	298	155	283	127	258	142: 434>	237	134	253	139	349	159	
440>	290	125	267	151	260	148	265	139: 448>	313	149	252	139	289	154	
454>	295	125	271	140	258	148	251	125: 462>	287	136	336	126	281	151	
468>	266	136	258	132	275	129	288	139: 476>	252	155	272	162	260	141	
482>	270	116	247	116	268	135	312	144: 490>	256	141	261	138	253	131	
496>	245	141	272	144	245	145	290	136: 504>	287	125	252	131	225	132	
510>	259	114	302	142	256	134	242	143: 518>	246	130	231	128	269	119	
524>	256	138	239	158	267	133	236	132: 532>	225	131	229	125	231	148	
538>	234	154	229	149	203	153	220	144: 546>	206	135	215	126	231	123	
552>	240	146	250	137	198	128	210	114: 560>	206	124	203	125	224	131	
566>	224	137	223	115	190	115	200	115: 574>	196	122	213	126	215	123	
580>	191	116	194	113	187	108	187	92: 588>	196	101	200	111	186	127	
594>	180	116	149	112	162	114	163	97: 602>	170	123	163	106	167	111	
608>	163	99	145	109	140	93	155	103: 616>	149	100	154	110	154	95	
622>	142	87	146	92	142	85	145	83: 630>	151	94	137	101	117	83	
636>	132	87	123	75	127	83	130	79: 644>	136	76	122	79	123	70	
650>	108	80	115	75	107	76	106	83: 658>	102	80	104	70	104	64	
664>	105	76	93	65	100	73	97	66: 672>	103	66	81	62	84	71	
678>	85	61	93	52	101	48	99	53: 686>	93	54	78	59	81	48	
692>	84	44	85	59	78	56	67	52: 700>	70	51	73	40	70	45	
706>	76	44	70	48	68	46	66	44: 714>	59	46	58	45	66	46	
720>	63	43	65	36	56	39	62	35: 728>	49	45	55	40	42	41	
734>	57	28	56	35	47	36	53	37: 742>	47	32	52	34	47	34	
748>	43	36	44	30	51	32	36	41: 756>	43	21	43	32	40	29	
762>	38	30	42	29	44	21	40	29: 770>	33	25	40	35	51	23	

B14006.SUM 1037 PKS W MIN. 1 CNTS. 17-JUN-93 14:21:45 SUM I: 0.2588E+05
 REPEAT REF #6 PFC (CONSOL) 0- 8 N AV MW: 436.6
 ACQUIRED 6-17-93 13:57:18 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 501.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 31 TO 502 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	U1	1	2	3	4	5
776>	35	26	40	19	35	20	39	23: 784>	26	23	27	28	28	23	
790>	35	17	30	20	25	21	31	21: 798>	25	21	31	16	29	22	
804>	23	20	24	24	17	19	31	16: 812>	23	21	19	21	19	23	
818>	20	17	23	18	21	14	24	13: 826>	20	18	21	13	18	17	
832>	21	12	26	9	22	12	14	16: 840>	15	17	14	19	14	16	
846>	15	10	19	15	12	13	15	17: 854>	11	15	9	15	13	13	
860>	12	14	16	8	17	12	13	8: 868>	16	11	14	9	17	11	
874>	14	10	9	10	15	6	11	13: 882>	9	12	11	9	10	9	
888>	11	10	11	11	12	7	13	10: 896>	10	10	12	4	8	11	
902>	10	8	11	8	9	7	12	9: 910>	6	9	5	9	6	13	
916>	5	0	13	7	7	6	8	6: 924>	6	8	6	9	7	4	
930>	9	10	4	9	8	2	10	3: 938>	11	3	7	5	6	8	
944>	7	6	7	6	7	5	8	5: 952>	6	6	6	5	7	5	
958>	8	6	6	8	1	5	9	2: 966>	5	4	7	3	5	4	
972>	5	6	4	7	2	5	7	1: 980>	8	1	5	8	6	3	
986>	5	5	5	2	5	4	6	2: 994>	5	3	4	3	6	3	
1000>	6	3	2	4	4	4	3	4: 1008>	4	2	7	3	3	0	
1014>	7	0	4	4	3	3	3	5: 1022>	4	2	3	3	3	7	
1028>	1	3	4	1	6	1	3	4: 1036>	2	2	4	2	3	2	
1042>	4	2	4	2	4	3	3	0: 1050>	3	5	2	0	6	0	
1056>	4	2	4	2	2	0	4	3: 1064>	2	5	0	4	1	4	
1070>	2	2	4	1	4	0	3	3: 1078>	0	5	0	4	1	0	
1084>	4	3	0	0	5	0	3	0: 1092>	4	0	3	2	3	2	
1098>	4	0	4	0	3	2	0	5: 1106>	0	0	0	0	5	0	
1112>	2	0	0	5	0	0	5	0: 1120>	1	2	0	2	0	4	
1126>	2	1	0	0	4	1	0	0: 1134>	3	0	3	1	0	0	
1140>	5	0	0	0	3	0	0	3: 1148>	1	4	0	0	2	0	
1154>	0	3	0	0	3	0	0	0: 1162>	0	0	0	0	4	0	
1168>	0	0	0	0	0	4	1	0: 1176>	0	0	0	0	0	3	
1182>	0	2	0	3	0	0	0	0: 1190>	0	0	0	0	0	0	
1196>	0	0	0	0	0	0	0	0: 1204>	0	0	0	0	0	0	
1210>	0	0	0	0	0	0	0	0: 1218>	0	0	0	0	0	0	
1224>	0	0	0	0	3	0	0	0: 1232>	0	0	0	0	0	0	
1238>	0	0	0	0	0	0	0	0: 1246>	0	0	0	0	0	0	
1252>	0	0	0	0	0	0	0	0: 1260>	0	0	0	0	0	0	
1266>	0	0	0	0	0	0	0	0: 1274>	0	0	0	0	0	0	
1280>	0	0	0	0	0	0	0	0: 1288>	0	0	0	0	0	0	
1294>	0	0	0	0	0	0	0	0: 1302>	0	0	0	0	0	0	
1308>	0	0	0	0	0	0	0	0: 1316>	0	0	0	0	0	0	
1322>	0	0	0	0	0	0	0	0: 1330>	0	0	0	0	0	0	
1336>	0	0	0	0	0	0	0	0: 1344>	0	0	0	0	0	0	
1350>	0	0	0	0	0	0	1	0: 1358>	0	0	0	0	0	0	

SUM ODD 4374.3 4471.5 4488.6 4381.2 4422.9 4452.2 4636.5
 EV 10340.9 9742.2 9982.6 9628.6 9517.1 9055.2 10189.9
 RATIO 0.42301 0.45899 0.44964 0.44576 0.46474 0.49168 0.45501
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.454833

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014006.SUM 1052 PKB W MIN. 5 CNTS. 05-AUG-93 15:33:53 SUM 1: 0.3947E+05
 REPEAT REF. NO 6 PFC 11A 0- 9 N AV MW: 444.2
 ACQUIRED 8- 2-93 16:23:48 CHAN.#3 0- 81911 6 MS/CHAN. WT AV MW: 509.5
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 29 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN: 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
			AR		U3		U2					RH		ROH	
48>	0	0	0	0	0	19	29	77: 56>	125	11	0	0	0	0	0
62>	0	12	0	0	0	0	38	30: 70>	50	0	0	0	0	0	0
76>	0	0	0	16	21	14	31	16: 84>	19	0	0	0	0	0	0
90>	0	0	11	0	22	14	16	10: 98>	0	14	0	0	0	0	0
104>	0	0	0	14	0	0	0	0: 112>	14	0	0	0	0	0	8
118>	0	0	0	0	15	0	13	7: 126>	10	0	0	0	0	9	0
132>	11	0	10	10	12	0	9	7: 140>	7	11	0	0	0	9	0
146>	12	10	10	11	12	7	9	0: 154>	8	0	0	0	0	13	11
160>	10	11	14	0	8	10	12	12: 168>	15	9	16	12	15	15	
174>	18	13	14	9	17	10	23	37: 182>	49	16	18	0	44	26	
188>	15	22	20	16	57	14	72	72: 196>	135	17	44	28	63	33	
202>	562	29	112	30	115	46	331	67: 210>	208	42	64	43	58	39	
216>	668	60	240	56	211	0	420	103: 224>	186	59	105	67	109	44	
230>	363	103	281	102	295	149	462	107: 238>	270	56	116	69	543	135	
244>	400	112	274	0	316	184	300	89: 252>	180	74	108	72	726	129	
258>	556	114	319	137	306	129	249	128: 266>	199	101	235	103	598	184	
272>	469	0	337	155	649	149	289	198: 280>	199	0	640	0	630	169	
286>	401	245	268	0	530	0	401	103: 294>	249	199	642	220	522	0	
300>	444	293	245	216	376	0	380	269: 308>	267	243	0	507	365	372	
314>	295	290	402	0	417	240	289	233: 322>	354	0	374	376	343	324	
328>	252	257	390	154	409	232	301	202: 336>	333	283	254	342	206	372	
342>	196	227	281	265	321	246	221	235: 350>	280	295	261	196	270	233	
356>	195	256	243	194	250	175	239	193: 364>	289	202	230	237	194	200	
370>	226	193	234	195	206	186	225	177: 378>	215	194	233	116	217	176	
384>	187	170	184	180	200	185	210	159: 392>	182	172	195	161	188	137	
398>	176	147	199	144	169	156	206	133: 406>	216	131	166	151	162	153	
412>	157	145	213	137	177	138	157	143: 420>	166	134	161	127	181	121	
426>	160	109	196	138	167	112	171	120: 434>	160	110	152	123	215	111	
440>	192	109	181	117	166	114	164	112: 448>	200	117	155	115	184	128	
454>	189	109	184	117	150	111	149	121: 462>	186	114	208	108	164	133	
468>	178	122	186	94	191	103	212	118: 476>	180	123	208	121	190	115	
482>	190	100	159	117	174	127	242	134: 490>	185	125	202	113	192	119	
496>	194	99	239	120	184	127	232	142: 504>	215	135	185	129	173	116	
510>	171	146	239	133	207	142	208	133: 518>	205	140	177	127	222	145	
524>	196	147	219	148	224	153	202	130: 532>	196	134	185	141	228	146	
538>	240	161	212	143	217	136	203	144: 546>	216	138	210	145	212	160	
552>	236	151	220	147	221	124	207	125: 560>	207	139	241	145	220	161	
566>	231	152	214	147	200	132	208	137: 574>	197	142	224	150	233	142	
580>	207	152	205	139	186	138	202	131: 588>	200	147	215	147	206	150	
594>	197	133	186	120	188	133	187	128: 602>	214	135	203	136	199	124	
608>	196	124	179	105	201	125	189	129: 616>	186	136	189	125	177	120	
622>	178	115	168	113	170	116	186	117: 630>	170	132	162	117	161	103	
636>	168	96	152	105	159	111	164	108: 644>	157	104	146	106	127	96	
650>	141	99	140	96	147	100	139	101: 658>	134	92	125	90	121	90	
664>	123	92	130	91	138	82	125	88: 672>	120	72	111	82	103	78	
678>	118	76	112	90	109	74	106	80: 686>	99	74	100	68	98	65	
692>	97	74	107	68	89	70	91	67: 700>	85	70	87	61	86	68	
706>	87	66	80	68	76	56	75	52: 714>	80	55	67	63	73	62	
720>	72	59	68	55	65	51	73	46: 728>	60	46	70	46	71	46	
734>	68	43	63	38	62	41	57	43: 742>	53	47	51	45	55	41	
748>	52	38	53	36	50	34	49	35: 756>	51	33	51	36	42	36	
762>	44	34	47	26	46	30	44	30: 770>	48	28	45	27	38	31	

C14004.SUM 1052 FKS W MIN. 5 CNTS. 05-AUG-93 15:34:36 SUM I: 0.3947E+05
 REPEAT REF. NO 6 PFC 11A 0-9 N AV MW: 444.2
 ACQUIRED 8- 2-93 16:23:48 CHAN.#S 0- 8191: 6 MS/CHAN. WT AV MW: 509.5
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 29 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN: 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
776>	37	31	33	29	36	33	39	30: 784>	34	28	33	28	33	22	
790>	36	28	29	23	33	23	32	20: 798>	34	24	30	22	33	21	
804>	27	21	28	26	24	27	22	15: 812>	31	20	26	19	23	22	
818>	21	16	30	15	23	17	22	15: 826>	26	16	20	16	21	17	
832>	22	11	19	16	17	16	21	11: 840>	20	15	15	13	19	17	
846>	12	13	17	10	21	11	18	11: 854>	15	16	15	13	13	14	
860>	13	12	16	12	17	9	11	13: 868>	16	6	15	13	9	12	
874>	11	11	15	7	16	5	16	5: 882>	11	10	6	12	12	10	
888>	10	6	15	6	10	7	11	5: 896>	9	9	9	5	13	5	
902>	8	11	7	8	8	8	10	9: 910>	9	8	6	5	11	5	
916>	8	11	3	11	5	9	6	8: 924>	6	7	4	9	6	9	
930>	5	8	6	9	5	7	7	5: 938>	6	5	6	5	6	8	
944>	3	6	6	6	5	6	4	8: 952>	2	3	4	6	5	6	
958>	2	6	6	5	3	5	5	5: 966>	4	5	4	6	3	4	
972>	4	3	6	3	3	4	5	5: 980>	3	4	3	5	1	5	
986>	3	3	4	3	3	3	4	4: 994>	3	2	4	3	5	4	
1000>	3	0	3	4	2	3	3	5: 1008>	2	3	0	5	5	2	
1014>	3	2	4	2	4	2	4	2: 1022>	4	3	2	3	2	4	
1028>	1	3	4	2	2	3	2	2: 1036>	2	3	2	3	1	3	
1042>	1	3	1	2	1	2	2	3: 1050>	2	2	2	2	2	3	
1056>	3	2	4	1	2	3	3	2: 1064>	0	1	2	3	2	3	
1070>	2	2	3	2	1	3	0	3: 1078>	1	2	0	3	2	0	
1084>	3	2	2	1	1	2	0	3: 1092>	1	2	1	0	4	0	
1098>	3	0	2	1	2	1	0	2: 1106>	1	1	1	2	1	0	
1112>	0	4	0	0	3	0	2	2: 1120>	1	1	2	0	0	3	
1126>	0	2	0	0	4	0	2	2: 1134>	0	0	0	0	0	0	
1140>	3	0	0	0	0	4	0	2: 1148>	0	0	2	1	1	0	
1154>	2	0	2	1	0	0	2	0: 1162>	2	0	0	0	3	0	
1168>	0	0	0	2	1	0	0	0: 1176>	0	0	0	0	0	0	
1182>	0	0	2	0	0	2	0	0: 1190>	0	0	0	0	0	3	
1196>	0	1	1	0	0	0	0	0: 1204>	2	0	0	0	0	0	
1210>	0	0	2	0	0	0	0	0: 1218>	3	0	0	0	0	2	
1224>	0	0	0	0	0	0	0	0: 1232>	0	0	0	0	1	0	
1238>	0	0	0	0	0	0	0	0: 1246>	0	0	0	0	0	0	
1252>	0	0	0	0	0	0	0	0: 1260>	2	0	0	0	0	0	
1266>	0	0	0	0	0	0	0	0: 1274>	0	0	0	0	0	0	
1280>	0	0	0	0	0	0	0	0: 1288>	0	0	2	0	1	0	
1294>	0	0	0	0	0	0	0	0: 1302>	0	0	0	2	0	0	
1308>	0	0	0	0	0	0	2	0: 1316>	0	0	0	0	0	0	
1322>	0	0	3	0	0	0	0	0: 1330>	0	0	0	0	0	0	
1336>	0	2	1	0	0	0	0	0: 1344>	0	0	0	0	0	0	
1350>	0	0	0	0	0	0	0	0: 1358>	0	0	0	0	0	0	
1364>	0	0	0	0	0	0	0	0: 1372>	0	0	0	0	0	0	
1378>	0	0	0	0	1	0	0	0: 1386>	0	0	0	0	0	0	

SUM ODD 5539.8 4621.1 5062.1 5576.7 5054.6 5597.0 5670.5
 EV 9828.8 8508.1 9150.7 9064.3 8228.7 7846.0 9498.2
 RATIO 0.56363 0.56665 0.55319 0.61524 0.61427 0.71337 0.59701
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.600758

AIM

Association for Information and Image Management

1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202

Centimeter

Inches

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2 of 2

E14007.SUM 1252 PKS W MIN. 1 CNTS. 14-JUN-93 11:34:00 SUM I: 0.2513E+05
 REF NO. 7 (CONSOL) 0- 8 N AV MW: 408.4
 ACQUIRED 6- 3-93 15:43:37 CHAN.#5 0- 8191: 6 MS/CHAN. WT AV MW: 503.7
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -66 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2					RH		ROH	
48>	0	0	0	0	0	0	0	0	56>	28	57	33	0	0	26
62>	0	0	0	0	0	0	0	19	70>	25	36	0	0	17	0
76>	0	0	0	0	0	0	0	12	84>	17	19	0	18	0	0
90>	0	12	0	0	48	0	0	21	98>	21	14	0	0	0	17
104>	0	0	17	0	57	0	31	0	112>	35	13	34	0	0	14
118>	0	12	0	27	61	11	27	16	126>	66	16	27	8	14	25
132>	18	0	57	5	70	8	28	12	140>	9	0	84	16	36	41
146>	53	25	112	20	62	12	16	12	154>	43	7	230	46	57	50
160>	103	41	152	20	46	9	56	59	168>	450	13	224	43	161	44
174>	176	35	98	17	239	22	207	117	182>	950	39	284	79	332	52
188>	218	38	100	30	424	21	423	140	196>	857	68	325	54	365	68
202>	1235	66	289	38	423	68	801	97	210>	722	53	387	58	419	35
216>	1074	102	549	57	479	94	837	86	224>	659	60	469	57	502	48
230>	725	121	616	67	514	99	650	67	238>	451	52	378	70	816	78
244>	598	123	455	91	450	82	442	54	252>	445	58	401	69	690	121
258>	545	98	398	71	393	78	330	61	266>	472	74	443	84	488	137
272>	476	105	331	89	597	80	329	71	280>	389	89	470	115	414	122
286>	354	92	258	71	472	99	353	74	294>	331	102	395	106	371	96
300>	295	82	264	64	376	101	348	102	308>	344	93	318	96	265	75
314>	222	83	383	90	342	118	308	112	322>	298	94	251	87	285	84
328>	222	97	355	95	326	105	277	101	336>	264	82	220	84	306	109
342>	245	82	294	108	280	108	248	130	350>	280	85	206	71	274	114
356>	250	106	257	109	229	99	207	95	364>	220	120	206	98	218	111
370>	240	102	218	113	209	94	185	107	378>	212	91	237	103	192	121
384>	201	127	173	108	175	98	227	103	392>	198	120	161	148	124	151
398>	173	144	162	117	147	112	190	106	406>	198	107	205	94	174	129
412>	158	94	206	100	155	132	184	97	420>	185	110	185	99	177	94
426>	157	101	194	97	181	102	181	113	434>	147	106	138	115	163	120
440>	139	150	124	151	116	124	134	140	448>	123	127	136	119	142	139
454>	114	149	156	146	123	137	124	122	462>	127	137	130	148	95	123
468>	137	142	129	139	118	147	106	140	476>	119	113	110	155	107	156
482>	111	156	104	131	125	125	122	165	490>	96	150	109	151	105	139
496>	100	131	146	124	109	137	93	143	504>	105	141	124	142	98	136
510>	94	116	113	135	102	138	115	152	518>	99	146	109	127	101	127
524>	100	145	91	151	81	141	102	138	532>	99	146	102	118	103	134
538>	97	132	107	149	100	139	92	132	546>	94	118	99	132	100	129
552>	106	131	108	113	110	127	93	137	560>	91	123	108	108	123	102
566>	123	123	105	112	111	112	95	110	574>	104	101	115	96	120	97
580>	121	84	146	84	121	97	111	87	588>	118	71	123	94	111	90
594>	110	93	124	91	113	83	111	78	602>	110	97	115	84	116	83
608>	112	92	109	78	105	72	99	89	616>	98	82	121	81	116	83
622>	97	86	90	83	89	83	88	80	630>	101	75	100	84	99	76
636>	97	73	87	77	81	68	91	79	644>	86	77	81	83	85	76
650>	85	68	85	70	88	74	75	71	658>	90	69	81	71	75	68
664>	79	62	75	61	73	66	71	73	672>	86	46	90	58	67	69
678>	67	60	74	58	69	63	63	63	686>	66	51	64	64	60	55
692>	70	53	74	54	57	55	62	58	700>	54	56	53	60	54	56
706>	59	61	60	51	58	47	56	52	714>	50	48	45	46	51	42
720>	61	33	56	46	46	46	43	36	728>	60	44	43	47	45	32
734>	53	38	51	44	47	44	40	39	742>	43	38	46	36	40	39
748>	45	37	41	33	46	38	40	36	756>	32	37	45	33	45	30
762>	40	33	40	29	43	30	35	34	770>	31	30	39	35	35	27

B14007.SUM 1252 PKS W MIN. 1 CNTS. 14-JUN-93 11:34:43 SUM I: 0.2513E+05
 REF NO. 7 (CONSOL) 0- 8 N AV MW: 408.4
 ACQUIRED 6- 3-93 15:43:37 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 503.7
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -66 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% FG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
776>	41	33	32	26	34	29	34	32	784>	32	29	30	31	28	33
790>	21	35	30	20	39	29	27	31	798>	33	23	30	29	25	25
804>	34	22	26	26	26	20	22	27	812>	34	22	21	25	21	25
818>	25	22	23	20	31	17	30	20	826>	28	24	21	25	18	22
832>	21	20	23	23	17	20	18	21	840>	21	19	19	21	16	21
846>	20	20	22	15	21	23	15	16	854>	24	16	20	17	20	17
860>	17	20	19	18	17	12	21	12	868>	27	11	15	13	15	16
874>	12	21	10	24	13	15	11	15	882>	16	14	14	16	10	13
888>	18	11	21	9	18	15	8	15	896>	12	14	11	12	17	8
902>	12	14	12	16	11	13	7	15	910>	9	13	10	12	12	12
916>	10	13	13	10	11	20	5	17	924>	8	14	10	14	7	11
930>	12	12	8	11	11	11	12	10	938>	10	11	9	9	10	6
944>	8	11	11	6	11	8	10	12	952>	9	10	7	10	9	7
958>	8	11	7	8	12	6	13	4	966>	9	8	9	9	9	7
972>	9	7	8	9	5	10	6	9	980>	7	6	10	9	5	7
986>	10	3	11	7	5	7	7	9	994>	7	7	5	5	7	7
1000>	3	6	7	6	7	7	5	7	1008>	9	5	7	9	9	1
1014>	8	7	4	9	3	0	9	6	1022>	6	3	8	6	6	5
1028>	5	5	6	5	7	7	1	9	1036>	4	6	4	9	3	4
1042>	5	5	3	6	6	4	7	4	1050>	5	5	6	2	7	5
1056>	3	7	1	5	5	4	4	3	1064>	3	7	2	6	2	7
1070>	1	6	4	3	5	1	8	2	1078>	4	4	7	0	5	3
1084>	4	2	3	7	1	6	3	3	1092>	3	7	2	4	3	3
1098>	4	3	7	2	3	2	5	3	1106>	3	4	0	3	2	5
1112>	2	5	1	3	4	4	2	3	1120>	3	3	3	4	1	3
1126>	2	3	3	3	3	5	0	2	1134>	5	2	5	2	4	3
1140>	5	2	3	2	4	3	5	2	1148>	2	2	4	2	3	1
1154>	4	3	4	3	4	2	2	4	1162>	1	6	1	1	3	4
1168>	1	6	0	2	3	2	3	3	1176>	2	2	4	1	4	0
1182>	3	3	0	3	1	4	1	0	1190>	0	6	1	0	4	0
1196>	3	1	3	2	0	0	7	0	1204>	2	2	3	0	3	1
1210>	0	3	2	0	4	0	4	4	1218>	0	2	4	0	4	0
1224>	3	0	3	1	0	5	0	2	1232>	3	1	2	0	4	0
1238>	3	0	2	3	0	0	0	0	1246>	0	6	0	0	0	0
1252>	0	5	0	0	4	0	0	4	1260>	0	0	4	0	2	0
1266>	0	6	0	0	3	2	2	2	1274>	0	0	4	0	2	1
1280>	2	0	4	0	0	0	3	0	1288>	0	0	0	5	0	1
1294>	0	0	4	0	0	0	5	0	1302>	0	0	4	0	3	0
1308>	3	0	0	0	4	0	0	0	1316>	0	0	5	0	2	0
1322>	3	0	3	0	1	0	0	0	1330>	0	0	0	0	0	0
1336>	0	0	0	0	0	0	0	0	1344>	0	0	0	0	0	0
1350>	0	0	0	0	0	0	0	3	1358>	1	1	0	0	0	0
1364>	0	0	0	4	0	1	2	0	1372>	0	2	0	0	0	0
1378>	0	0	0	0	0	0	0	0	1386>	0	0	0	0	1	0

SUM ODD 4491.0 4130.8 4253.1 4574.8 4218.0 4302.1 4482.6
 EV 10299.8 8576.4 9242.3 9268.8 10742.1 8821.8 9262.4
 RATIO 0.43603 0.48165 0.46126 0.49357 0.39266 0.48767 0.48396
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.460063

A14008.SUM 176 PKS W MIN. 1 CNTS. 21-JUN-93 15:11:14 SUM I: 0.2738E+04
 REF #8 SOH-ASOH (CONSOL) 1- 6 N AV MW: 161.4
 ACQUIRED 6-21-93 15:06:28 CHAN.#5 0- 4095; 6 MS/CHAN. WT AV MW: 179.2
 MAG. RET. TIME: 9999 MS, 8 SCANS/SPECTRM. 1 TO 1 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% C FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
46>	0	0	0	0	0	0	0	0	0: 56>	0	0	8030	653	0	0
62>	0	0	0	0	0	0	0	0	0: 70>	153	0	224	0	0	0
76>	0	0	150	0	0	0	0	0	0: 84>	2367	23	961	0	157	0
90>	0	0	478	0	241	0	0	0	0: 98>	2018	119	323	99	0	0
104>	0	0	855	287	523	47	0	164: 112>	1623	93	306	0	0	0	0
118>	303	0	962	374	840	0	482	80: 126>	1398	29	562	0	0	184	0
132>	2258	135	920	522	767	35	1040	52: 140>	725	74	1006	23	0	229	0
146>	4184	267	826	458	518	63	956	75: 154>	715	38	1239	72	565	234	0
160>	3716	453	893	257	454	32	913	71: 168>	1705	69	1049	173	2230	140	0
174>	2991	426	691	288	546	138	1044	64: 182>	1833	99	946	60	3043	152	0
188>	2802	236	495	101	900	32	1097	119: 196>	1440	57	641	133	1588	163	0
202>	1995	142	560	108	714	78	1231	129: 210>	1003	61	618	84	1011	124	0
216>	1154	75	508	50	545	27	1076	71: 224>	717	76	691	69	763	104	0
230>	505	65	373	44	455	43	730	82: 238>	475	21	453	44	482	73	0
244>	317	29	212	35	362	40	412	40: 252>	274	0	331	37	275	0	0
258>	228	0	130	0	162	0	239	13: 266>	161	0	228	0	132	0	0
272>	141	0	110	0	142	0	128	0: 280>	85	0	108	0	100	0	0
286>	0	0	0	0	0	0	72	0: 294>	73	0	91	0	0	0	0
300>	0	0	0	0	0	0	0	0: 308>	0	0	69	0	0	0	0
314>	0	0	0	0	0	0	0	0: 322>	0	0	0	0	0	0	0
328>	0	0	0	0	0	0	0	0: 336>	0	0	0	0	0	0	0
342>	0	0	0	0	0	0	0	0: 350>	0	0	0	0	155	0	0

SUM ODD 1829.2 2524.8 541.0 961.0 781.4 1467.4 1405.4
 EV 20593.6 8162.4 7169.2 9419.4 16764.5 17874.7 10506.0
 RATIO 0.08882 0.30932 0.07547 0.10202 0.04661 0.08209 0.13377
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.105097

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A14009.SUM 1274 FKS W MIN. 1 CNTS. 09-JUN-93 09:22:37 SUM I: 0.2645E+05
 REF NO. 9 (CONSOL) 0-10 N AV MW: 422.6
 ACQUIRED 6- 1-93 13:19:09 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 526.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -65 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	22	35:	56>	36	70	18	19	0	18
62>	0	0	0	0	0	0	0	26:	70>	26	16	0	0	0	16
76>	0	0	0	0	0	0	24	19:	84>	14	17	0	0	0	0
90>	0	0	0	0	22	0	0	18:	98>	21	0	0	0	0	0
104>	12	0	0	15	9	0	16	0:	112>	13	0	17	0	0	0
118>	0	18	12	17	21	0	0	0:	126>	20	0	16	7	0	27
132>	27	15	16	23	28	0	14	0:	140>	0	0	34	12	12	46
146>	109	45	32	39	20	16	0	12:	154>	22	0	66	23	41	53
160>	131	83	42	29	28	0	58	31:	168>	342	25	97	75	259	87
174>	185	97	40	37	78	16	242	102:	182>	778	49	157	152	743	164
188>	304	124	64	36	160	25	399	104:	196>	774	82	261	151	722	186
202>	1010	147	316	61	294	62	886	120:	210>	618	87	400	126	711	158
216>	770	121	372	66	389	105	932	125:	224>	599	90	479	113	620	107
230>	504	117	380	66	487	140	722	119:	238>	422	93	415	102	814	123
244>	468	82	363	84	425	111	484	97:	252>	298	67	300	91	582	130
258>	482	79	346	90	423	115	368	91:	266>	264	51	308	71	365	133
272>	383	90	321	106	600	122	347	68:	280>	230	77	444	100	330	119
286>	312	92	255	97	456	116	265	67:	294>	206	72	362	109	347	122
300>	312	92	236	110	306	108	253	86:	308>	218	94	309	106	314	96
314>	261	96	358	114	300	112	236	84:	322>	265	100	277	118	273	114
328>	215	108	336	116	304	98	220	90:	336>	250	95	276	109	302	119
342>	213	97	257	120	275	110	212	99:	350>	302	120	282	91	259	102
356>	264	95	224	96	251	95	223	108:	364>	261	125	253	111	204	102
370>	226	110	253	107	249	111	216	104:	378>	239	115	252	112	206	98
384>	232	102	237	106	227	109	244	96:	392>	220	107	220	104	204	98
398>	209	99	217	105	197	99	216	92:	406>	227	91	200	107	188	82
412>	194	103	247	124	188	110	180	109:	420>	205	109	178	104	219	98
426>	185	103	214	106	200	91	169	98:	434>	188	99	177	99	203	109
440>	183	95	196	91	185	107	178	109:	448>	204	111	173	90	175	115
454>	191	99	171	102	186	83	147	107:	462>	180	90	196	106	185	83
468>	187	87	168	96	181	104	199	89:	476>	172	113	171	103	178	90
482>	178	96	167	87	163	97	193	93:	490>	178	91	175	93	175	103
496>	167	90	212	98	159	96	192	103:	504>	179	84	151	90	150	92
510>	160	116	176	101	159	102	165	102:	518>	149	107	152	90	174	110
524>	157	106	171	101	159	94	145	96:	532>	147	83	153	102	179	102
538>	159	93	148	100	146	94	147	98:	546>	159	87	155	90	165	99
552>	151	99	163	81	167	81	141	88:	560>	148	91	169	89	160	87
566>	151	85	155	87	134	88	143	84:	574>	148	102	150	99	145	81
580>	136	103	115	86	136	79	130	100:	588>	145	94	127	93	123	87
594>	137	87	132	81	127	89	111	102:	602>	120	92	127	88	118	97
608>	119	83	117	72	124	80	122	83:	616>	123	77	128	81	114	79
622>	121	86	120	70	116	70	127	73:	630>	117	76	115	70	117	69
636>	105	76	105	74	111	76	111	73:	644>	98	73	105	65	115	70
650>	93	62	101	71	96	79	99	60:	658>	108	62	100	64	89	61
664>	87	77	84	67	90	64	89	61:	672>	92	60	91	62	93	59
678>	81	60	82	73	86	56	83	65:	686>	74	57	90	57	77	69
692>	74	60	75	59	76	59	62	63:	700>	64	59	65	61	67	50
706>	83	49	69	62	70	46	65	57:	714>	61	57	63	46	69	51
720>	69	47	64	53	65	47	64	44:	728>	69	37	61	47	60	44
734>	63	45	56	47	57	40	53	40:	742>	54	43	57	43	55	44
748>	50	46	62	44	47	41	50	37:	756>	47	34	53	37	50	39
762>	54	35	49	36	58	31	52	36:	770>	52	36	46	40	40	45

A14009.SUM 1274 PKS W MIN. 1 CNTS. 09-JUN-93 09:23:16 SUM I: 0.2645E+05
 REF NO. 9 (CONSOL) 0-10 N AV MW: 422.6
 ACQUIRED 6-1-93 13:19:09 CHAN.#5 0-8191; 6 MS/CHAN. WT AV MW: 526.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -65 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% FG. 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2		MASS	U1		RH		ROH	
776>	37	40	46	27	47	35	44	33	784>	45	36	32	37	37	37
790>	42	27	43	30	44	32	33	35	798>	40	30	37	34	40	31
804>	42	27	37	25	41	28	37	25	812>	37	29	33	35	28	32
818>	32	28	33	22	36	24	33	23	826>	32	33	24	29	30	27
832>	35	24	34	21	31	26	25	23	840>	24	24	24	25	32	20
846>	30	28	18	25	24	18	28	21	854>	26	22	26	24	17	27
860>	29	18	24	26	23	20	23	22	868>	24	21	22	18	27	21
874>	22	20	20	20	22	21	18	20	882>	16	17	27	11	19	23
888>	22	20	21	19	17	20	15	17	896>	23	11	22	17	20	19
902>	22	11	20	18	14	21	13	19	910>	18	17	15	18	16	20
916>	14	15	15	19	12	19	15	14	924>	18	12	20	14	16	19
930>	10	16	14	16	10	23	6	17	938>	15	14	15	16	14	13
944>	14	16	12	15	13	15	15	13	952>	10	15	11	10	19	8
958>	18	8	17	8	17	12	14	10	966>	12	8	11	16	9	12
972>	13	8	16	10	11	12	11	10	980>	11	11	12	7	14	4
986>	12	10	13	7	14	10	9	10	994>	10	9	0	21	0	14
1000>	12	10	9	5	15	7	9	11	1008>	7	12	9	8	7	12
1014>	6	14	9	5	15	5	10	7	1022>	8	10	10	7	9	7
1028>	12	5	10	9	5	11	0	16	1036>	2	9	6	11	4	12
1042>	5	7	12	6	5	11	4	9	1050>	5	0	15	3	12	6
1056>	7	6	7	8	5	5	9	6	1064>	5	7	9	7	5	5
1070>	4	8	10	4	10	3	7	3	1078>	9	4	8	5	7	5
1084>	6	9	3	7	4	6	6	6	1092>	5	8	6	3	7	3
1098>	9	0	9	4	4	0	12	1	1106>	6	6	5	4	5	6
1112>	7	3	3	5	3	5	4	4	1120>	5	3	3	5	5	6
1126>	1	8	3	5	0	8	1	5	1134>	3	3	8	2	4	6
1140>	2	6	4	4	4	6	2	4	1148>	3	3	7	0	7	1
1154>	5	4	4	5	3	5	3	3	1162>	5	1	8	0	4	4
1168>	2	3	4	5	1	4	0	8	1176>	1	2	5	3	2	4
1182>	3	5	2	3	3	2	6	1	1190>	2	6	0	3	4	0
1196>	6	1	5	3	3	3	4	1	1204>	5	1	4	2	3	3
1210>	4	2	4	2	5	0	3	4	1218>	3	0	2	5	1	3
1224>	2	2	3	0	4	2	4	2	1232>	3	1	3	3	3	2
1238>	2	2	6	0	2	2	1	3	1246>	3	2	2	4	1	3
1252>	0	1	2	3	0	5	1	2	1260>	2	1	3	5	0	5
1266>	0	3	1	2	4	0	1	2	1274>	3	1	3	0	5	4
1280>	1	2	4	1	4	2	2	1	1288>	2	1	4	0	3	0
1294>	0	0	0	0	4	1	3	2	1302>	0	3	0	3	1	2
1308>	0	4	0	3	0	3	0	0	1316>	4	0	2	1	4	0
1322>	2	2	0	0	0	4	0	2	1330>	2	1	2	0	0	3
1336>	0	0	0	4	0	0	4	1	1344>	0	5	0	0	0	4
1350>	0	2	1	0	0	0	5	1	1358>	3	0	0	4	0	0
1364>	3	0	0	3	0	0	0	5	1372>	0	0	0	3	0	2
1378>	0	0	3	2	0	0	3	0	1386>	0	0	4	0	0	0
1392>	1	2	0	0	0	0	0	0	1400>	0	0	0	0	0	0

SUM ODD 4426.0 4104.2 4109.9 4278.4 4072.2 4437.8 4767.4
 EV 10460.6 8596.4 9323.8 10254.8 10400.3 9131.2 11232.8
 RATIO 0.42311 0.47743 0.44080 0.41721 0.39155 0.48600 0.42442
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.435100

A14010.SUM 969 PKS W MIN. 1 CNTS. 08-JUN-93 10:11:49 SUM I: 0.1727E+05
 REF NO. 10 (CONSOL) 0- 9 N AV MW: 398.9
 ACQUIRED 6- 7-93 13:25:27 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 465.0
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2				U1		RH		ROH
48>	0	0	0	0	0	0	0	39:	56>	74	77	40	0	0	0
62>	0	0	0	0	0	0	0	0:	70>	33	45	0	0	21	0
76>	0	0	0	0	0	0	0	30:	84>	33	0	0	0	0	0
90>	0	0	0	0	31	0	18	33:	98>	19	0	0	0	0	0
104>	0	0	0	22	45	0	32	0:	112>	20	16	0	0	0	0
118>	0	0	20	0	48	18	19	0:	126>	23	0	0	0	0	18
132>	18	0	26	23	30	21	19	12:	140>	0	0	16	0	0	33
146>	35	41	38	23	26	21	12	0:	154>	0	0	40	19	34	46
160>	59	49	39	24	30	19	33	48:	168>	127	12	46	42	122	53
174>	69	63	79	26	78	29	111	90:	182>	359	46	97	72	354	100
188>	141	64	120	22	129	40	229	114:	196>	425	68	140	118	352	116
202>	792	102	391	52	232	63	614	146:	210>	383	82	279	70	360	105
216>	730	123	423	63	337	149	746	146:	224>	416	130	327	98	352	95
230>	439	100	403	91	409	219	613	147:	238>	307	114	309	129	790	162
244>	439	121	357	117	399	149	474	116:	252>	269	76	245	125	671	164
258>	569	113	393	114	415	143	363	133:	266>	285	74	318	115	436	172
272>	500	108	352	161	690	198	350	127:	280>	234	104	546	143	392	162
286>	382	115	309	147	540	169	349	107:	294>	226	101	486	148	469	118
300>	421	132	300	122	357	160	302	127:	308>	256	123	389	159	368	162
314>	339	138	501	140	379	133	270	131:	322>	312	129	345	160	353	162
328>	297	131	403	153	358	153	265	138:	336>	294	136	323	171	358	157
342>	289	126	322	158	346	128	268	127:	350>	433	158	357	131	328	128
356>	337	145	310	151	253	150	261	128:	364>	362	157	341	147	250	122
370>	296	145	340	127	335	139	261	131:	378>	315	172	336	133	256	127
384>	258	134	266	138	269	167	298	137:	392>	256	168	293	156	241	139
398>	312	123	273	155	243	170	283	150:	406>	281	142	238	141	245	129
412>	261	159	333	149	242	150	244	132:	420>	257	141	219	132	332	147
426>	243	164	286	159	257	134	233	129:	434>	227	140	208	144	296	152
440>	240	153	224	159	220	135	230	128:	448>	286	154	240	140	233	165
454>	245	125	243	122	206	124	202	137:	462>	259	154	276	130	220	145
468>	231	130	233	146	229	133	236	166:	476>	225	142	229	151	238	137
482>	219	116	182	113	236	129	255	140:	490>	223	126	214	127	224	113
496>	232	111	239	123	190	141	230	141:	504>	234	119	221	118	193	126
510>	171	125	232	122	195	147	184	131:	518>	166	136	166	117	194	124
524>	175	119	193	133	179	120	166	130:	532>	162	118	187	116	184	114
538>	188	102	170	112	189	106	172	114:	546>	161	106	166	104	158	113
552>	152	119	168	114	130	124	126	112:	560>	146	104	146	113	147	113
566>	142	115	142	106	136	85	138	82:	574>	138	88	143	94	124	85
580>	135	103	121	98	118	98	106	80:	588>	127	96	111	86	134	74
594>	120	93	119	85	115	85	101	88:	602>	108	79	115	74	89	84
608>	113	75	98	85	91	58	95	67:	616>	109	69	100	64	105	66
622>	101	68	95	61	92	68	83	62:	630>	95	64	86	75	87	59
636>	79	65	82	62	75	60	83	56:	644>	76	58	70	55	79	50
650>	61	66	62	52	69	54	63	47:	658>	70	50	63	47	68	55
664>	57	51	50	51	56	47	74	39:	672>	49	49	53	40	58	41
678>	57	39	49	44	43	58	40	37:	686>	53	39	43	46	43	46
692>	39	43	34	40	44	34	46	30:	700>	39	41	37	39	47	30
706>	42	33	42	27	38	32	46	23:	714>	40	33	38	35	35	27
720>	37	32	24	39	33	25	38	18:	728>	39	20	39	29	35	26
734>	24	29	31	26	26	23	29	25:	742>	35	18	35	0	43	17
748>	32	15	31	17	30	26	22	24:	756>	28	17	26	22	26	18
762>	26	19	22	24	18	22	25	16:	770>	16	24	23	27	38	21

A14010.SUM 969 FKS W MIN. 1 CNTS. 08-JUN-93 10:12:28 SUM I: 0.1727E+05
 REF NO. 10 (CONSOL) 0- 9 N AV MW: 398.9
 ACQUIRED 6- 7-93 13:25:27 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 465.0
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% F.G. 2

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
776>	22	18	14	23	15	24	16	16	784>	17	23	14	20	15	20
790>	17	19	17	14	20	18	16	12	798>	17	15	19	11	20	14
804>	16	15	11	17	20	11	15	18	812>	8	17	13	13	19	13
818>	16	8	19	12	14	8	22	10	826>	11	12	10	16	9	18
832>	6	15	8	15	9	10	15	10	840>	14	5	14	10	11	13
846>	10	12	11	11	13	9	6	10	854>	15	4	13	13	11	6
860>	14	6	12	5	12	4	13	6	868>	9	9	10	8	5	11
874>	7	5	15	3	14	8	6	9	882>	12	8	8	5	10	7
888>	7	12	4	6	11	9	4	10	896>	8	11	0	15	3	9
902>	6	7	7	8	8	6	7	9	910>	7	7	6	4	11	3
916>	5	6	8	4	11	2	12	3	924>	0	11	5	4	5	7
930>	7	5	8	4	7	6	3	7	938>	6	4	7	4	5	3
944>	8	2	8	6	6	2	10	1	952>	8	6	6	9	5	7
958>	2	6	8	2	7	2	7	2	966>	6	6	0	11	0	8
972>	1	8	5	5	2	6	6	0	980>	7	2	5	5	2	4
986>	3	2	7	6	1	6	3	0	994>	0	7	0	6	4	0
1000>	7	0	8	0	3	5	0	10	1008>	0	6	3	5	1	7
1014>	2	4	5	3	4	0	6	0	1022>	7	2	3	0	6	0
1028>	6	3	2	0	8	0	6	1	1036>	2	6	0	0	0	10
1042>	0	2	0	9	0	4	0	0	1050>	5	4	2	5	0	4
1056>	2	0	0	6	0	0	6	0	1064>	4	1	0	0	6	0
1070>	0	9	0	0	0	0	3	0	1078>	0	0	0	0	0	0
1084>	0	0	0	6	2	0	4	0	1092>	0	0	0	0	0	6
1098>	0	0	0	0	6	0	0	0	1106>	0	0	0	0	0	0
1112>	0	0	6	0	3	0	0	0	1120>	0	7	0	0	0	6
1126>	0	0	6	0	0	0	5	0	1134>	4	2	0	0	0	0
1140>	0	0	0	0	0	0	0	5	1148>	0	0	0	0	0	0
1154>	0	0	0	0	0	0	0	0	1162>	0	0	5	0	0	0
1168>	0	0	0	0	0	0	0	0	1176>	0	0	0	0	0	0
1182>	0	5	0	0	0	0	0	0	1190>	4	0	0	0	0	0
1196>	0	0	0	0	0	0	0	0	1204>	0	0	0	0	0	0
1210>	0	0	0	0	0	0	0	0	1218>	0	0	0	0	0	0
1224>	0	0	0	0	4	0	0	0	1232>	0	0	0	0	0	0
1238>	0	0	0	0	3	0	0	0	1246>	0	0	0	0	0	0
1252>	0	0	0	0	0	0	0	0	1260>	0	0	0	0	0	0
1266>	0	0	0	1	0	0	0	0	1274>	0	0	0	0	0	0

SUM ODD 4511.4 4465.7 4797.5 4648.0 4489.6 4568.7 4792.3
 EV 10312.5 9355.5 9438.1 9648.7 9284.0 8906.1 10333.0
 RATIO 0.43747 0.47733 0.50832 0.48173 0.48359 0.51299 0.46379
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.47704
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A14011.SUM 1311 PKS W MIN. 1 CNTS. 09-JUN-93 13:33:39 SUM I: 0.2031E+05
 REF NO. 11 (CONSOL) 3- 9 N AV MW: 464.4
 ACQUIRED 6- 1-93 16:19:24 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 567.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -16 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 85.00% C PG. 1

	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
MASS			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	0	33:	56>	0	38	81	0	0	23
62>	0	0	0	0	0	0	0	43:	70>	40	40	0	0	0	0
76>	0	0	0	0	0	0	19	0:	84>	25	14	0	0	0	0
90>	0	0	0	0	0	13	18	0:	98>	21	19	0	0	0	0
104>	0	0	18	13	0	21	17	27:	112>	0	22	0	35	0	0
118>	0	0	0	0	0	41	11	0:	126>	0	31	0	17	0	0
132>	14	0	13	0	15	17	0	0:	140>	0	0	0	0	0	23
146>	12	22	23	25	24	15	0	11:	154>	0	0	0	20	17	15
160>	23	25	37	20	17	22	12	41:	168>	24	20	14	52	27	38
174>	26	30	43	18	65	16	40	106:	182>	160	59	42	107	61	76
188>	42	49	52	21	128	35	195	137:	196>	346	114	102	107	122	90
202>	987	78	248	45	214	74	542	123:	210>	421	107	195	103	203	86
216>	854	114	382	55	342	127	733	138:	224>	564	101	324	78	292	75
230>	469	110	393	99	383	144	641	157:	238>	427	96	297	98	780	97
244>	531	112	387	82	400	132	442	114:	252>	364	84	277	104	591	120
258>	534	97	361	117	389	118	350	107:	266>	277	87	288	70	382	107
272>	435	107	340	113	591	135	328	106:	280>	241	92	393	114	329	111
286>	300	106	277	86	425	108	271	86:	294>	223	90	297	111	297	92
300>	302	83	220	83	282	107	238	108:	308>	221	83	272	103	246	105
314>	210	90	333	105	258	102	224	108:	322>	229	95	232	107	265	95
328>	198	82	288	100	266	100	202	99:	336>	199	104	204	89	253	126
342>	202	90	219	111	226	115	198	98:	350>	265	123	204	108	208	104
356>	240	101	211	111	202	104	179	95:	364>	229	114	222	91	185	111
370>	181	106	221	134	213	134	188	88:	378>	212	112	187	133	177	123
384>	165	144	161	107	174	0	191	196:	392>	109	192	130	178	128	180
398>	165	166	145	205	111	186	126	199:	406>	133	210	128	152	127	171
412>	122	138	135	237	139	192	120	186:	420>	124	204	135	178	129	221
426>	128	153	149	192	146	199	119	196:	434>	114	177	131	159	130	218
440>	127	177	144	193	126	173	123	192:	448>	134	216	119	170	128	214
454>	142	199	135	194	120	178	130	177:	462>	120	202	136	208	129	183
468>	144	155	135	196	107	214	113	204:	476>	134	190	132	180	122	199
482>	118	172	121	164	127	188	133	225:	490>	149	181	125	182	115	180
496>	113	175	121	195	141	168	128	210:	504>	122	211	123	177	120	157
510>	147	158	137	205	127	181	150	152:	518>	127	170	133	176	115	190
524>	134	172	141	189	120	176	129	176:	532>	124	172	127	160	134	179
538>	117	177	124	161	129	153	115	174:	546>	120	187	108	173	120	172
552>	125	170	124	163	128	160	137	137:	560>	119	155	121	166	116	164
566>	117	158	124	146	121	156	99	174:	574>	118	158	116	170	119	164
580>	123	161	107	161	111	142	115	171:	588>	102	159	104	161	109	135
594>	120	141	100	144	107	159	105	158:	602>	90	157	105	146	108	134
608>	106	136	104	143	101	134	111	139:	616>	85	149	107	153	97	128
622>	114	123	101	135	93	132	93	125:	630>	103	119	113	126	96	132
636>	92	115	94	125	75	133	89	133:	644>	76	120	74	124	84	112
650>	93	111	86	112	94	101	95	106:	658>	98	118	69	118	82	110
664>	85	105	90	112	71	108	88	93:	672>	80	111	75	97	77	95
678>	84	104	89	102	75	99	80	84:	686>	93	95	76	90	80	84
692>	82	84	69	92	71	81	83	92:	700>	62	83	62	93	68	86
706>	65	90	67	78	72	81	74	73:	714>	70	78	64	80	61	88
720>	62	75	60	83	57	76	51	73:	728>	62	58	69	69	55	70
734>	64	75	48	68	54	72	62	64:	742>	60	54	61	66	55	73
748>	39	74	58	53	64	45	67	62:	756>	52	55	57	59	54	58
762>	63	59	53	54	47	61	41	71:	770>	35	58	48	54	41	50

A14011.SUM 1311 PKS W MIN. 1 CNTS. 09-JUN-93 13:34:21 SUM I: 0.2031E+05
 REF NO. 11 (CONSOL) 3- 9 N AV MW: 464.4
 ACQUIRED 6- 1-93 16:19:24 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 567.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -16 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2		MASS>	U1		RH		ROH	
776>	51	46	53	47	54	46	48	52: 784>	51	39	47	45	44	45	
790>	46	47	42	50	42	48	40	48: 798>	33	51	40	58	32	46	
804>	36	38	45	36	47	48	31	50: 812>	29	46	34	47	38	33	
818>	51	33	35	45	39	40	32	43: 826>	41	26	39	39	31	41	
832>	39	29	38	36	35	35	30	39: 840>	30	36	27	28	43	36	
846>	40	33	31	29	33	44	22	36: 854>	29	33	34	32	33	27	
860>	38	28	27	33	24	39	22	33: 868>	24	30	24	32	30	26	
874>	27	33	19	37	27	17	26	24: 882>	28	19	37	21	23	30	
888>	15	34	20	25	23	22	29	25: 896>	22	30	26	17	30	30	
902>	18	27	26	20	26	22	26	27: 910>	17	30	16	20	20	30	
916>	14	32	15	30	20	18	26	17: 924>	21	28	0	31	15	21	
930>	24	20	21	21	23	19	17	18: 938>	16	19	18	20	18	19	
944>	22	18	13	21	15	19	19	15: 952>	20	20	16	17	16	20	
958>	17	14	19	20	21	15	14	21: 966>	18	14	24	12	18	15	
972>	16	16	18	15	18	12	3	9: 980>	19	13	19	9	21	8	
986>	18	14	14	11	14	16	16	16: 994>	11	18	16	12	21	5	
1000>	22	7	14	11	16	7	16	13: 1008>	13	10	12	12	15	12	
1014>	11	15	10	15	8	14	8	17: 1022>	0	19	8	13	10	12	
1028>	16	7	12	15	12	13	4	13: 1036>	10	13	13	10	11	12	
1042>	10	14	11	8	15	8	12	11: 1050>	12	8	8	11	9	9	
1056>	9	11	6	11	7	12	8	9: 1064>	9	8	10	10	9	9	
1070>	7	9	7	9	11	6	11	5: 1078>	10	10	9	3	14	5	
1084>	8	13	7	12	5	10	10	3: 1092>	14	6	6	8	9	7	
1098>	9	12	5	10	5	8	5	6: 1106>	10	7	6	7	6	11	
1112>	5	6	10	5	3	11	5	10: 1120>	7	4	9	5	7	8	
1126>	5	9	8	6	4	8	7	4: 1134>	0	15	2	7	2	9	
1140>	4	8	10	0	11	4	9	0: 1148>	9	3	10	2	11	3	
1154>	8	5	7	5	10	4	8	1: 1162>	12	2	8	7	3	8	
1168>	3	8	2	4	4	5	4	8: 1176>	5	6	6	6	6	3	
1182>	9	2	4	7	3	5	3	5: 1190>	3	9	0	10	0	10	
1196>	2	4	6	5	4	5	5	5: 1204>	7	4	5	5	0	3	
1210>	7	5	5	5	4	3	5	3: 1218>	3	7	2	3	7	2	
1224>	3	4	7	4	0	9	0	6: 1232>	1	5	4	8	1	3	
1238>	5	2	5	2	7	3	4	4: 1246>	3	3	4	3	6	2	
1252>	4	4	5	3	4	4	3	1: 1260>	4	6	1	3	5	0	
1266>	4	3	2	5	2	3	4	2: 1274>	5	1	4	4	4	4	
1280>	1	6	2	3	5	0	5	2: 1288>	4	5	0	0	0	10	
1294>	0	3	5	1	5	3	0	4: 1302>	2	1	5	1	4	0	
1308>	4	2	3	2	3	2	4	1: 1316>	3	4	3	1	0	6	
1322>	0	4	2	2	4	2	4	1: 1330>	3	2	1	3	3	0	
1336>	0	6	3	1	5	2	0	7: 1344>	2	1	0	5	3	0	
1350>	0	6	1	2	2	4	1	3: 1358>	2	0	6	1	1	0	
1364>	0	6	0	3	3	3	2	4: 1372>	1	0	5	1	3	0	
1378>	2	4	1	0	6	0	3	1: 1386>	0	5	0	0	4	1	
1392>	1	0	0	1	2	2	0	0: 1400>	0	0	0	0	0	0	

SUM ODD 5817.3 5976.2 6047.3 6493.7 6295.6 6098.3 6147.1
 EV 9246.5 7684.7 7969.9 8383.3 7867.6 7043.5 7823.9
 RATIO 0.62914 0.77767 0.75877 0.77461 0.80020 0.86581 0.78568
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.765370

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B14011.SUM 1237 PPS W MIN. 1 CNTS. 18-JUN-93 11:36:51 SUM I: 0.1260E+05
 REPEAT REF #11 INT (CONSOL) 0-9 N AV MW: 451.3
 ACQUIRED 6-17-93 16:47:50 CHAN.#5 0-8191; 6 MS/CHAN. WT AV MW: 555.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -67 TO 498 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2					RH		ROH	
48>	0	0	0	0	0	0	0	0	56>	0	101	0	0	41	0
62>	0	0	0	0	0	0	0	0	70>	36	50	0	0	0	0
76>	0	0	0	0	0	0	0	0	84>	0	36	0	0	0	0
90>	0	0	0	0	89	0	0	0	98>	37	0	0	0	0	0
104>	0	0	0	24	73	0	0	0	112>	0	35	61	30	0	0
118>	0	0	0	20	90	0	0	0	126>	99	0	46	0	0	36
132>	53	32	58	31	92	15	0	0	140>	0	0	66	31	55	45
146>	87	52	97	16	64	26	20	17	154>	37	16	106	47	52	62
160>	112	84	134	31	68	0	48	44	168>	327	33	140	100	140	80
174>	139	84	100	25	100	16	169	95	182>	729	74	188	143	355	104
188>	169	71	81	44	194	35	295	118	196>	749	96	240	125	416	128
202>	906	95	207	50	223	58	581	116	210>	533	96	278	90	353	86
216>	745	85	307	61	305	84	622	96	224>	509	119	335	90	316	76
230>	413	111	318	68	333	124	550	116	238>	343	70	284	90	465	176
244>	340	104	264	99	322	90	374	96	252>	250	78	216	119	346	190
258>	361	145	245	136	246	113	253	103	266>	201	107	215	130	242	170
272>	242	148	221	128	396	162	241	98	280>	177	94	244	139	206	194
286>	202	157	170	136	316	158	214	120	294>	178	128	234	136	211	174
300>	194	140	163	118	196	163	199	115	308>	142	117	241	126	197	153
314>	146	143	264	155	216	125	197	149	322>	202	159	172	174	205	144
328>	170	155	243	184	199	123	182	154	336>	156	119	186	175	201	139
342>	179	154	186	157	194	174	170	168	350>	210	155	189	139	194	163
356>	182	143	186	188	174	136	162	178	364>	190	178	204	128	182	169
370>	174	139	169	143	199	155	172	141	378>	203	161	208	146	164	133
384>	162	160	161	150	176	199	166	155	392>	166	175	149	150	173	130
398>	156	159	179	158	171	141	177	154	406>	167	157	133	143	154	125
412>	151	159	190	140	143	140	157	115	420>	169	131	152	133	176	132
426>	148	126	152	139	155	129	160	112	434>	142	158	138	148	163	154
440>	148	132	154	145	144	150	140	135	448>	167	94	167	115	158	132
454>	132	148	150	111	143	129	119	143	462>	139	145	149	117	147	137
468>	131	120	152	136	129	134	154	121	476>	127	136	155	126	146	118
482>	129	126	136	131	152	130	137	138	490>	131	110	130	113	127	141
496>	140	125	144	104	143	128	139	132	504>	131	132	111	124	134	118
510>	109	138	138	134	112	146	113	143	518>	107	122	121	119	134	126
524>	135	131	128	132	127	115	129	109	532>	132	131	128	106	140	127
538>	141	134	119	121	123	113	118	121	546>	138	110	123	114	138	126
552>	126	135	122	122	123	114	125	126	560>	113	109	121	136	116	119
566>	127	126	121	102	126	120	119	126	574>	114	126	126	114	135	121
580>	123	119	122	108	117	130	110	104	588>	137	105	107	91	137	106
594>	120	102	119	116	122	99	109	121	602>	109	99	103	106	113	109
608>	103	105	106	98	130	96	105	118	616>	102	103	115	104	85	120
622>	100	113	95	113	111	106	103	111	630>	96	93	0	145	66	120
636>	91	106	98	108	101	101	92	93	644>	93	93	102	90	94	99
650>	87	89	99	97	97	79	94	116	658>	76	99	79	117	92	83
664>	95	89	90	86	99	82	97	91	672>	79	85	83	88	87	89
678>	70	78	84	80	76	72	78	80	686>	85	71	95	66	0	120
692>	76	76	83	77	75	76	81	66	700>	78	82	73	71	81	69
706>	72	68	68	63	77	64	81	71	714>	68	59	64	75	57	68
720>	75	57	69	0	113	44	62	80	728>	52	64	66	59	55	65
734>	56	52	59	74	44	35	54	61	742>	61	64	46	65	53	60
748>	52	57	65	47	69	41	63	38	756>	57	52	45	49	39	65
762>	52	58	43	65	41	56	53	36	770>	60	60	35	59	45	43

B14011.SUM 1237 PKS W MIN. 1 CNTS. 18-JUN-93 11:37:32 SUM I: 0.1260E+05
 REPEAT REF #11 INT (CONSOL) 0- 9 N AV MW: 451.3
 ACQUIRED 6-17-93 16:47:50 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 555.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -67 TO 498 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00%C FG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	U1	1	2	3	4	5
			AR		U3		U2				RH		ROH		
776>	63	31	52	47	39	50	48	37: 784>	46	43	50	51	41	45	
790>	31	57	32	55	35	54	42	43: 798>	43	26	50	40	23	55	
804>	33	44	45	22	48	35	42	38: 812>	48	24	52	34	28	42	
818>	38	33	39	25	35	43	23	42: 826>	37	33	29	37	34	30	
832>	35	27	38	23	44	29	31	38: 840>	24	36	33	27	32	41	
846>	21	34	37	22	35	25	28	38: 854>	19	32	36	26	27	38	
860>	17	35	25	22	31	18	34	28: 868>	22	28	24	30	28	27	
874>	24	26	21	30	28	17	25	39: 882>	17	24	30	19	27	20	
888>	25	28	21	22	21	31	15	32: 896>	18	20	21	32	17	16	
902>	19	28	20	19	32	12	25	15: 910>	21	19	18	17	25	23	
916>	17	17	19	32	6	25	9	27: 924>	21	17	17	15	24	16	
930>	22	20	17	15	17	18	25	15: 938>	24	14	23	9	19	18	
944>	20	12	18	20	16	16	21	15: 952>	11	27	8	21	14	11	
958>	16	23	1	15	25	6	16	16: 966>	10	20	10	19	12	14	
972>	15	17	13	11	19	12	12	15: 980>	13	9	22	13	10	24	
986>	5	12	14	9	16	8	15	7: 994>	15	15	8	17	11	11	
1000>	9	14	5	17	14	13	9	15: 1008>	8	19	9	11	13	8	
1014>	15	7	6	16	13	11	9	12: 1022>	12	9	11	15	3	14	
1028>	9	12	10	9	15	4	15	10: 1036>	11	12	12	5	12	10	
1042>	9	10	6	6	15	8	7	14: 1050>	8	10	11	7	10	13	
1056>	4	15	8	11	3	16	1	8: 1064>	16	9	4	15	3	11	
1070>	5	10	6	8	13	4	11	5: 1078>	14	7	3	8	12	6	
1084>	7	5	7	10	7	11	9	9: 1092>	7	4	8	7	9	7	
1098>	7	3	7	11	3	13	3	10: 1106>	6	10	3	11	0	15	
1112>	0	0	16	4	4	0	19	0: 1120>	10	3	6	9	4	6	
1126>	8	6	4	11	6	9	3	9: 1134>	2	11	0	11	0	13	
1140>	7	9	3	5	8	1	12	2: 1148>	10	3	4	6	4	9	
1154>	4	4	9	0	8	1	10	0: 1162>	9	4	0	10	4	4	
1168>	9	5	6	7	5	5	0	0: 1176>	7	6	4	5	5	5	
1182>	5	7	4	3	7	5	1	6: 1190>	7	0	6	5	3	4	
1196>	3	4	6	2	0	6	3	6: 1204>	2	3	0	0	11	4	
1210>	0	11	5	4	0	2	3	4: 1218>	0	0	0	10	1	6	
1224>	8	0	0	7	3	0	0	10: 1232>	2	0	9	2	2	0	
1238>	0	13	0	0	8	0	0	8: 1246>	0	7	0	8	2	0	
1252>	7	0	5	0	5	6	0	6: 1260>	0	8	0	6	2	1	
1266>	0	9	0	0	10	0	4	0: 1274>	0	0	0	8	0	0	
1280>	0	11	0	2	0	9	0	0: 1288>	7	0	0	0	5	3	
1294>	4	2	0	7	0	0	0	0: 1302>	0	0	0	0	9	1	
1308>	0	0	6	2	0	3	0	0: 1316>	0	0	0	8	0	0	
1322>	5	0	5	0	0	0	0	0: 1330>	0	0	0	0	0	7	
1336>	3	0	6	3	0	0	0	0: 1344>	8	0	3	0	0	0	
1350>	0	9	0	0	0	0	0	0: 1358>	8	0	0	0	0	8	
1364>	0	0	0	0	0	0	7	0: 1372>	0	0	6	0	0	0	
1378>	0	0	0	0	0	0	0	0: 1386>	0	0	0	0	0	2	
1392>	2	0	0	0	0	0	0	2: 1400>	0	0	0	0	0	0	

SUM ODD 5747.0 5315.7 5284.0 5513.6 5497.7 5672.5 6025.3
 EV 8443.4 7194.3 7927.9 8118.6 8948.2 7297.1 7892.7
 RATIO 0.68065 0.73887 0.66650 0.67915 0.61440 0.77736 0.76340
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.699651

A14012.SUM 176 PKS W MIN. 1 CNTS. 21-JUN-93 16:40:38 SUM I: 0.2237E+04
 REF #12 SOH-ASOH (CONSOL) 0- 5 N AV MW: 167.6
 ACQUIRED 6-21-93 16:37:18 CHAN.#S 0- 4075; 6 MS/CHAN. WT AV MW: 181.9
 MAG. RET. TIME: 9999 MS, 8 SCANS/SPECTRM. 0 TO 0 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% FG. 1

	0	1	2	3	4	5	6	7	0	1	2	3	4	5
MASS			AR		U3		U2		MASS>	U1		RH		ROH
48>	0	0	0	0	0	0	0	0:	56>	0	0	3470	567	0
62>	0	0	0	0	0	0	0	0:	70>	0	0	169	0	0
76>	0	0	269	0	0	0	0	0:	84>	2061	96	819	0	0
90>	0	0	292	246	379	0	119	0:	98>	1755	66	317	0	0
104>	0	0	634	552	669	0	227	0:	112>	1579	73	269	0	100
118>	222	0	933	970	994	39	618	95:	126>	1353	72	409	0	263
132>	2373	287	944	953	692	127	991	53:	140>	827	90	777	121	397
146>	3452	907	997	775	427	95	958	0:	154>	568	66	704	92	365
160>	3152	1107	846	600	476	72	961	144:	168>	1747	40	692	215	395
174>	2934	625	820	431	652	44	1160	188:	182>	1664	160	772	258	383
188>	2781	637	676	267	623	61	1062	83:	196>	1314	136	758	192	329
202>	1993	363	628	130	624	101	1145	78:	210>	785	161	609	93	240
216>	1040	212	493	92	489	98	968	125:	224>	762	69	607	96	135
230>	666	80	335	77	454	68	687	126:	238>	466	0	477	87	61
244>	390	35	198	0	295	15	449	47:	252>	254	42	334	0	61
258>	218	0	148	0	237	0	233	0:	266>	169	0	214	0	0
272>	128	0	123	0	146	0	153	0:	280>	116	0	143	27	0
286>	0	0	0	0	74	0	71	0:	294>	90	0	0	0	0
300>	72	0	0	0	0	0	67	0:	308>	0	0	0	0	0
314>	0	0	0	0	0	0	0	0:	322>	0	0	0	0	0
328>	0	0	0	0	0	0	0	0:	336>	0	0	0	34	0
342>	0	0	0	0	0	0	0	0:	350>	0	0	0	0	123

SUM ODD 4253.4 5092.8 719.9 939.4 1070.7 1782.0 2728.5
 EV 19420.0 8337.4 7229.5 9867.6 15509.2 11540.9 11508.6
 RATIO 0.21902 0.61083 0.09958 0.09520 0.06904 0.15441 0.23708
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.198850

A14013.SUM 1338 PKS W MIN. 1 CNTS. 09-JUN-93 16:07:14 SUM I: 0.2943E+05
 REF NO. 13 (CONSOL) 0-11 N AV MW: 435.4
 ACQUIRED 6- 2-93 12:42:46 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 557.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -66 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	0	32:	56>	35	70	0	0	0	0
62>	0	0	0	0	0	0	0	13:	70>	21	39	0	0	0	0
76>	0	0	0	0	0	0	12	20:	84>	0	19	0	0	0	0
90>	0	0	0	0	26	9	12	16:	98>	20	12	0	0	0	0
104>	0	0	0	0	0	13	0	19:	112>	11	9	0	13	0	13
118>	0	0	18	0	0	14	0	16:	126>	20	0	9	0	0	0
132>	12	0	12	0	12	0	0	0:	140>	0	0	20	0	15	14
146>	61	13	14	16	14	0	16	0:	154>	16	8	36	10	24	16
160>	119	14	18	13	17	9	27	18:	168>	163	16	55	13	199	11
174>	134	15	30	9	64	9	99	20:	182>	446	10	63	32	539	18
198>	261	15	31	13	131	8	236	37:	196>	445	22	134	36	664	17
202>	1021	54	333	18	276	28	994	45:	210>	447	34	450	29	637	32
216>	825	33	378	28	414	46	1016	31:	224>	529	34	687	48	785	33
230>	488	30	397	33	564	54	792	25:	238>	463	41	755	52	1302	58
244>	539	38	497	46	607	53	617	34:	252>	401	33	582	63	919	71
258>	580	41	520	40	646	35	505	60:	266>	381	18	524	33	640	66
272>	511	39	495	57	775	56	481	39:	280>	336	41	664	62	507	61
286>	407	55	434	38	595	56	396	41:	294>	304	32	578	52	528	41
300>	401	42	380	42	436	39	347	32:	308>	328	31	445	51	441	51
314>	336	70	516	68	421	52	297	41:	322>	359	56	396	59	398	54
328>	325	58	465	68	424	45	290	41:	336>	355	63	412	67	397	53
342>	322	48	370	68	367	50	301	37:	350>	391	59	392	65	368	55
356>	364	68	333	60	319	46	299	43:	364>	349	66	372	66	299	56
370>	328	56	358	59	328	61	273	56:	378>	327	56	334	67	274	53
384>	291	67	306	64	270	60	299	59:	392>	295	67	296	63	258	60
398>	293	48	293	55	276	55	256	53:	406>	309	48	273	56	240	59
412>	266	49	288	56	251	65	238	63:	420>	260	60	245	51	249	62
426>	260	54	257	59	246	53	234	48:	434>	238	62	206	53	252	54
440>	242	57	230	66	227	50	230	59:	448>	255	43	222	56	210	67
454>	232	59	215	50	184	53	212	55:	462>	216	62	217	56	204	59
468>	212	64	199	45	204	54	223	58:	476>	207	54	200	57	210	55
482>	205	49	191	46	188	49	211	60:	490>	184	58	182	41	194	54
496>	195	50	183	52	176	57	181	56:	504>	178	45	177	49	164	53
510>	172	64	170	62	163	52	161	64:	518>	155	58	155	49	159	60
524>	171	51	153	59	153	68	154	46:	532>	150	44	157	44	162	48
538>	159	56	149	51	156	51	163	34:	546>	156	39	160	43	147	52
552>	136	48	137	51	143	57	142	49:	560>	136	41	146	54	131	61
566>	140	52	138	49	135	44	137	48:	574>	122	57	126	48	139	40
580>	135	42	129	43	125	48	135	43:	588>	126	52	118	43	126	44
594>	133	36	117	51	120	42	117	48:	602>	119	47	112	52	113	46
608>	118	37	128	43	117	44	93	62:	616>	96	49	112	46	105	44
622>	99	50	99	44	109	46	93	45:	630>	100	49	103	44	104	53
636>	102	36	102	51	99	33	96	46:	644>	85	53	84	52	88	48
650>	80	44	104	42	86	50	87	40:	658>	93	39	92	45	91	43
664>	86	42	79	46	83	44	80	44:	672>	83	34	85	38	79	45
678>	84	44	75	42	82	34	79	42:	686>	67	42	76	44	78	42
692>	84	34	75	33	82	31	81	30:	700>	73	47	74	23	76	43
706>	67	45	64	44	63	30	72	32:	714>	58	46	59	43	65	37
720>	62	38	68	27	69	34	63	37:	728>	43	45	56	39	65	38
734>	56	39	69	28	61	28	63	32:	742>	59	28	63	28	61	33
748>	54	30	59	33	54	36	58	24:	756>	60	29	58	30	53	36
762>	56	25	51	31	57	31	55	37:	770>	51	24	53	32	52	29

A14013.SUM 1338 FKS W MIN. 1 CNTS. 09-JUN-93 16:07:53 SUM I: 0.2943E+05
 REF NO. 13 (CONSOL) 0-11 N AV MW: 435.4
 ACQUIRED 6- 2-93 12:42:46 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 557.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -66 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2	MASS>		U1		RH		ROH	
776>	55	24	56	26	57	22	52	27: 784>	56	29	43	42	37	35	
790>	43	31	39	35	45	27	47	33: 798>	41	25	47	25	46	27	
804>	51	22	39	0	56	25	39	29: 812>	41	27	47	19	51	25	
818>	43	23	41	24	43	25	41	30: 826>	35	24	38	28	34	23	
832>	43	24	38	23	41	25	46	20: 840>	34	30	36	24	37	25	
846>	35	34	23	36	26	26	34	22: 854>	34	27	30	23	32	33	
860>	24	26	34	21	42	16	36	18: 868>	30	22	36	25	30	22	
874>	31	27	28	25	32	19	30	25: 882>	29	23	25	26	24	22	
888>	26	25	29	19	37	14	33	16: 896>	33	18	23	26	26	21	
902>	33	18	24	23	25	24	23	23: 910>	20	24	22	22	28	19	
916>	26	23	21	25	21	25	21	19: 924>	25	16	22	25	20	19	
930>	25	21	20	20	23	19	22	23: 938>	22	21	16	23	19	16	
944>	22	19	22	17	24	12	21	16: 952>	21	19	19	13	29	14	
958>	21	22	16	20	18	19	19	20: 966>	17	20	14	22	19	12	
972>	23	16	22	12	22	17	18	15: 980>	19	13	18	14	21	16	
986>	18	15	18	16	20	11	20	8: 994>	24	11	19	13	21	10	
1000>	18	18	14	19	13	16	21	14:1008>	12	18	14	16	17	11	
1014>	17	17	13	13	19	11	12	14:1022>	14	16	13	11	16	14	
1028>	14	12	15	14	10	18	10	16:1036>	9	20	8	17	13	12	
1042>	14	17	11	15	13	15	6	12:1050>	14	13	14	11	14	13	
1056>	13	12	16	6	14	13	12	17:1064>	0	23	4	18	0	21	
1070>	11	12	11	10	15	8	14	8:1078>	13	10	15	9	11	13	
1084>	7	10	11	15	9	11	9	14:1092>	10	11	8	14	5	15	
1098>	10	10	9	9	15	5	17	5:1106>	13	8	13	9	8	10	
1112>	11	7	10	6	14	0	23	2:1120>	10	6	14	5	14	4	
1126>	13	11	10	7	10	12	6	10:1134>	8	0	16	4	14	5	
1140>	10	10	8	8	11	8	6	10:1148>	10	6	11	8	7	7	
1154>	12	6	10	5	12	4	10	4:1162>	11	7	8	9	7	6	
1168>	10	5	9	9	8	9	7	9:1176>	5	9	3	10	8	6	
1182>	10	6	9	6	7	11	4	9:1190>	3	10	4	10	4	11	
1196>	3	10	3	8	7	7	6	8:1204>	4	11	3	8	7	7	
1210>	6	7	7	2	10	5	5	8:1218>	7	5	6	3	6	7	
1224>	2	9	4	5	9	4	7	7:1232>	3	5	8	5	5	9	
1238>	3	8	5	4	8	4	6	6:1246>	6	3	9	1	8	6	
1252>	7	9	4	0	7	5	5	3:1260>	10	1	7	5	2	9	
1266>	2	8	1	7	6	0	10	1:1274>	8	3	5	6	1	7	
1280>	2	6	3	7	4	3	7	1:1288>	4	5	4	3	6	5	
1294>	4	4	5	5	2	10	0	7:1302>	1	6	3	3	4	6	
1308>	2	6	0	9	1	4	5	1:1316>	3	7	5	7	2	3	
1322>	5	2	4	4	2	8	0	5:1330>	5	3	6	1	3	4	
1336>	2	4	5	2	6	2	5	3:1344>	0	6	3	4	3	3	
1350>	6	0	7	2	3	4	3	1:1358>	2	5	2	1	0	6	
1364>	1	4	4	2	5	3	2	6:1372>	0	5	1	5	1	3	
1378>	2	4	4	3	3	4	2	2:1386>	3	2	3	2	4	2	
1392>	1	2	2	2	2	3	0	0:1400>	0	0	0	0	0	0	

SUM ODD 2593.1 2550.5 2513.7 2576.7 2662.1 2674.0 2703.0
 EV 11964.9 10418.0 11185.0 11748.1 10792.2 11473.3 13479.3
 RATIO 0.21673 0.24482 0.22473 0.21932 0.24667 0.23306 0.20053
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.225423

A14014.SUM 1334 PKS W MIN. 1 CNTS. 10-JUN-93 09:07:43 SUM I: 0.2207E+05
 REF NO. 14 (CONSOL) 0-10 N AV MW: 435.7
 ACQUIRED 6- 2-93 15:52:46 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 546.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -64 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
			AR		U3		U2				U1		RH		ROH
48>	21	0	0	0	0	0	0	0	56>	35	77	0	0	50	68
62>	0	0	0	0	0	0	20	0	70>	38	33	0	0	24	0
76>	0	0	0	0	0	35	19	32	84>	24	41	0	0	0	0
90>	0	0	20	0	38	0	23	25	98>	32	0	0	0	0	19
104>	0	0	18	0	25	0	35	25	112>	30	18	52	18	0	19
118>	0	0	27	0	24	0	0	15	126>	94	18	33	0	0	14
132>	16	0	18	11	21	0	21	14	140>	11	0	28	0	48	18
146>	34	15	21	16	27	0	19	0	154>	12	0	44	9	31	11
160>	67	10	26	12	20	0	22	9	168>	115	18	55	11	132	21
174>	92	18	20	14	45	9	77	22	182>	309	12	52	19	361	20
188>	152	18	31	18	109	12	180	39	196>	374	27	97	29	392	44
202>	982	46	321	19	222	27	915	58	210>	416	37	352	39	507	41
216>	748	19	342	33	347	45	926	28	224>	528	33	632	35	679	23
230>	444	35	370	18	472	63	739	47	238>	455	38	697	60	1275	42
244>	537	25	424	45	527	76	576	29	252>	357	36	549	47	893	70
258>	586	54	485	31	557	62	473	45	266>	350	38	457	55	583	57
272>	490	30	454	58	776	58	446	46	280>	337	32	654	61	501	56
286>	368	43	376	65	591	46	362	37	294>	286	45	600	49	538	59
300>	383	60	378	56	408	53	338	47	308>	313	45	439	60	418	51
314>	338	67	538	48	409	50	292	38	322>	352	47	392	65	410	55
328>	296	68	478	74	392	42	292	39	336>	338	66	393	74	424	64
342>	309	51	363	65	351	63	291	49	350>	398	57	381	77	400	78
356>	364	58	371	54	302	51	285	54	364>	370	56	373	66	297	69
370>	339	62	345	58	340	45	298	52	378>	322	63	358	61	295	44
384>	312	57	324	60	278	84	290	70	392>	318	74	314	52	286	57
398>	315	61	300	69	245	78	298	62	406>	293	76	261	61	271	57
412>	275	65	317	73	261	67	257	66	420>	276	88	236	70	239	73
426>	269	55	293	56	256	69	236	63	434>	265	67	253	47	276	63
440>	238	81	240	66	232	58	243	53	448>	277	62	224	70	239	61
454>	247	75	222	69	208	65	212	72	462>	248	79	243	54	227	69
468>	222	70	211	49	233	55	246	63	476>	227	63	229	53	230	67
482>	222	66	191	66	202	64	235	77	490>	201	63	184	74	198	54
496>	197	72	208	71	198	66	192	72	504>	201	50	198	53	187	64
510>	196	62	218	58	200	57	179	76	518>	179	60	175	66	183	75
524>	173	71	185	54	186	71	176	71	532>	165	55	166	52	203	44
538>	182	52	170	55	163	60	171	55	546>	165	59	182	52	177	52
552>	173	57	163	58	172	49	158	51	560>	153	65	162	52	157	76
566>	146	67	152	64	148	56	143	51	574>	144	50	140	72	150	52
580>	145	57	127	53	142	59	133	56	588>	145	53	131	59	134	62
594>	132	56	124	45	130	54	130	51	602>	124	50	125	57	128	45
608>	117	53	127	47	118	55	127	49	616>	114	56	115	48	120	45
622>	115	51	112	45	95	54	108	53	630>	113	47	110	47	117	39
636>	107	50	101	50	101	43	110	50	644>	111	50	105	43	91	55
650>	96	47	89	46	92	46	95	41	658>	96	59	94	50	99	43
664>	98	40	93	34	96	37	85	43	672>	84	42	95	40	96	31
678>	98	35	82	47	76	46	80	38	686>	77	37	79	40	77	40
692>	90	41	75	42	77	36	75	49	700>	76	26	88	32	76	30
706>	82	29	75	36	68	42	72	42	714>	75	38	72	44	62	42
720>	76	33	74	34	71	37	58	41	728>	67	31	64	40	74	38
734>	59	37	61	39	57	31	70	23	742>	67	24	66	40	52	37
748>	66	28	61	31	63	32	54	33	756>	57	33	51	33	49	37
762>	52	31	61	29	55	23	59	32	770>	54	34	56	28	50	24

A14014.SUM 1334 PKS W MIN. 1 CNTS. 10-JUN-93 09:08:21 SUM I: 0.2207E+05
 REF NO. 14 (CONSOL) 0-10 N AV MW: 435.7
 ACQUIRED 6- 2-93 15:52:46 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 546.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -64 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN: 86.00% FG. 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2	MASS>	U1		RH		ROH		
776>	55	31	51	26	60	24	46	34: 784>	52	30	47	30	51	28	
790>	56	26	48	22	53	22	45	29: 798>	45	28	46	26	43	21	
804>	41	28	43	27	44	29	32	31: 812>	47	24	40	32	38	25	
818>	33	33	31	31	42	17	42	24: 826>	38	20	36	27	27	37	
832>	28	31	37	19	41	22	37	22: 840>	37	26	36	24	33	26	
846>	31	28	33	22	34	18	40	14: 854>	30	25	33	22	37	15	
860>	33	20	31	21	21	26	21	28: 868>	20	25	32	21	33	21	
874>	30	27	29	26	28	21	29	17: 882>	27	18	32	13	30	18	
888>	30	13	35	20	26	24	30	17: 896>	28	21	20	29	25	18	
902>	25	19	26	20	26	16	23	20: 910>	20	19	29	15	24	17	
916>	28	18	23	21	22	14	28	16: 924>	24	14	29	12	25	16	
930>	24	18	24	10	24	18	27	6: 938>	29	9	25	20	20	18	
944>	19	15	21	19	14	19	20	14: 952>	24	12	20	17	16	14	
958>	24	13	18	18	17	16	20	12: 966>	24	9	22	12	20	13	
972>	13	20	8	16	19	12	14	8: 980>	20	19	6	21	13	14	
986>	16	16	12	14	21	12	14	11: 994>	17	12	17	16	12	8	
1000>	17	10	15	9	16	14	11	19:1008>	10	15	8	11	17	6	
1014>	18	12	16	6	14	17	10	14:1022>	11	15	10	17	8	13	
1028>	15	13	12	14	11	11	14	12:1036>	11	8	15	12	11	14	
1042>	15	10	5	19	7	12	8	10:1050>	12	14	8	13	13	8	
1056>	17	10	10	8	10	14	4	15:1064>	8	7	12	7	10	11	
1070>	10	5	13	9	12	6	10	8:1078>	10	11	9	9	11	5	
1084>	10	7	12	5	7	9	12	3:1092>	15	6	11	6	10	5	
1098>	12	6	12	5	14	7	9	3:1106>	12	9	4	10	14	8	
1112>	8	10	5	9	11	8	6	9:1120>	5	9	10	4	10	1	
1126>	11	6	8	10	6	8	5	6:1134>	7	10	6	11	2	9	
1140>	3	9	5	10	2	12	2	12:1148>	1	9	8	5	8	5	
1154>	9	6	4	10	8	2	7	7:1162>	7	6	3	7	7	6	
1168>	4	7	8	5	4	10	4	8:1176>	2	7	6	7	4	10	
1182>	3	8	5	6	4	6	6	4:1190>	8	1	7	4	7	5	
1196>	3	8	3	8	4	5	3	6:1204>	2	7	2	7	5	2	
1210>	4	6	5	3	6	3	3	8:1218>	1	7	2	7	5	2	
1224>	6	5	4	6	3	7	1	4:1232>	7	2	8	3	5	3	
1238>	7	4	4	4	6	4	4	3:1246>	3	5	4	4	4	4	
1252>	4	5	2	3	6	4	3	3:1260>	6	3	2	7	2	4	
1266>	3	5	4	3	2	3	5	5:1274>	4	3	3	1	4	3	
1280>	4	6	2	2	5	3	3	4:1288>	4	0	6	0	4	2	
1294>	4	2	5	2	5	2	3	5:1302>	2	4	1	4	3	4	
1308>	0	6	3	5	3	2	2	5:1316>	1	3	1	4	1	2	
1322>	4	4	0	4	2	3	4	2:1330>	2	0	5	3	3	0	
1336>	3	3	2	1	6	0	2	5:1344>	0	6	0	5	1	2	
1350>	2	0	7	0	5	0	4	3:1358>	2	4	1	2	3	2	
1364>	0	0	6	0	4	0	4	0:1372>	3	0	0	6	0	3	
1378>	2	1	2	2	1	2	3	0:1386>	4	0	0	6	1	2	
1392>	0	1	1	2	2	2	2	0:1400>	0	0	0	0	0	0	

SUM ODD 2704.2 2643.6 2717.6 2740.7 2808.1 2781.7 2829.3
 EV 11750.9 10532.1 10905.6 11562.0 10911.8 11475.0 13124.1
 RATIO 0.23013 0.25101 0.24919 0.23704 0.25734 0.24242 0.21558
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.239533

A14015.SUM 203 PKS W MIN. 1 CNTS. 21-JUN-93 17:54:54 SUM I: 0.4301E+04
 REF #15 SOH-ASOH (CONSOL) 0- 4 N AV MW: 172.3
 ACQUIRED 6-21-93 17:51:04 CHAN.#S 0- 4095; 6 MS/CHAN. WT AV MW: 192.4
 MAG. RET. TIME: 9999 MS, 8 SCANS/SPECTRM. 1 TO 1 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
48>	0	0	0	0	0	0	0	0	56>	0	0	8060	554	98	0
62>	0	0	0	0	0	0	0	0	70>	0	0	115	0	0	0
76>	0	0	159	0	0	0	109	124	84>	2373	0	865	0	0	0
90>	0	0	554	64	79	0	88	132	98>	2015	33	232	0	0	0
104>	0	0	884	100	180	0	78	0	112>	1477	55	176	0	0	0
118>	373	0	1051	105	253	65	611	36	126>	1512	12	216	0	0	0
132>	1884	103	783	145	269	0	1105	47	140>	1024	35	406	45	0	0
146>	3270	81	778	71	216	39	1161	44	154>	737	16	513	50	375	70
160>	3073	145	599	60	226	30	1091	33	168>	1272	35	365	68	1653	107
174>	2181	38	542	32	550	63	1229	33	182>	1799	15	434	130	3220	13
188>	2263	125	391	44	875	36	1481	41	196>	1489	7	565	82	3018	128
202>	1949	84	455	84	972	15	1550	42	210>	1207	3	1015	62	2504	84
216>	1617	0	649	19	780	40	1264	40	224>	797	25	1143	101	2237	27
230>	1016	64	637	69	824	46	806	39	238>	407	38	812	49	1399	50
244>	925	0	507	20	736	0	544	23	252>	304	16	399	21	710	0
258>	450	27	271	24	437	37	371	0	266>	205	35	228	27	293	0
272>	215	4	178	17	187	10	202	17	280>	149	0	161	0	155	0
286>	111	21	122	0	126	22	72	0	294>	104	0	76	0	61	0
300>	44	0	73	0	54	0	41	0	308>	66	0	55	0	0	0
314>	0	0	0	0	0	0	36	0	322>	0	0	39	0	0	0
328>	0	0	0	0	0	0	0	0	336>	0	0	0	0	0	21
342>	0	0	28	0	0	0	0	0	350>	0	0	0	0	85	0

SUM ODD 692.2 855.2 401.9 651.9 325.9 1187.7 625.4
 EV 19373.2 8663.5 6763.6 11838.3 16937.5 15875.9 15807.8
 RATIO 0.03573 0.09871 0.05942 0.05507 0.01924 0.07481 0.03956
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.049761

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A14014.SUM 1321 PKS W MIN. 1 CNTS. 06-AUG-93 12:16:04 SUM I: 0.3086E+05
 REF NO. 16 (CONSOL) 0- 9 N AV MW: 431.6
 ACQUIRED 6- 3-93 12:45:31 CHAN.#6 0- 8191; 6 MS/CHAN. WT AV MW: 537.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -66 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

0	1	2	3	4	5	6	7	0	1	2	3	4	5
MASS		AR		U3		U2	MASS	U1		RH		ROH	
48>	0	0	0	0	0	0	20: 56>	34	60	0	0	0	17
62>	0	0	0	0	0	0	18: 70>	0	34	0	0	0	0
76>	0	0	0	0	0	0	0: 84>	17	27	0	0	0	0
90>	0	0	0	0	18	0	13: 98>	22	0	0	11	7	12
104>	8	0	0	0	0	0	0: 112>	22	0	36	0	0	0
118>	0	0	0	0	0	12	0: 126>	60	0	23	8	0	0
132>	10	0	15	0	13	0	0: 140>	8	0	10	10	29	11
146>	28	7	10	0	17	0	0: 154>	14	0	24	9	16	11
160>	44	16	19	11	18	6	7: 168>	177	13	45	14	124	17
174>	95	11	31	11	39	8	33: 182>	392	16	73	24	376	24
188>	131	17	28	9	112	15	38: 196>	398	27	112	30	398	34
202>	1415	22	306	22	179	40	24: 210>	401	29	299	28	420	33
216>	1054	17	354	16	360	49	64: 224>	511	40	484	28	535	22
230>	536	27	370	14	457	67	54: 238>	489	37	523	113	1352	75
244>	597	46	435	40	517	50	43: 252>	360	29	440	80	910	68
258>	672	53	446	58	516	51	70: 266>	386	25	454	68	611	56
272>	531	47	450	83	875	77	48: 280>	339	52	686	76	552	52
286>	435	48	397	44	689	62	46: 294>	316	48	568	90	589	53
300>	461	58	355	45	479	77	69: 308>	322	53	459	81	439	77
314>	343	54	667	79	444	58	48: 322>	369	58	415	74	444	70
328>	334	76	533	90	463	65	53: 336>	340	78	401	86	449	96
342>	331	62	380	75	365	76	57: 350>	435	77	396	85	353	77
356>	355	75	333	76	315	66	70: 364>	381	84	368	85	300	65
370>	316	73	359	54	347	75	63: 378>	309	80	370	76	291	66
384>	244	76	299	64	303	69	61: 392>	295	69	307	76	258	63
398>	264	80	303	71	262	82	74: 406>	295	77	253	62	230	64
412>	244	69	306	94	246	59	71: 420>	265	61	250	60	288	83
426>	237	76	243	80	242	68	76: 434>	236	63	217	78	239	77
440>	245	65	228	80	209	63	71: 448>	264	55	212	66	199	65
454>	226	69	223	69	198	57	68: 462>	223	76	223	68	192	64
468>	194	68	185	76	194	79	64: 476>	198	78	205	71	194	68
482>	185	70	178	64	183	80	75: 490>	178	64	186	67	178	63
496>	184	72	183	76	169	76	70: 504>	172	70	159	57	152	79
510>	163	67	187	67	180	61	66: 518>	170	62	161	61	167	69
524>	153	68	163	69	154	79	61: 532>	151	63	156	56	160	71
538>	166	60	150	67	146	67	70: 546>	144	64	150	72	144	67
552>	138	74	149	71	143	68	68: 560>	147	59	142	72	134	72
566>	126	80	129	68	127	65	72: 574>	131	63	143	60	134	64
580>	131	60	132	62	128	57	57: 588>	134	69	131	58	124	58
594>	122	63	124	62	117	63	70: 602>	114	51	139	51	116	56
608>	112	61	110	62	111	50	61: 616>	99	60	106	57	110	60
622>	109	62	111	48	108	53	51: 630>	99	54	91	55	103	51
636>	103	51	101	51	94	48	49: 644>	102	56	86	59	90	61
650>	92	53	93	49	95	54	63: 658>	87	47	87	60	85	49
664>	83	47	85	61	86	45	44: 672>	84	53	78	57	79	61
678>	74	46	77	57	80	51	38: 686>	66	42	85	45	72	53
692>	72	45	71	53	68	45	39: 700>	75	46	66	59	54	55
706>	61	52	73	40	66	45	33: 714>	68	37	69	39	74	41
720>	66	42	69	38	60	44	42: 728>	67	36	58	43	62	37
734>	62	42	63	39	60	38	37: 742>	53	43	55	34	57	33
748>	56	38	57	35	57	35	42: 756>	57	35	47	42	46	38
762>	55	27	57	36	53	23	37: 770>	50	29	53	35	52	30

A14016.SCH 1321 PMS W MIN. 1 CNTS. 06-AUG-93 12:16:46 SUM I: 0.3066E+05
 REF NO. 1: (CONSOL) 0-9 N AV MW: 431.6
 ACQUIRED 6-3-93 12:45:31 CHAN.#3 0-8191 6 MS/CHAN. WT AV MW: 537.9
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -66 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 85.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
776>	45	32	55	34	51	29	49	37	784>	42	34	43	32	46	31
790>	41	28	49	23	42	35	43	31	798>	35	32	42	30	42	28
804>	46	27	42	29	37	37	37	30	812>	38	35	35	31	34	31
818>	42	30	37	29	32	36	38	27	826>	36	25	35	29	41	28
832>	37	27	30	29	33	25	38	25	840>	36	21	37	26	35	25
846>	36	19	35	27	27	30	24	28	854>	20	31	27	24	33	19
860>	32	23	29	28	28	23	27	28	868>	25	24	20	30	24	22
874>	31	23	31	16	33	20	27	22	882>	26	16	27	21	24	23
888>	26	19	29	20	23	21	26	20	896>	25	17	25	26	20	21
902>	23	20	25	21	24	20	22	15	910>	28	18	19	19	23	21
916>	19	18	22	18	26	15	19	19	924>	20	19	17	20	27	13
930>	26	14	21	15	18	19	14	22	938>	16	10	26	13	22	13
944>	19	16	21	13	20	15	20	15	952>	17	18	13	18	18	19
958>	17	13	18	15	13	17	16	11	966>	15	17	15	10	15	14
972>	13	12	13	0	27	7	22	9	980>	19	10	17	7	20	13
986>	12	12	15	11	16	13	14	16	994>	10	16	11	15	14	14
1000>	12	10	14	14	13	10	16	11	1008>	12	17	6	13	12	14
1014>	13	7	15	10	11	13	13	12	1022>	11	13	9	12	12	11
1028>	11	9	12	11	15	9	10	13	1036>	10	10	9	8	14	4
1042>	16	5	12	8	10	12	10	7	1050>	10	9	8	13	11	9
1056>	12	6	13	7	10	8	13	6	1064>	10	9	7	9	8	9
1070>	11	8	8	6	13	7	9	8	1078>	4	13	6	8	9	4
1084>	11	5	9	7	10	9	9	6	1092>	10	5	9	5	13	3
1098>	7	6	10	5	12	7	6	7	1106>	7	10	7	4	12	2
1112>	10	6	7	5	9	4	8	7	1120>	6	6	9	5	10	3
1126>	9	5	6	5	5	7	5	7	1134>	4	8	5	9	4	3
1140>	7	8	4	5	10	3	7	5	1148>	6	4	8	3	5	8
1154>	5	6	4	7	5	4	5	5	1162>	8	4	8	0	8	1
1168>	9	5	6	2	5	6	3	6	1176>	4	6	6	3	4	7
1182>	2	5	5	6	2	7	2	5	1190>	4	6	2	6	3	6
1196>	4	8	3	5	1	9	1	5	1204>	7	1	6	3	5	3
1210>	5	4	5	2	3	6	3	3	1218>	5	3	2	5	2	5
1224>	3	4	5	2	6	2	5	2	1232>	4	1	7	1	6	2
1238>	5	3	3	5	4	1	5	2	1246>	5	3	3	2	3	5
1252>	3	5	2	2	5	3	2	3	1260>	4	2	4	4	2	4
1266>	3	3	5	0	7	0	5	3	1274>	2	3	6	0	2	4
1280>	2	5	1	5	2	3	2	3	1298>	3	2	3	0	4	2
1294>	3	2	2	3	4	1	3	2	1302>	3	2	3	3	1	5
1308>	4	0	4	4	0	4	2	3	1316>	0	3	3	1	3	1
1322>	2	2	3	2	3	1	4	1	1330>	3	4	0	0	6	1
1336>	0	1	2	0	1	3	2	3	1344>	1	3	0	3	1	1
1350>	2	3	1	2	3	1	1	3	1358>	2	2	0	3	0	2
1364>	2	0	3	2	1	2	1	3	1372>	1	1	3	0	4	0
1378>	3	1	1	2	0	3	2	1	1386>	2	2	1	0	5	0
1392>	0	1	2	2	1	0	0	0	1400>	0	0	0	0	0	0

SUM ODD 2864.4 2911.4 2995.0 2961.4 2949.0 3186.5 3051.5
 EV 12330.3 10272.9 10767.0 11243.7 10711.0 10649.4 12594.7
 RATIO 0.23231 0.26340 0.27765 0.26336 0.27532 0.29734 0.24228
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.265929

A14017.SUM 1246 PKS W MIN. 1 CNTS. 08-JUN-93 11:06:03 SUM I: 0.2416E+05
 REF NO. 17 (CONSOL) 0- 8 N AV MW: 436.9
 ACQUIRED 6- 7-93 15:46:32 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 522.6
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 500 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	0	25: 56>	42	45	0	0	20	15	
62>	0	0	0	0	0	0	15	21: 70>	23	26	0	0	0	0	
76>	0	0	0	0	0	0	22	0: 84>	44	17	0	0	11	0	
90>	0	0	0	0	27	0	0	21: 98>	14	0	0	0	0	0	
104>	0	0	0	11	26	0	17	9: 112>	21	12	22	0	0	0	
118>	13	0	18	0	17	0	12	0: 126>	35	0	18	0	0	11	
132>	15	0	0	0	0	0	13	0: 140>	0	8	19	9	23	0	
146>	20	0	16	14	13	13	0	0: 154>	9	0	13	0	0	13	
160>	18	10	19	12	14	0	14	0: 168>	34	11	19	0	23	20	
174>	21	15	30	9	23	8	28	22: 182>	67	18	23	19	65	14	
188>	19	0	31	12	72	10	60	39: 196>	118	22	39	25	80	20	
202>	1118	33	235	19	145	28	460	29: 210>	184	26	120	23	94	22	
216>	968	43	328	29	254	53	578	43: 224>	306	36	241	26	211	27	
230>	472	41	317	27	356	66	597	61: 238>	334	38	307	80	1150	116	
244>	509	54	380	39	429	83	482	61: 252>	323	29	342	92	881	86	
258>	654	57	415	62	477	59	446	90: 266>	379	35	437	70	590	76	
272>	528	51	429	67	1033	92	483	49: 280>	338	53	754	95	576	74	
286>	438	57	389	68	721	73	441	51: 294>	348	56	607	102	626	83	
300>	536	63	385	67	485	82	381	63: 308>	351	61	481	86	488	74	
314>	396	138	682	103	501	59	377	56: 322>	427	57	436	78	513	116	
328>	359	100	549	118	462	87	328	75: 336>	383	74	431	90	552	104	
342>	372	78	400	111	377	91	315	70: 350>	521	82	398	97	430	83	
356>	445	84	390	83	325	92	289	103: 364>	418	105	409	101	322	75	
370>	368	102	396	92	371	108	313	78: 378>	344	85	397	104	303	66	
384>	310	93	334	75	309	109	374	103: 392>	299	100	303	83	305	74	
398>	336	79	331	100	292	107	299	79: 406>	315	91	262	90	259	73	
412>	293	94	381	118	273	104	261	86: 420>	277	79	246	86	320	97	
426>	265	96	283	79	256	89	222	97: 434>	214	96	228	100	295	103	
440>	271	101	254	86	227	87	223	86: 448>	302	107	228	90	241	115	
454>	239	103	230	86	208	86	207	105: 462>	236	118	244	89	209	92	
468>	203	97	217	80	232	86	236	105: 476>	217	96	218	93	227	76	
482>	185	102	169	97	212	96	244	93: 490>	202	103	160	106	200	86	
496>	197	92	223	88	196	84	233	77: 504>	191	91	166	86	154	97	
510>	174	96	218	93	181	97	177	89: 518>	167	85	169	89	135	119	
524>	179	82	185	97	172	89	155	86: 532>	160	88	137	85	173	85	
538>	178	104	145	80	168	74	112	90: 546>	154	83	163	80	153	82	
552>	158	85	150	88	134	69	152	79: 560>	145	83	153	91	136	83	
566>	131	67	105	102	110	76	145	80: 574>	134	87	137	74	136	74	
580>	131	83	107	77	120	78	128	82: 588>	122	71	125	82	108	91	
594>	107	72	109	85	116	74	121	72: 602>	112	78	108	72	107	75	
608>	98	78	106	83	98	92	106	63: 616>	107	63	119	69	87	77	
622>	105	66	103	68	99	72	102	72: 630>	97	64	103	72	95	85	
636>	88	77	92	64	93	71	87	57: 644>	88	68	86	55	102	59	
650>	87	67	74	67	72	69	79	61: 658>	85	62	83	65	84	58	
664>	81	58	75	57	75	66	70	70: 672>	63	0	106	54	67	68	
678>	64	57	67	67	53	68	52	80: 686>	45	72	55	75	45	72	
692>	55	65	50	60	48	63	55	64: 700>	61	49	62	48	60	52	
706>	52	57	61	60	47	56	43	56: 714>	48	46	52	52	54	48	
720>	45	61	42	52	50	48	47	48: 728>	50	45	52	44	44	54	
734>	45	49	38	55	44	54	44	46: 742>	43	48	42	49	35	58	
748>	34	59	30	52	32	41	40	50: 756>	32	40	37	46	31	43	
762>	37	41	37	42	35	41	35	41: 770>	39	36	37	36	36	53	

A14017.SUM 1246 PKS W MIN. 1 CNTS. 08-JUN-93 11:06:42 SUM I: 0.2416E+05
 REF NO. 17 (CONSOL) 0- 8 N AV MW: 436.9
 ACQUIRED 6- 7-93 15:46:32 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 522.6
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 500 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2				U1		RH		ROH
776>	26	53	23	44	35	37	26	41: 784>	36	34	33	36	30	30	30
790>	31	0	56	29	30	40	25	35: 798>	22	34	33	32	31	31	32
804>	30	34	32	25	40	26	29	32: 812>	31	28	25	35	29	27	27
818>	31	28	25	33	16	30	27	30: 826>	27	25	27	29	27	24	24
832>	26	34	16	29	23	24	29	25: 840>	26	25	29	17	38	18	18
846>	24	22	28	25	20	27	24	23: 854>	22	18	23	0	39	21	21
860>	19	17	26	21	22	25	18	23: 868>	15	30	17	22	22	18	18
874>	19	24	19	17	21	20	23	22: 882>	14	19	18	20	18	18	18
888>	24	9	25	18	25	11	25	17: 896>	17	21	17	15	16	16	16
902>	21	0	30	10	15	18	16	13: 910>	14	20	13	15	16	16	16
916>	14	20	12	12	18	14	13	16: 924>	14	14	18	15	16	15	15
930>	13	13	16	17	13	17	13	19: 938>	12	10	22	8	16	15	15
944>	12	10	12	15	10	14	17	8: 952>	16	14	14	7	14	11	11
958>	15	14	10	14	9	15	12	10: 966>	13	9	12	13	8	13	13
972>	13	11	11	12	7	16	8	12: 980>	12	8	10	10	10	10	10
986>	8	10	14	8	11	9	0	24: 994>	2	14	9	10	10	10	10
1000>	5	13	7	10	12	7	11	7: 1008>	11	11	10	8	8	10	10
1014>	8	7	9	11	7	7	11	9: 1022>	7	8	5	12	8	5	5
1028>	9	5	8	7	7	6	10	6: 1036>	10	8	4	10	7	6	6
1042>	6	8	7	5	10	5	7	12: 1050>	2	13	3	8	8	6	6
1056>	7	4	11	7	4	8	8	5: 1064>	10	7	5	8	5	5	5
1070>	8	9	3	7	5	9	6	5: 1078>	8	7	6	7	5	5	5
1084>	7	4	6	6	5	4	5	7: 1092>	4	7	4	7	4	7	7
1098>	4	5	7	4	5	5	7	5: 1106>	5	6	4	4	3	7	7
1112>	1	8	4	9	0	9	3	7: 1120>	3	3	7	4	6	4	4
1126>	2	5	2	6	0	9	1	6: 1134>	6	4	0	6	4	4	4
1140>	3	2	6	4	4	3	3	3: 1148>	4	4	4	5	3	4	4
1154>	5	1	4	2	7	0	4	5: 1162>	1	7	1	6	0	7	7
1168>	1	4	4	4	4	3	4	2: 1176>	3	3	0	6	3	6	6
1182>	2	1	5	4	3	2	5	5: 1190>	0	5	3	3	3	2	2
1196>	3	3	0	7	2	3	4	3: 1204>	4	2	0	3	3	4	4
1210>	2	1	5	0	5	0	4	2: 1218>	1	4	0	3	1	5	5
1224>	1	3	3	3	0	3	3	2: 1232>	3	0	6	0	0	4	4
1238>	0	5	2	0	4	2	0	0: 1246>	5	0	3	1	3	0	0
1252>	4	2	0	0	0	5	1	1: 1260>	3	1	0	0	6	0	0
1266>	3	2	3	0	0	0	0	5: 1274>	1	0	4	1	3	0	0
1280>	3	0	2	2	0	0	5	1: 1288>	0	0	3	2	0	0	0
1294>	0	0	4	0	4	1	1	3: 1302>	0	3	0	0	4	0	0
1308>	2	0	0	3	1	2	0	3: 1316>	0	1	0	0	6	0	0
1322>	0	4	0	2	0	3	0	0: 1330>	0	0	5	0	0	0	0
1336>	4	0	1	0	0	0	4	0: 1344>	0	4	0	3	1	0	0
1350>	0	0	0	0	0	0	0	3: 1358>	0	0	4	0	0	0	0
1364>	0	0	0	0	0	0	0	0: 1372>	3	0	0	0	0	0	0
1378>	0	0	0	0	4	0	0	3: 1386>	0	2	0	0	0	0	0
1392>	0	1	0	0	1	0	0	1: 1400>	0	0	0	0	0	0	0

SUM ODD 3504.0 3532.6 3587.8 3545.5 3382.5 3546.1 3637.1
 EV 11830.2 10085.0 10487.5 10128.0 9453.1 9795.3 11293.8
 RATIO 0.29619 0.35028 0.34210 0.35007 0.35782 0.36202 0.32204
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.332506

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A14018.SUM 206 FKS W MIN. 1 CNTS. 21-JUN-93 19:06:45 SUM I: 0.4245E+04
 REF #18 SDH-ASDH (CONSOL) 0- 4 N AV MW: 174.2
 ACQUIRED 6-21-93 19:03:12 CHAN.#5 0- 4095; 6 MS/CHAN. WT AV MW: 195.1
 MAG. RET. TIME: 9999 MS, 8 SCANS/SPECTRM. 2 TO 0 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	U1	RH	ROH	5
48>	0	0	0	0	0	0	118	0:	56>	0	0	8588	765
62>	0	0	0	0	0	0	0	0:	70>	127	0	144	0
76>	0	0	193	0	0	0	159	104:	84>	2106	0	550	0
90>	0	0	501	97	88	0	232	92:	98>	1563	41	231	0
104>	0	0	760	167	144	0	111	69:	112>	1224	42	170	0
118>	343	0	841	108	321	39	555	81:	126>	981	11	201	0
132>	1760	53	796	85	391	47	893	16:	140>	909	13	504	0
146>	2871	107	752	95	291	19	993	40:	154>	580	20	527	70
160>	2628	84	635	94	302	20	925	32:	168>	1623	9	541	36
174>	2015	121	557	46	521	48	1061	69:	182>	2174	82	503	110
188>	2199	108	472	47	813	39	1309	98:	196>	1779	53	695	82
202>	2181	73	629	33	843	37	1993	78:	210>	1338	57	1104	44
216>	1308	73	552	4	677	66	1513	36:	224>	1241	75	1346	55
230>	1014	0	550	21	705	46	944	32:	238>	829	7	1096	75
244>	765	17	474	31	573	17	606	51:	252>	418	32	594	19
258>	489	58	317	22	414	0	374	1:	266>	236	0	346	0
272>	327	9	204	11	322	22	228	17:	280>	140	24	124	0
286>	133	0	108	20	124	0	121	0:	294>	84	0	80	0
300>	60	0	52	0	99	0	68	0:	308>	45	0	47	0
314>	0	0	0	0	0	0	34	0:	322>	0	0	0	0
328>	0	0	0	0	0	0	0	0:	336>	0	0	0	0
342>	0	0	0	0	0	0	0	0:	350>	0	0	0	102

SUM ODD 702.6 877.7 400.1 814.9 485.1 1262.2 702.2
 EV 18092.4 8393.4 6628.9 12235.0 17296.8 17391.2 14717.6
 RATIO 0.03883 0.10457 0.06036 0.06661 0.02804 0.07257 0.04771
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.055350

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INDIVIDUAL SPECTRA AND PATTERN TABLES FOR PFL SAMPLE 5

A14005.000 -62 to -29°C No. Av. MW = 184. Wt. Av. MW = 188.
REF NO. 5 (CONSOL)

111

A14005.001 -32 to -17°C No. Av. MW = 194. Wt. Av. MW = 197.
REF NO. 5 (CONSOL)

A14005.002 -19 to -7°C No. Av. MW = 207. Wt. Av. MW = 210.
REF NO. 5 (CONSOL)

A14005.003 -8 to 17°C No. Av. MW = 217. Wt. Av. MW = 220.
REF NO. 5 (CONSOL)

114

A14005.004 22 to 56°C No. Av. MW = 245. Wt. Av. MW = 250.
REF NO. 5 (CONSOL)

115

A14005.005 58 to 93°C No. Av. MW = 293. Wt. Av. MW = 299.
REF NO. 5 (CONSOL)

A14005.006 98 to 159°C No. Av. MW = 373. Wt. Av. MW = 386.
REF NO. 5 (CONSOL)

117

A14005.007 173 to 227°C No. Av. MW = 468. Wt. Av. MW = 486.
REF NO. 5 (CONSOL)

A14005.008 233 to 293°C No. Av. MW = 562. Wt. Av. MW = 589.
REF NO. 5 (CONSOL)

A14005.009 299 to 359°C No. Av. MW = 641. Wt. Av. MW = 672.
REF NO. 5 (CONSOL)

A14005.010 365 to 471°C No. Av. MW = 689. Wt. Av. MW = 720.
REF NO. 5 (CONSOL)

A14005.011 483 to 501°C No. Av. MW = 716. Wt. Av. MW = 738.
REF NO. 5 (CONSOL)

A14005.012 501 to 501°C No. Av. MW = 705. Wt. Av. MW = 710.
REF NO. 5 (CONSOL)

A14005.SUM -62 to 501°C No. Av. MW = 429. Wt. Av. MW = 531.
REF NO. 5 (CONSOL) ¹³C-Corrected

A14005.000 94 PKS W MIN. 1 CNTS. 08-JUN-93 15:04:23 SUM I: 0.9659E+03
 REF NO. 5 (CONSOL) N AV MW: 184.8
 ACQUIRED 5-28-93 11:51:14 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 188.1
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO -29 DEG. C SF= 0

ABSOLUTE INTENSITIES C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
132>	6	2	0	2	4	0	0	0	0: 140>	0	0	14	0	0	3
146>	31	3	2	4	3	0	0	0	0: 154>	6	0	28	2	13	1
160>	58	5	4	2	3	0	11	0	0: 168>	40	0	19	2	71	2
174>	58	4	8	2	11	0	18	0	0: 182>	34	1	14	0	76	1
188>	50	2	7	1	17	0	20	0	0: 196>	18	0	13	0	40	1
202>	26	1	9	0	19	0	16	1	1: 210>	8	1	9	1	18	0
216>	13	0	9	0	13	0	13	1	1: 224>	5	0	6	0	9	0
230>	5	0	6	0	7	0	6	0	0: 238>	3	0	4	0	4	0
244>	3	0	2	0	3	0	2	0	0: 252>	0	0	2	0	0	0
258>	0	0	0	0	0	0	0	0	0: 266>	0	0	0	0	0	0
272>	0	0	0	0	0	0	0	0	0: 280>	0	0	0	0	0	0
286>	0	0	0	0	0	0	0	0	0: 294>	0	0	0	0	0	0
300>	0	0	0	0	0	0	0	0	0: 308>	0	0	0	0	0	0
314>	0	0	0	0	0	0	0	0	0: 322>	0	0	0	0	0	0
328>	0	0	0	0	0	0	0	0	0: 336>	0	0	0	0	0	0
342>	0	0	0	0	0	0	0	0	0: 350>	0	0	0	0	1	0

SUM ODD 17.9 11.3 0.9 2.2 1.7 4.9 8.1
 EV 250.2 47.2 80.3 85.1 114.8 108.9 232.3
 RATIO 0.07172 0.23978 0.01063 0.02543 0.01495 0.04543 0.03476
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.051176

A14005.001 120 PKS W MIN. 1 CNTS. 08-JUN-93 15:04:48 SUM I: 0.1796E+04
 REF NO. 5 (CONSOL) N AV MW: 194.0
 ACQUIRED 5-28-93 12:03:08 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 197.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -32 TO -17 DEG. C SF= 0

ABSOLUTE INTENSITIES C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
118>	0	0	0	0	2	0	0	0	0: 126>	0	0	0	0	0	2
132>	4	0	0	0	5	0	0	0	0: 140>	0	0	6	1	0	6
146>	15	4	5	4	5	0	0	0	0: 154>	6	0	23	3	6	7
160>	27	8	6	2	4	0	10	1	1: 168>	98	1	38	4	83	8
174>	52	9	8	2	15	2	32	1	1: 182>	114	3	38	3	157	4
186>	83	6	9	1	19	1	31	0	0: 196>	54	3	27	0	95	3
202>	77	0	16	0	31	1	38	3	1: 210>	30	1	26	1	52	2
216>	34	2	21	1	29	0	30	1	1: 224>	17	0	17	1	26	0
230>	14	1	16	0	21	0	16	1	1: 238>	9	0	10	1	11	2
244>	7	1	8	0	10	0	7	0	0: 252>	3	0	4	0	5	0
258>	2	0	3	0	4	0	4	0	0: 266>	2	0	2	0	2	0
272>	2	0	2	0	0	0	2	0	0: 280>	0	0	1	0	0	0

SUM ODD 29.9 9.6 3.6 7.2 7.8 14.1 32.8
 EV 318.8 93.8 145.2 169.2 333.6 192.7 437.3
 RATIO 0.09364 0.10199 0.02509 0.04279 0.02341 0.07310 0.07504
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.062116

A14005.002 115 PKS W MIN. 1 CNTS. 08-JUN-93 15:05:08 SUM I: 0.1655E+04
 REF NO. 5 (CONSOL) N AV MW: 207.3
 ACQUIRED 5-28-93 12:15:01 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 210.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -19 TO -7 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
132>	0	0	0	0	0	0	0	0	0: 140>	0	0	0	0	0	2
146>	0	0	2	0	0	0	0	0	0: 154>	0	0	0	0	0	4
160>	0	0	4	0	0	0	5	2: 168>	43	1	7	6	12	5	
174>	2	5	3	0	15	1	33	4: 182>	143	2	24	6	100	7	
188>	23	7	5	2	13	0	40	3: 196>	88	2	37	6	110	8	
202>	61	5	16	3	14	2	41	2: 210>	43	1	37	2	78	5	
216>	51	3	29	0	31	1	33	4: 224>	23	0	28	1	43	2	
230>	27	0	25	0	32	0	25	2: 238>	11	2	15	1	22	0	
244>	11	1	16	1	18	0	13	1: 252>	7	1	7	0	7	1	
256>	6	1	7	0	10	1	6	0: 266>	3	0	4	0	3	0	
272>	3	0	4	0	5	0	3	0: 280>	2	0	3	0	2	0	
286>	0	0	2	0	2	0	0	0: 294>	1	0	0	0	0	0	

SUM ODD 23.0 6.0 4.7 17.3 9.4 22.0 34.4
 EV 182.9 112.1 139.2 198.7 364.2 163.8 377.0
 RATIO 0.12573 0.05315 0.03347 0.08717 0.02588 0.13439 0.09118
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.075914

A14005.003 109 PKS W MIN. 1 CNTS. 08-JUN-93 15:05:33 SUM I: 0.1544E+04
 REF NO. 5 (CONSOL) N AV MW: 217.4
 ACQUIRED 5-28-93 12:26:55 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 220.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -8 TO 17 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
160>	0	0	0	0	0	0	0	3: 168>	5	0	0	3	0	4	
174>	0	0	3	0	12	0	17	5: 182>	66	6	4	7	23	9	
188>	4	4	4	0	17	3	49	6: 196>	98	8	25	5	53	0	
202>	43	8	22	3	17	4	61	6: 210>	62	7	47	5	74	9	
216>	39	6	17	1	17	3	44	7: 224>	39	5	43	4	62	5	
230>	29	4	21	3	22	0	29	3: 238>	21	3	27	5	31	5	
244>	20	3	20	2	20	4	13	3: 252>	12	0	15	4	13	1	
258>	9	2	9	3	14	2	10	1: 266>	6	0	6	2	4	0	
272>	4	2	4	3	5	1	4	1: 280>	2	0	4	0	2	0	
286>	0	0	2	0	2	1	2	0: 294>	0	0	2	0	0	0	
300>	1	0	0	0	0	0	0	0: 308>	0	0	0	0	0	0	

SUM ODD 28.8 14.8 18.3 34.6 28.5 34.9 33.4
 EV 148.4 101.8 126.7 228.4 310.8 171.6 262.6
 RATIO 0.19387 0.14505 0.14425 0.15171 0.09167 0.20349 0.12702
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.143102

A14005.004 162 PKS W MIN. 1 CNTS. 08-JUN-93 15:05:57 SUM I: 0.3198E+04
 REF NO. 5 (CONSOL) N AV MW: 245.7
 ACQUIRED 5-28-93 12:38:49 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 250.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 22 TO 56 DEG. C SF= 0

ABSOLUTE INTENSITIES									C13XN, 86.00%C					PG. 1	
	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2	MASS>		U1		RH		ROH	
160>	0	0	0	0	0	0	0	3: 168>	0	0	0	0	0	0	0
174>	0	0	0	0	0	0	0	12: 182>	3	1	0	6	0	3	0
188>	0	0	0	0	15	3	19	16: 196>	22	6	2	8	3	0	0
202>	82	16	50	1	40	5	74	20: 210>	41	10	13	9	13	0	0
216>	109	14	64	12	69	0	127	24: 224>	64	9	37	8	20	30	0
230>	60	7	68	9	81	19	132	20: 238>	57	12	47	16	68	16	0
244>	49	9	39	23	67	8	85	14: 252>	46	10	42	13	51	13	0
258>	46	10	39	7	55	14	51	15: 266>	34	1	31	17	32	13	0
272>	25	5	28	12	39	9	35	12: 280>	24	13	26	7	18	6	0
286>	18	11	17	7	20	7	17	0: 294>	19	0	19	5	13	4	0
300>	10	5	11	3	12	4	11	0: 308>	12	6	12	2	10	2	0
314>	6	3	8	2	7	2	7	0: 322>	6	4	6	0	6	3	0
328>	5	2	5	2	3	2	4	0: 336>	4	2	3	2	4	1	0
342>	2	0	3	0	3	0	2	2: 350>	2	3	2	0	2	0	0
356>	2	0	0	0	0	0	0	0: 364>	2	0	2	0	0	0	0
370>	0	0	1	0	0	0	0	0: 378>	1	0	0	0	0	0	0

SUM ODD 82.5 79.6 72.5 137.5 77.6 93.3 91.6
 EV 414.2 334.1 411.2 563.3 339.3 241.6 239.6
 RATIO 0.19929 0.23833 0.17622 0.24402 0.22861 0.38629 0.38247
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.249522

A14005.005 197 PKS W MIN. 1 CNTS. 08-JUN-93 15:06:22 SUM I: 0.2804E+04
 REF NO. 5 (CONSOL) N AV MW: 293.6
 ACQUIRED 5-28-93 12:50:42 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 299.3
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 58 TO 93 DEG. C SF= 0

ABSOLUTE INTENSITIES									C13XN, 86.00%C					PG. 1	
	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2		MASS>	U1		RH		ROH	
216>	8	5	2	0	2	8	1	3: 224>	0	2	0	0	0	3	0
230>	25	7	18	3	9	15	5	6: 238>	2	2	0	0	0	93	9
244>	50	11	28	10	21	14	11	7: 252>	12	2	10	4	99	17	
258>	77	15	44	14	26	18	21	9: 266>	15	6	22	9	62	14	
272>	88	12	58	19	57	15	28	0: 280>	21	22	41	24	49	16	
286>	61	19	51	16	45	14	34	7: 294>	18	16	38	33	36	0	
300>	51	11	43	12	33	15	26	6: 308>	21	0	31	5	37	8	
314>	40	5	38	11	28	9	18	0: 322>	18	0	21	6	23	16	
328>	18	7	22	7	17	18	12	13: 336>	9	14	4	18	3	17	
342>	0	16	7	13	9	13	8	11: 350>	6	12	4	11	6	8	
356>	3	11	0	10	5	10	5	8: 364>	4	9	3	9	3	7	
370>	0	7	4	8	3	5	4	4: 378>	4	6	4	5	3	4	
384>	3	5	2	4	2	5	2	4: 392>	3	3	3	4	1	3	
398>	2	4	2	2	2	4	1	0: 406>	3	2	2	2	2	2	
412>	1	2	0	2	0	2	0	2: 420>	1	0	2	1	0	2	
426>	0	1	1	0	1	0	0	0: 434>	0	2	0	0	0	0	
440>	0	0	0	1	0	0	0	0: 448>	0	1	0	0	0	0	

SUM ODD 137.4 132.5 164.4 78.7 98.7 131.1 123.1
 EV 428.2 319.2 260.8 176.3 136.8 184.8 421.6
 RATIO 0.32090 0.41501 0.63043 0.44629 0.72160 0.70940 0.29203
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.449201

A14005.006 383 PKS W MIN. 1 CNTS. 08-JUN-93 15:06:51 SUM I: 0.5556E+04
 REF NO. 5 (CONSOL) N AV MW: 373.5

ACQUIRED 5-28-93 13:02:36 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 386.0
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 98 TO 159 DEG. C SF= 0

ABSOLUTE INTENSITIES									C13XN, 86.00% PG. 1						
	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2		MASS>	U1		RH		ROH	
230>	0	0	0	0	1	0	0	0:	238>	0	0	0	0	2	0
244>	0	2	0	0	0	0	0	0:	252>	2	2	2	2	5	4
258>	1	0	0	0	0	1	2	2:	266>	8	0	7	7	11	11
272>	7	5	2	7	58	7	14	4:	280>	18	5	43	10	22	16
286>	10	7	5	8	53	10	31	8:	294>	26	11	57	18	31	18
300>	36	14	14	9	42	11	46	13:	308>	46	12	58	24	43	17
314>	27	16	69	15	50	15	51	16:	322>	60	18	58	26	52	19
328>	32	15	73	18	67	19	54	19:	336>	68	20	61	21	59	18
342>	41	14	65	17	69	18	58	23:	350>	60	25	60	22	49	14
356>	60	13	65	17	56	19	63	18:	364>	55	22	48	19	37	16
370>	48	15	57	17	58	16	54	18:	378>	49	17	44	15	41	10
384>	43	13	53	13	49	15	42	15:	392>	39	15	34	14	35	9
398>	39	10	39	14	41	14	37	11:	406>	37	12	30	11	24	10
412>	32	11	34	9	34	9	30	10:	420>	28	8	27	7	22	8
426>	24	9	27	8	23	9	23	8:	434>	21	9	21	5	17	7
440>	21	6	23	6	19	9	20	6:	448>	17	3	17	5	16	4
454>	15	4	17	5	16	5	14	5:	462>	12	4	13	3	12	3
468>	13	4	14	5	11	5	12	5:	476>	11	4	10	4	11	4
482>	10	3	10	4	9	3	9	4:	490>	11	2	7	4	9	4
496>	9	2	8	2	9	2	9	2:	504>	7	3	7	2	7	2
510>	6	3	7	2	6	2	4	3:	518>	6	3	5	2	5	2
524>	6	2	5	2	5	1	5	2:	532>	4	1	3	2	4	1
538>	6	1	4	2	4	1	4	2:	546>	3	2	2	1	3	1
552>	4	2	4	1	3	2	4	0:	560>	4	1	3	1	3	1
566>	3	1	2	1	2	2	2	1:	574>	3	1	2	1	2	1
580>	3	1	2	1	2	2	2	1:	588>	2	1	2	0	2	1
594>	3	0	2	0	2	0	2	0:	602>	2	0	2	1	3	0
608>	2	0	2	1	1	1	2	0:	616>	1	0	1	0	2	0
622>	2	1	1	1	1	0	1	0:	630>	1	0	2	0	2	0
636>	1	0	0	0	0	0	1	1:	644>	1	0	0	0	2	0
650>	0	1	0	0	1	0	0	1:	658>	0	0	0	0	1	0
664>	1	0	0	0	0	0	1	0:	672>	0	0	0	0	0	0

SUM ODD	175.8	184.5	197.1	196.3	200.1	229.2	202.9
EV	505.7	607.0	693.3	597.9	602.0	626.1	536.6
RATIO	0.34770	0.30400	0.28425	0.32839	0.33245	0.36612	0.37811
OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.332493							

A14005.007 483 PKS W MIN. 1 CNTS. 08-JUN-93 15:07:32 SUM 1: 0.3861E+04
 REF NO. 5 (CONSOL) N AV MW: 468.4
 ACQUIRED 5-28-93 13:14:30 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 486.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 173 TO 227 IEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
244>	0	0	0	0	0	0	0	0	0: 252>	0	0	0	1	0	0
258>	0	0	0	0	0	0	0	0	0: 266>	0	0	0	0	0	0
272>	0	0	0	0	0	0	0	0	0: 280>	1	0	0	0	0	0
286>	0	0	0	0	0	2	1	0	0: 294>	0	2	0	2	0	0
300>	0	0	1	1	0	0	0	0	0: 308>	0	0	0	0	0	0
314>	0	2	3	2	2	2	0	2	2: 322>	1	1	0	2	6	2
328>	4	3	5	5	3	4	2	2	2: 336>	1	2	1	1	15	6
342>	8	5	9	7	4	4	3	3	3: 350>	23	5	8	4	15	5
356>	22	6	17	7	8	8	4	4	4: 364>	25	6	20	6	16	8
370>	29	10	15	13	20	10	14	6	4: 378>	21	8	29	10	28	9
384>	31	13	23	13	17	11	24	11	5: 392>	25	8	31	10	34	12
398>	34	13	25	14	18	11	26	10	6: 406>	35	12	39	14	33	14
412>	33	14	32	14	25	13	25	11	7: 420>	34	13	32	11	35	13
426>	33	15	27	11	26	11	28	9	8: 434>	30	13	30	13	30	15
440>	28	13	25	12	23	10	28	11	9: 448>	31	12	28	15	27	13
454>	25	11	27	10	26	8	26	10	10: 462>	28	13	24	11	24	11
468>	21	10	23	8	21	9	23	9	11: 476>	25	10	25	9	19	11
482>	21	8	19	7	19	8	22	8	12: 490>	20	9	19	9	20	9
496>	17	10	14	7	18	5	18	8	13: 504>	19	9	18	7	17	6
510>	15	7	14	5	16	5	16	7	14: 518>	13	6	16	6	13	5
524>	12	6	15	5	13	4	13	6	15: 532>	10	7	12	4	13	6
538>	10	5	11	4	11	5	13	6	16: 546>	10	4	10	5	9	6
552>	10	4	10	4	9	6	10	4	17: 560>	9	4	8	4	8	4
566>	9	3	8	4	8	4	7	2	18: 574>	8	3	6	0	8	4
580>	8	3	6	4	8	1	7	4	19: 588>	6	3	7	2	7	2
594>	7	2	7	2	6	4	6	2	20: 602>	6	2	5	2	7	2
608>	6	2	5	2	6	2	6	1	21: 616>	6	2	4	3	4	3
622>	5	2	5	2	4	2	5	2	22: 630>	5	2	4	1	3	3
636>	3	2	4	2	3	3	4	1	23: 644>	4	0	4	2	4	2
650>	4	1	4	2	3	1	3	2	24: 658>	3	1	3	2	3	2
664>	4	1	4	1	3	1	3	1	25: 672>	2	2	4	1	3	1
678>	3	2	1	2	2	1	3	1	26: 686>	2	1	3	1	2	1
692>	3	1	3	1	2	0	2	1	27: 700>	2	2	2	1	1	2
706>	1	2	2	1	2	1	3	1	28: 714>	2	1	2	1	1	1
720>	2	1	2	1	2	1	2	1	29: 728>	1	1	1	1	1	1
734>	0	3	0	1	1	1	2	0	30: 742>	1	0	2	0	1	1
748>	1	1	1	1	1	0	1	0	31: 756>	1	1	1	0	1	2
762>	1	0	1	0	1	1	1	0	32: 770>	1	0	2	0	1	0
776>	1	1	1	0	0	0	1	1	33: 784>	0	0	0	0	1	0
790>	1	0	1	0	0	0	0	1	34: 798>	0	0	1	0	0	0
804>	0	1	0	0	1	0	1	0	35: 812>	0	0	0	0	1	1
818>	0	0	0	0	1	1	0	0	36: 826>	0	0	0	0	0	0
832>	0	0	0	0	0	0	0	0	37: 840>	0	0	0	0	0	0
846>	0	0	0	1	0	0	0	0	38: 854>	0	0	0	0	0	0

SUM ODD 184.1 179.4 159.9 148.3 162.3 161.7 181.7
 EV 410.9 370.8 333.0 350.7 410.7 391.2 412.3
 RATIO 0.44813 0.48379 0.48005 0.42287 0.39506 0.41341 0.44071
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.439381

A14005.008 662 PKS W MIN. 1 CNTS. 08-JUN-93 15:08:25 SUM I: 0.3759E+04
 REF NO. 5 (CONSOL) N AV MW: 562.8
 ACQUIRED 5-28-93 13:26:23 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 589.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 233 TO 293 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		RDH	
216>	2	0	0	0	0	0	0	0	0: 224>	0	0	0	0	0	0
230>	0	0	0	0	0	0	0	0	0: 238>	0	0	0	0	0	0
244>	0	0	0	0	0	0	0	0	0: 252>	0	0	0	0	2	0
258>	0	0	0	0	0	0	0	0	0: 266>	0	0	0	2	0	0
272>	0	0	0	0	0	1	0	0	0: 280>	0	0	2	0	0	2
286>	0	0	1	0	0	0	0	0	0: 294>	0	2	0	0	0	0
300>	0	0	0	0	0	0	2	0	0: 308>	0	0	0	0	0	0
314>	0	2	0	0	2	2	1	0	0: 322>	0	0	0	0	0	0
328>	0	2	0	2	0	2	2	0	0: 336>	0	0	0	0	0	2
342>	0	1	0	0	0	0	0	0	0: 350>	1	0	0	0	2	2
356>	1	0	0	2	1	1	0	1	1: 364>	2	1	0	2	1	2
370>	0	2	0	2	4	2	2	1	1: 378>	3	2	1	2	3	1
384>	0	2	1	2	5	3	6	3	3: 392>	2	4	3	3	2	2
398>	6	3	8	2	5	3	9	5	5: 406>	5	3	4	5	2	3
412>	3	6	14	6	10	5	12	7	7: 420>	8	4	4	4	16	4
426>	7	4	19	6	15	7	13	8	8: 434>	9	7	7	4	17	8
440>	13	7	17	9	18	10	13	11	11: 448>	15	7	13	7	15	6
454>	23	11	21	7	22	10	16	10	10: 462>	12	9	20	6	19	7
468>	22	10	23	13	22	10	20	10	10: 476>	16	9	21	9	24	8
482>	24	11	24	12	23	12	18	12	12: 490>	17	10	18	9	22	11
496>	24	10	24	11	19	11	18	11	11: 504>	20	8	18	11	21	13
510>	24	11	24	10	22	12	19	10	10: 518>	19	7	19	9	20	14
524>	21	10	20	11	20	9	22	8	8: 532>	17	9	19	9	23	11
538>	19	12	16	11	16	11	17	7	7: 546>	18	8	17	9	20	8
552>	18	12	19	8	18	8	14	8	8: 560>	16	9	17	9	17	9
566>	16	10	16	8	15	7	15	6	6: 574>	15	7	15	10	15	9
580>	17	7	12	9	15	7	11	8	8: 588>	12	6	14	8	15	8
594>	13	8	12	8	11	8	10	7	7: 602>	12	5	14	6	13	6
608>	13	7	10	8	9	6	12	4	4: 616>	12	5	12	8	10	6
622>	11	6	11	4	12	4	11	5	5: 630>	9	6	11	5	9	7
636>	9	5	9	6	8	7	7	4	4: 644>	10	5	9	5	6	6
650>	7	4	8	6	8	5	9	3	3: 658>	9	4	8	4	7	4
664>	7	5	6	4	7	4	7	4	4: 672>	6	3	7	4	6	3
678>	6	3	6	3	7	3	7	3	3: 686>	7	3	6	4	6	5
692>	5	3	6	2	6	3	5	3	3: 700>	4	4	4	2	5	4
706>	4	4	4	3	4	2	5	3	3: 714>	4	2	4	3	4	2
720>	5	2	4	2	4	3	3	3	3: 728>	4	2	5	2	4	3
734>	3	3	4	3	3	2	4	2	2: 742>	4	2	3	2	3	2
748>	3	2	4	1	4	1	2	2	2: 756>	4	1	4	1	4	2
762>	3	2	3	3	3	2	2	2	2: 770>	3	1	3	2	2	2
776>	3	1	3	1	4	1	3	2	2: 784>	1	2	2	2	2	2
790>	2	1	2	1	2	1	3	2	2: 798>	2	1	3	1	3	1
804>	2	2	2	2	1	2	1	1	1: 812>	2	1	3	0	3	1
818>	1	2	1	1	2	1	2	1	1: 826>	2	1	2	1	2	2
832>	1	1	3	1	2	2	1	2	2: 840>	2	0	1	1	2	1
846>	1	1	2	1	2	0	2	1	1: 854>	1	1	2	1	2	1
860>	1	1	1	1	1	1	2	0	0: 868>	2	1	1	1	2	0
874>	0	2	1	1	1	1	0	1	1: 882>	1	1	1	1	1	1
888>	1	1	0	2	1	1	0	1	1: 896>	1	1	1	1	0	1
902>	0	1	0	0	2	1	1	1	1: 910>	1	1	1	1	1	1
916>	1	1	1	0	1	0	1	1	1: 924>	1	1	1	0	1	1
930>	0	2	1	0	1	0	1	0	0: 938>	1	1	1	1	0	0

A14005.008 662 FKS W MIN. 1 CNTS. 08-JUN-93 15:09:01 SUM I: 0.3759E+04
 REF NO. 5 (CONSOL) N AV MW: 562.8
 ACQUIRED 5-28-93 13:26:23 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 589.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 233 TO 293 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
944>	0	1	0	1	0	1	1	0	0: 952>	1	0	0	1	0	0
958>	1	1	1	1	1	0	1	1	1: 966>	0	0	2	0	1	0
972>	1	0	1	0	1	0	1	1	1: 980>	0	1	0	1	1	1
986>	0	1	0	1	1	1	0	1	1: 994>	1	1	0	1	0	1
1000>	0	1	0	0	1	0	0	0	0:1008>	1	0	0	1	0	0
1014>	0	0	0	0	0	0	0	0	0:1022>	0	0	1	0	1	0
1028>	0	0	0	0	0	0	0	0	0:1036>	0	0	0	0	1	0
1042>	0	0	0	0	0	0	0	0	0:1050>	0	0	0	0	0	0
1056>	0	0	0	0	0	0	0	0	0:1064>	0	0	0	0	0	0
1070>	0	0	0	0	0	0	0	0	0:1078>	0	0	0	0	0	0

SUM ODD	205.0	195.2	196.3	189.8	172.2	183.2	196.9
EV	345.8	366.5	358.0	333.3	316.4	320.6	357.0
RATIO	0.59296	0.53271	0.54831	0.56932	0.54415	0.57145	0.55173

OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.558341

A14005.009 785 PKS W MIN. 1 CNTS. 08-JUN-93 15:09:35 SUM I: 0.4077E+04
 REF NO. 5 (CONSOL) N AV MW: 641.0
 ACQUIRED 5-28-93 13:38:17 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 672.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 299 TO 359 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
244>	0	0	0	0	0	0	0	0:	252>	0	0	0	3	0	0
258>	0	0	0	0	0	0	0	0:	266>	0	0	2	0	0	2
272>	0	0	2	0	0	0	0	0:	280>	0	0	0	0	0	1
286>	0	2	0	0	0	0	0	0:	294>	0	2	0	0	2	2
300>	0	0	0	0	0	0	2	0:	308>	0	0	0	0	0	2
314>	0	0	0	2	0	0	0	0:	322>	0	0	0	0	2	0
328>	1	2	0	0	2	0	0	0:	336>	0	0	0	2	0	0
342>	0	2	0	0	2	1	0	2:	350>	1	0	0	0	3	2
356>	0	0	0	0	2	0	0	0:	364>	2	0	0	0	0	1
370>	0	2	1	0	2	0	1	1:	378>	2	0	0	2	1	1
384>	1	0	0	2	1	2	1	1:	392>	1	2	0	0	2	0
398>	1	0	0	0	0	2	1	1:	406>	1	1	0	2	1	0
412>	2	2	1	2	1	1	2	1:	420>	2	2	1	1	4	1
426>	2	1	2	2	1	2	0	2:	434>	0	3	2	3	5	3
440>	2	3	3	1	2	2	2	1:	448>	7	2	3	3	5	3
454>	3	3	3	3	1	1	1	3:	462>	8	4	10	3	7	5
468>	5	4	2	4	8	3	10	4:	476>	8	6	11	7	8	5
482>	5	6	2	5	7	6	18	7:	490>	13	5	14	9	10	6
496>	9	6	12	5	9	6	17	10:	504>	18	8	14	8	10	6
510>	7	7	16	6	17	7	17	9:	518>	17	10	15	9	15	8
524>	14	7	15	9	18	10	20	11:	532>	16	11	14	10	12	14
538>	12	10	16	9	19	10	20	12:	546>	19	12	15	12	13	11
552>	17	10	17	11	19	12	23	13:	560>	21	11	18	11	16	9
566>	17	9	21	9	23	12	21	10:	574>	19	13	15	12	16	10
580>	16	10	19	11	22	11	19	13:	588>	15	12	18	11	15	9
594>	17	14	16	12	21	10	19	10:	602>	15	13	15	12	16	9
608>	17	12	15	13	17	12	15	11:	616>	14	12	14	11	17	9
622>	18	10	18	9	15	10	16	10:	630>	16	8	14	11	12	11
636>	15	10	18	8	14	9	15	8:	644>	16	8	14	8	13	9
650>	14	9	13	12	11	10	12	9:	658>	12	8	13	7	14	8
664>	14	7	13	7	14	7	12	7:	672>	11	8	12	8	12	8
678>	12	7	13	5	11	8	11	7:	686>	10	9	9	9	10	5
692>	13	6	10	7	10	7	11	6:	700>	10	7	9	8	9	7
706>	10	5	11	7	8	6	9	7:	714>	10	5	9	6	8	6
720>	9	6	8	6	8	5	10	5:	728>	8	5	9	6	10	4
734>	8	6	6	6	9	5	8	4:	742>	7	5	7	5	8	5
748>	6	6	6	5	7	3	6	5:	756>	6	6	5	6	6	5
762>	7	5	5	6	5	4	6	4:	770>	7	4	6	4	5	3
776>	6	5	4	5	5	4	4	0:	784>	8	1	5	4	6	3
790>	6	3	4	5	4	5	6	4:	798>	4	4	3	4	4	3
804>	5	4	4	3	4	4	4	4:	812>	3	5	4	3	4	1
818>	4	3	4	3	4	3	4	3:	826>	5	2	4	3	3	3
832>	3	4	3	2	4	3	4	2:	840>	3	3	3	3	4	1
846>	3	3	3	2	3	3	2	3:	854>	4	2	2	3	2	3
860>	2	4	2	2	4	2	2	3:	868>	3	1	4	2	2	2
874>	3	2	3	2	4	1	3	2:	882>	2	2	3	2	3	2
888>	2	2	1	3	1	2	2	2:	896>	2	2	3	1	2	2
902>	2	1	2	2	2	2	2	2:	910>	2	1	3	1	2	1
916>	2	1	2	2	1	2	1	2:	924>	2	2	2	1	1	1
930>	2	2	2	1	2	1	2	1:	938>	2	0	2	1	2	1
944>	2	0	2	0	2	1	1	1:	952>	2	2	1	0	2	2
958>	0	2	1	1	1	2	1	1:	966>	1	1	2	1	1	1

A14005.009 785 PKS W MIN. 1 CNTS. 08-JUN-93 15:10:12 SUM I: 0.4077E+04
 REF NO. 5 (CONSOL) N AV MW: 641.0
 ACQUIRED 5-28-93 13:38:17 CHAN.#5 0- 8191; 6 MS/CHAN. WT AV MW: 672.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 299 TO 359 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% FG. 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2	MASS>		U1		RH		ROH	
972>	1	2	0	1	1	1	1	1: 980>	1	1	1	1	1	1	1
986>	1	1	1	1	1	2	1	2: 994>	0	1	1	1	1	1	1
1000>	1	1	1	1	1	1	0	1:1008>	1	1	1	0	1	1	0
1014>	0	1	1	1	1	1	1	0:1022>	1	1	0	2	0	1	1
1028>	0	1	0	1	1	0	1	0:1036>	1	1	1	1	1	1	0
1042>	1	1	1	1	1	1	0	1:1050>	1	1	0	1	0	1	1
1056>	0	0	1	0	1	0	0	2:1064>	0	1	1	0	1	1	0
1070>	0	1	0	0	1	1	1	0:1078>	1	0	1	0	0	1	1
1084>	0	1	1	0	1	0	1	0:1092>	0	1	0	0	1	1	0
1096>	0	1	0	1	0	1	0	0:1106>	1	0	0	0	1	1	1
1112>	0	1	0	0	1	0	0	0:1120>	0	1	0	0	0	0	0
1126>	0	0	1	0	0	0	1	0:1134>	1	0	0	1	0	0	0
1140>	1	0	0	1	0	0	0	1:1148>	0	0	0	1	0	0	0
1154>	1	0	0	1	0	0	0	1:1162>	0	0	0	1	0	0	0
1168>	0	1	0	1	0	0	0	0:1176>	0	0	0	0	0	0	0
1182>	1	0	0	0	0	0	0	0:1190>	1	0	0	0	1	0	0
1196>	1	0	0	0	0	0	0	0:1204>	0	0	0	0	0	0	0
1210>	0	0	0	0	0	0	0	0:1218>	0	0	0	0	0	0	0
1224>	0	0	0	0	0	0	0	0:1232>	0	0	0	0	0	0	0
1238>	1	0	0	0	0	0	0	0:1246>	0	0	0	0	0	0	0

SUM ODD	234.9	228.3	225.2	235.5	239.6	246.1	226.1
EV	327.8	333.1	355.0	370.1	361.9	333.1	333.1
RATIO	0.71654	0.68514	0.63437	0.63629	0.66209	0.73870	0.67878
OVERALL RATIO OF ODD TO EVEN MASS PEAKS	0.677508						

A14005.010 760 PKS W MIN. 1 CNTS. 08-JUN-93 15:10:49 SUM I: 0.2819E+04
 REF NO. 5 (CONSOL) N AV MW: 689.1
 ACQUIRED 5-28-93 13:50:11 CHAN.#S 0- 8191: 6 MS/CHAN. WT AV MW: 720.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 365 TO 471 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
258>	0	0	0	0	0	0	0	0	0: 266>	0	0	0	2	1	0
272>	0	0	0	0	0	0	0	0	0: 280>	0	0	0	0	0	0
286>	0	0	0	0	0	0	0	0	0: 294>	0	0	0	0	0	0
300>	0	0	0	0	0	0	0	0	0: 308>	0	0	0	0	0	0
314>	0	0	0	0	0	0	0	0	0: 322>	0	2	0	0	0	0
328>	1	1	0	0	0	0	0	1	1: 336>	0	0	0	0	0	0
342>	1	0	0	0	0	0	2	0	0: 350>	2	1	0	0	2	0
356>	0	0	0	2	0	0	0	0	0: 364>	0	0	2	0	0	1
370>	0	2	0	0	0	2	1	0	0: 378>	2	0	2	1	1	0
384>	1	0	0	1	1	0	0	2	1: 392>	1	0	0	0	1	1
398>	0	0	2	1	0	2	0	1	1: 406>	1	0	1	0	2	1
412>	0	0	0	2	1	0	1	0	0: 420>	2	0	0	0	2	0
426>	1	2	1	1	1	1	0	2	2: 434>	0	2	0	2	1	1
440>	1	1	0	2	1	1	0	2	2: 448>	1	0	2	1	1	1
454>	2	1	0	1	1	2	1	1	1: 462>	1	1	2	1	1	1
468>	2	1	1	0	2	1	2	2	2: 476>	1	1	2	2	1	2
482>	1	1	1	1	2	3	2	3	3: 490>	2	2	1	2	1	1
496>	3	2	4	2	4	1	4	2	2: 504>	2	2	2	2	1	3
510>	3	3	7	5	4	4	4	4	4: 518>	2	2	2	2	6	4
524>	6	3	9	5	5	4	3	4	4: 532>	2	2	4	3	9	5
538>	10	5	8	6	8	5	3	4	4: 546>	5	2	8	4	10	6
552>	11	9	9	7	5	6	5	4	4: 560>	6	4	12	5	10	7
566>	13	8	10	7	7	6	6	5	5: 574>	6	5	13	6	14	6
580>	14	7	11	9	5	7	8	4	4: 588>	11	5	12	8	16	10
594>	11	10	10	7	8	6	8	0	0: 602>	15	7	14	10	13	9
608>	15	6	11	8	8	6	9	8	8: 616>	11	9	14	8	15	8
622>	13	7	11	5	12	4	12	7	7: 630>	12	8	14	9	13	9
636>	11	8	9	8	8	8	13	6	6: 644>	13	8	13	7	13	7
650>	9	9	8	7	10	6	10	9	9: 658>	13	8	9	9	10	8
664>	9	8	7	7	9	5	12	0	0: 672>	14	8	11	7	10	7
678>	9	7	9	6	10	6	11	7	7: 686>	11	6	11	4	9	8
692>	8	6	10	7	8	7	9	7	7: 700>	8	8	9	7	8	7
706>	7	7	9	4	10	5	8	7	7: 714>	8	6	8	7	6	7
720>	8	6	7	6	8	6	8	5	5: 728>	8	7	6	6	5	6
734>	6	5	7	6	8	6	6	6	6: 742>	7	5	6	6	5	4
748>	7	4	8	4	8	5	6	5	5: 756>	6	3	6	5	6	4
762>	5	5	6	5	5	4	6	5	5: 770>	6	5	4	4	5	5
776>	7	4	6	3	6	5	4	3	3: 784>	6	4	5	4	4	4
790>	5	4	4	5	4	3	6	3	3: 798>	4	3	5	4	4	4
804>	5	3	5	3	4	3	4	4	4: 812>	5	3	4	4	2	4
818>	3	4	4	4	4	2	4	3	3: 826>	4	3	4	2	4	2
832>	3	4	3	3	4	3	3	4	4: 840>	2	3	3	3	4	1
846>	4	4	2	4	3	2	3	3	3: 854>	2	4	3	2	4	2
860>	3	2	2	2	3	3	3	1	1: 868>	3	2	5	2	2	2
874>	2	3	3	2	3	2	3	3	3: 882>	2	1	3	2	2	3
888>	2	3	2	3	1	3	2	2	2: 896>	2	2	2	3	2	3
902>	2	2	3	2	2	1	2	1	1: 910>	2	2	2	2	2	2
916>	1	2	2	1	3	1	4	1	1: 924>	3	0	2	2	2	1
930>	2	2	1	1	3	1	2	2	2: 938>	2	2	1	2	1	1
944>	2	1	1	1	2	1	1	1	1: 952>	2	1	1	2	1	0
958>	2	1	1	2	2	1	1	2	2: 966>	1	2	0	1	2	1
972>	2	1	2	1	2	1	1	1	1: 980>	1	1	2	1	1	1

A14005.010 760 PKS W MIN. 1 CNTS. 08-JUN-93 15:11:30 SUM I: 0.2819E+04
 REF NO. 5 (CONSOL) N AV MW: 689.1
 ACQUIRED 5-28-93 13:50:11 CHAN.#8 0- 8191 6 MS/CHAN. WT AV MW: 720.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 365 TO 471 DEG. C SF= 0

ABSOLUTE INTENSITIES									C13XN, 86.00%C					FG. 2		
	0	1	2	3	4	5	6	7		0	1	2	3	4	5	
MASS			AR		U3		U2	MASS>		U1		RH		ROH		
986>	1	1	1	1	2	1	1	1: 994>	2	2	0	0	2	1		
1000>	2	1	1	1	1	1	1	1:1008>	1	1	1	1	0	2		
1014>	0	2	1	1	0	1	1	1:1022>	1	1	0	1	1	1		
1028>	1	1	1	2	1	1	1	0:1036>	1	1	0	1	1	1		
1042>	1	1	0	0	1	1	0	1:1050>	1	0	1	1	1	1		
1056>	1	0	0	1	0	1	1	0:1064>	1	0	1	0	2	0		
1070>	1	1	1	1	1	1	1	1:1078>	0	1	1	0	0	0		
1084>	1	0	1	0	0	1	0	1:1092>	0	1	0	1	0	1		
1098>	0	1	1	0	0	1	0	0:1106>	1	0	1	0	1	0		
1112>	0	1	0	1	0	0	1	1:1120>	1	0	1	0	1	0		
1126>	1	0	1	1	1	0	1	0:1134>	0	0	0	0	1	0		
1140>	0	0	0	1	0	1	0	1:1148>	0	1	1	0	0	0		
1154>	1	0	0	1	0	0	0	1:1162>	0	1	0	0	0	1		
1168>	0	0	0	0	0	0	0	1:1176>	0	0	0	1	0	0		
1182>	0	0	0	0	0	0	0	0:1190>	0	1	0	0	0	0		
1196>	0	0	0	0	0	0	0	0:1204>	0	0	0	0	0	1		
1210>	0	0	0	0	0	0	0	0:1218>	0	0	0	0	0	1		
1224>	0	0	0	0	0	0	0	0:1232>	0	0	0	0	0	0		
1238>	0	0	0	0	0	1	0	0:1246>	0	0	0	0	0	0		
1252>	0	0	0	0	0	0	0	0:1260>	0	0	0	0	0	0		
1266>	0	0	0	0	0	0	0	0:1274>	0	0	0	0	0	0		
1280>	0	0	0	0	0	0	0	0:1288>	0	0	0	0	0	0		
1294>	0	0	0	0	0	0	0	0:1302>	0	0	0	0	0	0		
1308>	0	0	0	0	1	0	0	0:1316>	0	0	0	0	0	0		
1322>	0	0	0	0	0	0	0	0:1330>	0	0	0	0	0	0		
1336>	0	0	0	0	0	0	0	0:1344>	0	0	0	0	0	0		

SUM ODD	180.1	176.0	162.7	153.3	158.9	171.9	179.3
EV	244.9	224.9	215.0	208.5	229.9	238.9	244.8
RATIO	0.73511	0.78245	0.75656	0.73512	0.69131	0.71946	0.73219

OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.735570

A14005.011 544 PKS W MIN. 1 CNTS. 08-JUN-93 15:12:08 SUM 1: 0.1201E+04
 REF NO. 5 (CONSOL) N AV MW: 716.5
 ACQUIRED 5-28-93 14:02:05 CHAN.#5 0- 81911 6 MS/CHAN. WT AV MW: 738.8
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 483 TO 501 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00XC FG. 1

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48	0	0	0	0	0	0	0	0	56	0	4	0	0	0	0
62	0	0	0	0	0	0	0	0	70	0	0	0	0	0	0
76	0	0	0	0	0	0	0	0	84	0	0	0	0	0	0
90	0	0	0	0	0	0	0	0	98	0	0	0	0	0	0
104	0	0	0	0	0	0	0	0	112	0	0	0	0	0	0
118	0	0	0	0	0	0	0	0	126	0	0	0	0	0	0
132	0	0	0	0	0	0	0	0	140	0	0	0	0	0	0
146	0	0	0	0	0	0	0	0	154	0	0	0	0	0	0
160	0	0	0	0	0	0	0	0	168	0	0	0	0	0	0
174	0	0	0	0	0	0	0	0	182	0	0	0	0	0	0
188	0	0	0	0	0	0	0	0	196	0	0	0	0	0	0
202	0	0	0	0	0	0	0	0	210	0	0	0	0	0	0
216	0	0	0	0	0	0	0	0	224	0	0	0	0	0	0
230	0	0	0	0	0	0	0	0	238	0	0	0	0	0	0
244	0	0	0	0	0	0	0	0	252	0	0	0	0	0	0
258	0	0	0	0	0	0	0	0	266	0	0	0	0	0	0
272	0	0	0	0	0	0	0	0	280	0	0	0	0	0	0
286	0	0	0	0	0	0	0	0	294	0	0	0	0	0	0
300	0	0	1	0	0	0	0	0	308	0	0	0	0	0	0
314	0	0	0	0	0	0	0	0	322	0	0	0	0	0	0
328	0	0	0	0	0	0	0	0	336	0	0	0	0	1	0
342	0	0	0	0	0	0	0	0	350	0	0	0	0	0	0
356	0	0	0	0	2	0	0	0	364	0	0	0	0	0	0
370	0	0	0	0	0	0	0	0	378	0	0	0	0	0	0
384	0	0	0	0	0	0	0	0	392	0	0	0	0	0	0
398	0	0	0	0	0	0	0	0	406	0	0	0	0	0	0
412	0	0	0	0	0	0	0	0	420	0	0	0	0	0	0
426	0	0	1	1	0	0	0	0	434	0	0	0	0	0	0
440	0	0	0	0	0	1	1	0	448	1	0	0	0	0	0
454	0	0	0	0	0	0	0	0	462	0	0	0	0	0	0
468	0	0	0	0	1	0	0	0	476	0	0	0	0	0	0
482	0	0	0	0	0	0	0	1	490	0	0	0	0	0	0
496	0	0	1	0	0	0	1	0	504	1	0	0	0	1	0
510	0	0	0	2	1	1	0	0	518	1	0	0	0	2	1
524	2	0	0	2	1	0	1	0	532	1	1	0	1	2	1
538	1	0	2	1	1	1	1	2	546	2	0	3	2	2	2
552	2	2	2	1	1	1	2	1	560	3	2	3	3	2	2
566	1	3	1	1	2	1	3	3	574	4	2	5	2	4	2
580	2	1	2	1	2	3	4	3	588	4	3	4	3	4	2
594	2	3	3	1	3	3	4	4	602	6	3	4	4	3	3
608	2	3	3	2	4	3	6	3	616	6	4	4	4	4	2
622	4	2	3	3	6	3	5	5	630	3	5	4	3	4	2
636	3	3	4	3	6	5	6	5	644	5	3	5	3	2	3
650	4	2	5	4	6	4	5	4	658	4	4	4	3	4	4
664	4	4	5	4	5	4	5	3	672	5	4	3	3	4	3
678	4	3	4	4	5	3	5	3	686	5	4	4	3	5	3
692	4	3	6	3	5	5	4	4	700	3	3	3	2	5	4
706	5	3	5	3	4	4	2	3	714	3	4	3	2	4	4
720	4	2	4	3	4	3	3	3	728	3	3	3	3	3	2
734	4	4	4	3	4	3	3	3	742	3	2	3	3	2	4
748	3	3	3	2	3	3	3	2	756	3	2	3	3	2	4
762	2	2	4	2	3	2	3	3	770	3	2	3	4	2	4

A14005.011 544 PKS W MIN. 1 CNTS. 08-JUN-93 15:12:45 SUM I: 0.1201E+04
 REF NO. 5 (CONSOL) N AV MW: 716.5
 ACQUIRED 5-28-93 14:02:05 CHAN.#5 0- 81911 6 MS/CHAN. WT AV MW: 738.8
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 483 10 501 DEG. C SF= 0

ABSOLUTE INTENSITIES C13XN, 86.00XC FG, 2

	0	1	2	3	4	5	6	7		0	1	2	3	4	5
MASS			AR		U3		U2	MASS		U1		RH		ROH	
776>	3	3	3	2	3	3	3	2: 784>	3	3	3	3	2	3	
790>	2	3	1	2	3	2	3	3: 798>	2	2	4	2	3	2	
804>	2	2	3	2	2	3	1	3: 812>	2	1	3	2	2	2	
818>	2	2	2	2	2	1	2	2: 826>	2	2	2	1	3	2	
832>	1	2	2	2	2	1	2	1: 840>	3	1	2	2	1	2	
846>	1	2	2	1	2	2	1	2: 854>	1	2	2	1	2	1	
860>	3	1	2	1	1	2	1	1: 868>	2	1	1	2	1	1	
874>	2	1	1	2	1	1	2	1: 882>	2	1	1	1	1	1	
888>	1	1	1	1	1	2	1	1: 896>	1	1	2	0	2	0	
902>	1	2	1	1	1	2	1	1: 910>	2	1	1	1	1	1	
916>	2	0	2	1	1	1	1	1: 924>	1	1	1	1	1	1	
930>	1	0	1	1	1	0	2	1: 938>	1	1	1	0	1	1	
944>	1	0	1	1	1	1	1	1: 952>	1	1	1	1	1	0	
958>	2	0	1	1	0	1	0	1: 966>	1	1	1	1	1	1	
972>	1	0	1	0	1	0	1	1: 980>	0	1	0	0	1	0	
986>	0	1	1	0	1	0	1	0: 994>	1	0	1	0	1	0	
1000>	1	0	0	1	0	1	1	0: 1008>	1	0	0	0	1	1	
1014>	1	1	0	0	0	0	0	1: 1022>	0	1	0	0	0	1	
1028>	0	1	1	0	0	0	0	0: 1036>	0	1	0	0	1	0	
1042>	1	0	1	0	0	0	1	0: 1050>	1	0	1	0	0	0	
1056>	0	1	0	0	0	0	1	0: 1064>	0	0	0	0	0	0	
1070>	0	1	0	0	1	0	0	0: 1078>	0	0	0	0	0	0	
1084>	0	0	0	0	0	1	0	0: 1092>	0	0	0	0	0	0	
1098>	0	0	0	0	0	0	0	0: 1106>	0	0	0	0	0	0	

SUM ODD 66.8 67.1 78.8 77.3 74.6 70.6 72.4
 EV 77.8 89.7 94.6 92.6 96.6 88.6 89.0
 RATIO 0.85863 0.74803 0.83268 0.83470 0.77185 0.79715 0.81316
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.807011

A14005.012 146 PKS W MIN. 1 CNTS. 08-JUN-93 15:13:17 SUM I: 0.1425E+03
 REF NO. 5 (CONSOL) N AV MW: 705.1
 ACQUIRED 5-28-93 14:13:58 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 710.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 501 TO 501 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% FB. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
580>	0	0	0	0	0	1	0	0:	588>	0	0	0	0	0	0
594>	0	1	0	0	1	0	1	0:	602>	1	0	0	0	0	0
608>	0	0	0	0	2	1	1	0:	616>	1	0	0	0	0	0
622>	0	1	1	1	1	1	1	1:	630>	0	0	0	0	0	0
636>	0	2	1	1	1	0	2	0:	644>	0	0	0	0	0	0
650>	0	2	1	0	1	1	1	1:	658>	1	1	0	1	2	0
664>	1	0	2	1	2	0	1	1:	672>	0	1	1	1	1	1
678>	1	1	1	1	1	1	1	1:	686>	0	1	1	1	1	2
692>	1	1	1	0	1	0	1	1:	700>	1	1	1	1	1	2
706>	1	1	1	1	0	1	0	2:	714>	1	0	1	1	0	1
720>	0	2	1	1	1	1	1	0:	728>	1	1	1	1	1	0
734>	2	1	1	1	1	0	0	0:	742>	2	1	1	1	1	1
748>	1	1	1	1	1	0	1	1:	756>	1	1	1	0	0	1
762>	0	0	1	1	1	1	1	0:	770>	1	1	1	1	0	1
776>	1	0	1	0	0	0	0	1:	784>	0	1	0	0	1	1
790>	0	0	0	1	0	0	1	0:	798>	1	0	0	0	0	0
804>	0	0	1	0	1	0	0	1:	812>	0	0	0	1	0	0
818>	0	0	0	0	0	0	0	0:	826>	0	0	0	0	0	0
832>	0	0	0	0	0	0	0	0:	840>	0	0	0	0	0	0
846>	0	0	0	0	0	0	0	0:	854>	0	0	0	0	1	0
860>	0	0	1	0	0	1	0	0:	868>	0	0	0	0	0	0

SUM ODD 12.3 9.6 9.4 8.0 8.2 10.7 9.1
 EV 6.8 14.2 13.3 14.3 11.1 6.3 8.4
 RATIO 1.81407 0.67492 0.70729 0.55997 0.74034 1.69811 1.07593
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.904408

A14005.SUM 1289 PKS W MIN. 1 CNTS. 08-JUN-93 15:14:04 SUM 1: 0.3512E+05
 REF NO. 5 (CONSOL) 0-12 N AV MW: 429.2
 ACQUIRED 5-28-93 14:13:58 CHAN.#S 0- 8191 6 MS/CHAN. WT AV MW: 531.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
48>	0	0	0	0	0	0	0	23:	56>	34	59	0	0	0	0
62>	0	0	0	0	0	0	0	22:	70>	0	24	0	19	10	13
76>	0	0	0	0	0	0	14	15:	84>	17	17	0	0	0	0
90>	0	0	0	0	21	0	16	13:	98>	0	18	0	0	0	0
104>	13	13	12	11	16	0	15	13:	112>	13	0	0	0	0	0
118>	11	0	0	10	16	11	0	0:	126>	15	9	10	11	12	20
132>	36	13	15	14	35	8	10	0:	140>	12	0	62	19	0	39
146>	143	28	36	34	35	8	15	0:	154>	42	10	157	21	64	43
160>	255	47	47	18	34	10	81	37:	168>	533	14	194	51	481	59
174>	331	62	69	23	164	14	298	79:	182>	1031	38	246	71	1027	76
188>	464	69	77	20	244	21	459	83:	196>	807	63	301	63	872	89
202>	968	59	328	23	355	47	742	90:	210>	557	68	381	50	686	71
216>	772	85	449	36	489	90	761	106:	224>	452	53	414	48	523	51
230>	487	64	442	54	505	114	611	87:	238>	327	50	321	75	637	90
244>	411	85	377	39	413	83	388	72:	252>	249	51	251	61	533	77
258>	420	80	322	91	357	112	295	75:	266>	214	45	240	84	352	106
272>	392	78	296	94	498	84	241	83:	280>	198	53	396	72	315	107
286>	275	105	237	99	393	86	259	68:	294>	182	83	359	99	312	90
300>	291	78	220	75	271	94	264	65:	308>	239	70	300	108	269	90
314>	227	87	347	102	268	88	242	87:	322>	257	81	255	111	263	95
328>	186	94	312	99	289	96	235	85:	336>	265	88	249	90	282	96
342>	203	80	271	98	268	88	224	99:	350>	296	109	247	100	247	79
356>	279	81	279	97	248	91	236	86:	364>	271	100	238	94	182	94
370>	249	103	243	97	270	100	223	88:	378>	239	87	253	96	226	73
384>	239	92	240	92	242	95	228	99:	392>	206	100	215	88	221	82
398>	247	83	227	100	199	94	228	84:	406>	238	87	205	96	194	85
412>	207	98	244	94	211	84	200	87:	420>	218	83	191	78	226	82
426>	198	95	225	88	200	88	192	86:	434>	181	98	177	84	204	99
440>	191	94	204	85	180	100	184	91:	448>	210	74	183	89	190	89
454>	198	87	204	78	190	80	171	88:	462>	182	96	199	73	175	89
468>	184	88	181	90	185	82	193	84:	476>	179	86	199	89	189	80
482>	183	84	167	84	179	89	206	97:	490>	183	88	171	93	177	94
496>	179	87	176	84	168	76	187	98:	504>	192	83	179	89	173	84
510>	162	95	200	86	188	87	176	97:	518>	162	83	169	80	169	100
524>	163	86	181	94	185	82	187	88:	532>	141	94	150	84	183	111
538>	168	98	162	93	168	99	168	91:	546>	164	90	156	99	162	97
552>	171	114	179	90	159	95	169	87:	560>	165	91	174	90	163	96
566>	172	97	168	90	162	95	157	84:	574>	154	90	158	102	167	97
580>	173	84	152	102	162	85	153	95:	588>	152	87	174	91	170	94
594>	159	102	152	86	154	90	144	86:	602>	154	91	151	105	151	87
608>	155	87	140	95	130	88	141	82:	616>	143	95	133	105	154	79
622>	151	81	144	74	143	74	138	92:	630>	133	89	141	86	121	100
636>	123	84	121	87	113	89	136	61:	644>	148	70	133	81	116	77
650>	114	78	115	93	114	80	120	84:	658>	122	77	108	76	114	80
664>	110	79	99	77	115	64	112	69:	672>	100	76	105	71	106	85
678>	103	72	96	68	100	66	105	64:	686>	109	61	99	64	97	84
692>	98	60	101	64	90	64	92	63:	700>	87	67	80	71	85	71
706>	84	60	93	58	79	60	75	63:	714>	81	54	81	56	69	58
720>	83	51	76	56	74	50	79	53:	728>	73	50	77	55	69	49
734>	66	56	64	55	75	49	65	45:	742>	63	48	63	51	64	40
748>	62	48	64	42	68	40	55	46:	756>	58	38	60	38	58	43
762>	55	48	48	51	48	38	56	40:	770>	58	40	55	39	55	39

A14005.SUM 1289 PKS W MIN. 1 CNTS. 08-JUN-93 15:14:42 SUM I: 0.3512E+05
 REF NO. 5 (CONSOL) 0-12 N AV MW: 429.2
 ACQUIRED 5-28-93 14:13:58 CHAN.#5 0- 81911 6 MS/CHAN. WT AV MW: 531.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. -62 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00% FG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2				U1		RH		ROH
776>	59	41	52	39	51	40	39	42: 784>	48	35	47	35	51	33	
790>	51	30	41	43	40	36	52	35: 798>	35	38	43	31	43	26	
804>	43	32	43	30	41	34	36	32: 812>	35	38	37	33	35	27	
818>	38	31	35	28	37	26	38	28: 826>	38	23	40	25	29	28	
832>	33	32	32	24	34	28	30	29: 840>	28	25	29	32	27	21	
846>	28	31	26	26	26	25	24	24: 854>	26	25	29	19	33	22	
860>	25	25	21	26	27	21	29	19: 868>	24	21	28	22	24	16	
874>	26	23	27	17	29	14	26	17: 882>	21	19	22	20	21	21	
888>	20	20	15	25	17	19	20	21: 896>	19	18	20	16	14	24	
902>	17	20	14	19	19	14	23	14: 910>	17	15	21	13	20	14	
916>	17	15	19	16	17	17	18	13: 924>	16	14	16	15	14	8	
930>	21	15	14	12	18	13	14	12: 938>	16	9	15	11	15	14	
944>	12	14	11	18	10	13	14	11: 952>	10	18	9	13	14	13	
958>	14	10	14	12	11	16	8	14: 966>	11	13	12	13	10	12	
972>	10	11	11	8	11	11	9	13: 980>	9	9	10	11	7	14	
986>	8	10	8	7	12	9	9	9: 994>	12	6	11	6	15	2	
1000>	9	10	9	10	8	4	12	6: 1008>	9	7	10	9	4	15	
1014>	1	13	6	7	8	6	9	8: 1022>	7	8	5	13	2	12	
1028>	5	11	6	8	7	7	6	9: 1036>	8	5	7	7	9	8	
1042>	6	8	3	9	8	5	6	9: 1050>	4	8	3	8	6	3	
1056>	11	3	6	6	8	2	8	5: 1064>	4	7	5	8	6	4	
1070>	7	2	9	2	7	5	5	6: 1078>	4	6	5	6	3	5	
1084>	7	5	5	7	2	5	6	4: 1092>	4	6	0	9	2	6	
1098>	4	4	7	1	8	1	7	4: 1106>	5	3	4	3	4	4	
1112>	5	2	6	4	5	4	4	4: 1120>	2	7	4	3	3	5	
1126>	3	5	1	7	2	2	7	0: 1134>	8	1	5	4	2	5	
1140>	0	5	3	4	2	5	4	2: 1148>	5	1	6	2	5	1	
1154>	4	2	5	2	4	4	1	3: 1162>	1	6	0	7	3	4	
1168>	2	5	3	3	2	4	4	2: 1176>	2	4	2	4	2	5	
1182>	0	4	1	4	1	5	0	4: 1190>	1	2	3	1	3	2	
1196>	3	2	2	5	0	4	0	3: 1204>	4	0	3	2	1	3	
1210>	0	3	4	0	3	2	2	4: 1218>	0	4	2	3	2	3	
1224>	2	0	3	1	2	3	2	2: 1232>	2	2	2	3	0	2	
1238>	4	2	2	1	4	3	0	6: 1246>	0	3	2	1	2	3	
1252>	1	3	0	3	2	2	1	4: 1260>	0	2	1	2	3	2	
1266>	0	2	3	0	2	2	0	2: 1274>	2	0	3	1	1	2	
1280>	2	1	3	0	2	1	2	0: 1288>	3	1	1	2	2	0	
1294>	3	1	0	0	5	0	0	0: 1302>	0	4	0	2	0	4	
1308>	1	2	0	0	3	1	0	3: 1316>	1	1	1	2	1	1	
1322>	1	0	3	0	2	1	1	2: 1330>	0	2	0	3	0	1	
1336>	0	0	3	0	2	0	2	2: 1344>	1	2	0	2	0	0	
1350>	0	4	0	1	0	3	0	0: 1358>	2	1	0	0	0	0	
1364>	3	0	1	0	2	0	2	1: 1372>	0	0	0	3	1	0	
1378>	0	0	3	0	1	0	3	0: 1386>	1	0	0	3	0	0	
1392>	0	1	0	1	0	1	1	0: 1400>	0	0	0	0	0	0	

SUM ODD 4058.3 3863.7 3843.7 4007.7 3797.6 3998.8 4102.1
 EV 11110.7 9083.4 9771.8 10227.4 10754.5 9322.7 11800.3
 RATIO 0.36526 0.42536 0.39334 0.39186 0.35312 0.42893 0.34762
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.383952

INDIVIDUAL SPECTRA AND PATTERN TABLES FOR PFC SAMPLE 6

A14006.000 30 to 29°C No. Av. MW = 206. Wt. Av. MW = 210.
REF NO. 6(CONSOL)

142

A14006.001 29 to 37°C No. Av. MW = 214. Wt. Av. MW = 218.
REF NO. 6(CONSOL)

143

A14006.002 38 to 46°C No. Av. MW = 222. Wt. Av. MW = 225.
REF NO. 6(CONSOL)

144

A14006.003 47 to 53°C No. Av. MW = 235. Wt. Av. MW = 238.
REF NO. 6(CONSOL)

A14006.004 53 to 64°C No. Av. MW = 250. Wt. Av. MW = 254.
REF NO. 6(CONSOL)

A14006.005 65 to 89°C No. Av. MW = 282. Wt. Av. MW = 288.

REF NO. 6(CONSOL)

A14006.006 94 to 156°C No. Av. MW = 336. Wt. Av. MW = 349.
REF NO. 6(CONSOL)

A14006.007 161 to 239°C No. Av. MW = 405. Wt. Av. MW = 426.
REF NO. 6(CONSOL)

A14006.008 244 to 305°C No. Av. MW = 476. Wt. Av. MW = 501.
REF NO. 6(CONSOL)

A14006.009 310 to 399°C No. Av. MW = 541. Wt. Av. MW = 572.
REF NO. 6(CONSOL)

A14006.010 408 to 468°C No. Av. MW = 576. Wt. Av. MW = 613.
REF NO. 6(CONSOL)

A14006.011 474 to 501°C No. Av. MW = 519. Wt. Av. MW = 575.
REF NO. 6(CONSOL)

A14006.SUM 30 to 501°C No. Av. MW = 401. Wt. Av. MW = 473.
REF NO. 6(CONSOL) ¹³C-Corrected

A14006.000 128 PKS W MIN. 1 CNTS. 14-JUN-93 11:06:36 SUM I: 0.1971E+04
 REF NO. 6(CONSOL) N AV MW: 206.0
 ACQUIRED 6-4-93 13:58:21 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 210.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 29 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
76>	0	0	0	0	0	0	0	0	84>	7	0	5	0	8	0
90>	3	0	0	0	0	0	0	0	98>	0	0	0	0	0	0
104>	0	0	0	0	0	0	0	0	112>	0	0	0	0	0	0
118>	0	0	0	0	0	0	0	0	126>	0	0	0	0	0	0
132>	3	0	0	0	0	0	0	0	140>	0	0	4	0	0	2
146>	14	0	0	0	5	0	0	0	154>	0	0	8	2	5	4
160>	18	3	3	0	5	0	7	0	168>	41	2	13	3	41	6
174>	25	5	15	1	20	1	29	0	182>	106	0	25	6	99	6
188>	35	3	27	2	23	2	42	5	196>	82	5	33	4	93	3
202>	57	10	31	3	26	6	55	3	210>	56	4	48	3	72	3
216>	37	5	29	2	28	2	47	2	224>	35	6	41	3	52	4
230>	31	0	22	2	28	1	28	2	238>	18	3	27	1	26	2
244>	17	2	16	1	15	2	15	2	252>	11	2	16	2	12	2
258>	10	0	9	1	8	0	7	0	266>	6	1	9	2	5	0
272>	3	0	5	0	5	0	2	0	280>	3	0	3	0	2	0
286>	2	0	2	0	2	0	0	0	294>	0	0	0	0	0	0

SUM ODD 29.0 12.7 13.8 14.7 22.7 24.6 32.9
 EV 253.2 159.3 164.1 231.6 365.1 232.7 414.5
 RATIO 0.11436 0.07993 0.08386 0.06338 0.06212 0.10560 0.07949
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.082577

A14006.001 97 PKS W MIN. 1 CNTS. 14-JUN-93 11:07:01 SUM I: 0.8182E+03
 REF NO. 6(CONSOL) N AV MW: 214.8
 ACQUIRED 6-4-93 14:10:15 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 218.0
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 29 TO 37 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
146>	0	0	0	0	0	0	0	0	154>	0	0	3	0	0	0
160>	4	1	0	0	0	0	0	0	168>	14	2	3	0	9	3
174>	5	0	2	0	5	0	8	3	182>	39	1	5	4	21	3
188>	8	0	2	0	10	1	21	3	196>	41	2	11	2	24	6
202>	33	0	14	0	11	2	42	2	210>	29	2	18	1	26	3
216>	16	3	10	0	12	2	35	1	224>	27	0	22	3	23	1
230>	12	1	8	1	10	1	16	2	238>	13	0	16	1	19	1
244>	9	1	7	0	7	0	10	0	252>	6	0	9	0	9	1
258>	5	0	5	0	5	0	4	0	266>	3	0	5	0	3	0
272>	2	0	4	0	3	0	3	0	280>	3	0	3	1	0	0
286>	0	0	2	0	2	0	1	0	294>	0	0	0	0	0	0

SUM ODD 5.8 0.6 6.1 11.2 6.2 12.3 17.1
 EV 94.1 54.6 66.2 139.2 174.2 96.3 134.4
 RATIO 0.06120 0.01078 0.09139 0.08048 0.03554 0.12808 0.12684
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.077962

A14006.002 115 PKS W MIN. 1 CNTS. 14-JUN-93 11:07:21 SUM I: 0.1248E+04
 REF NO. 6(CONSOL) N AV MW: 222.5
 ACQUIRED 6- 4-93 14:22:09 CHAN.*S 0- 8191; 6 MS/CHAN. WT AV MW: 225.7
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 38 TO 46 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
160>	0	0	0	0	0	0	0	2: 168>	10	2	3	0	6	2	
174>	2	0	0	0	6	0	11	4: 182>	33	4	4	7	17	5	
188>	5	3	3	0	15	2	24	6: 196>	38	3	6	4	24	5	
202>	59	3	32	1	21	3	67	7: 210>	39	6	20	5	22	6	
216>	39	3	25	1	26	3	65	3: 224>	31	5	31	3	29	2	
230>	17	2	15	2	27	1	45	2: 238>	24	2	24	0	26	0	
244>	15	2	12	0	12	2	19	0: 252>	17	1	19	1	15	3	
258>	7	2	9	0	12	0	10	0: 266>	7	1	10	1	9	1	
272>	6	0	7	0	7	0	6	0: 280>	4	0	6	0	4	2	
286>	3	0	4	0	3	0	2	0: 294>	4	0	2	0	0	0	
300>	2	0	2	0	2	0	0	0: 308>	0	0	0	0	0	0	

SUM ODD 14.5 4.3 10.7 23.9 23.0 21.8 25.7
 EV 154.3 102.8 131.1 247.4 207.5 123.2 152.2
 RATIO 0.09395 0.03920 0.08168 0.09679 0.11091 0.17699 0.16862
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.110188

A14006.003 137 PKS W MIN. 1 CNTS. 14-JUN-93 11:07:45 SUM I: 0.1961E+04
 REF NO. 6(CONSOL) N AV MW: 235.0
 ACQUIRED 6- 4-93 14:34:02 CHAN.*S 0- 8191; 6 MS/CHAN. WT AV MW: 238.7
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 47 TO 53 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
160>	0	0	0	0	0	0	0	3: 168>	4	0	0	0	0	0	
174>	0	0	0	0	5	0	5	7: 182>	13	3	2	3	6	4	
188>	2	0	4	0	13	1	15	11: 196>	25	0	5	4	11	7	
202>	110	3	42	3	30	3	59	10: 210>	29	5	12	8	13	6	
216>	85	0	54	6	59	7	97	12: 224>	44	5	25	6	25	4	
230>	35	3	45	4	61	6	91	0: 238>	47	7	34	5	33	7	
244>	24	4	24	4	42	3	64	7: 252>	28	5	28	4	27	2	
258>	19	3	16	3	24	4	31	3: 266>	24	2	25	1	14	3	
272>	12	0	11	1	18	2	14	3: 280>	17	1	16	1	14	0	
286>	8	2	9	0	10	1	10	1: 294>	8	2	10	1	7	0	
300>	5	0	5	0	4	0	6	0: 308>	4	0	7	0	3	1	
314>	3	0	4	0	3	0	0	0: 322>	2	0	2	1	0	0	
328>	2	0	0	0	1	0	0	0: 336>	1	0	0	0	0	0	
342>	0	0	0	0	0	0	0	0: 350>	0	0	1	0	0	0	

SUM ODD 15.0 20.0 27.1 56.5 29.2 34.5 35.9
 EV 305.2 111.2 270.4 391.6 243.6 167.4 153.3
 RATIO 0.04898 0.09482 0.10006 0.14417 0.11987 0.20623 0.23392
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.125132

A14006.004 164 PKS W MIN. 1 CNTS. 14-JUN-93 11:08:10 SUM I: 0.2350E+04
 REF NO. 6(CONSOL) N AV MW: 250.1
 ACQUIRED 6- 4-93 14:45:56 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 254.8
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 53 TO 64 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
160>	0	0	0	0	0	0	0	2	168>	2	0	0	2	0	3
174>	0	1	0	0	0	0	0	11	182>	5	1	0	3	3	3
188>	3	0	0	0	6	2	4	10	196>	9	3	2	3	3	6
202>	71	7	22	3	11	8	25	14	210>	13	5	6	3	4	4
216>	108	10	56	8	37	19	51	15	224>	17	8	8	4	11	6
230>	61	7	68	0	64	26	74	15	238>	22	8	12	9	51	14
244>	57	6	60	5	70	17	60	13	252>	23	4	20	5	29	10
258>	42	8	43	10	63	6	57	9	266>	24	4	18	7	24	3
272>	24	3	31	3	39	7	41	4	280>	24	3	20	5	18	3
286>	16	2	17	4	21	5	22	1	294>	16	3	18	2	11	3
300>	9	0	12	3	15	2	13	4	308>	11	8	6	0	10	0
314>	6	2	6	0	10	2	7	2	322>	7	0	9	2	5	0
328>	5	2	6	0	5	2	4	1	336>	3	2	5	0	4	0
342>	0	4	1	1	0	3	2	0	350>	3	2	0	3	0	0
356>	0	0	0	2	1	0	0	1	364>	0	1	0	0	0	0

SUM ODD 52.5 37.8 99.6 102.9 52.8 47.6 55.8
 EV 403.9 321.7 341.7 359.6 179.1 122.4 173.1
 RATIO 0.12989 0.11735 0.29158 0.28609 0.29469 0.38902 0.32256
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.236108

A14006.005 216 PKS W MIN. 1 CNTS. 14-JUN-93 11:08:36 SUM I: 0.3355E+04
 REF NO. 6(CONSOL) N AV MW: 282.4
 ACQUIRED 6- 4-93 14:57:50 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 288.5
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 65 TO 89 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
174>	0	0	0	0	0	0	0	4	182>	4	0	0	0	3	0
188>	0	0	0	0	0	0	2	4	196>	4	1	2	1	0	0
202>	23	3	5	0	3	4	6	7	210>	5	3	3	0	3	3
216>	35	7	17	4	7	17	9	11	224>	3	3	3	3	8	4
230>	40	10	36	6	22	22	14	14	238>	6	4	3	5	128	16
244>	63	17	51	12	37	21	23	11	252>	15	4	10	10	105	20
258>	109	20	67	17	51	20	26	14	266>	19	0	25	8	79	13
272>	97	17	74	0	86	18	44	11	280>	19	6	53	10	71	7
286>	77	9	64	16	59	14	32	9	294>	19	8	41	8	44	11
300>	42	13	50	9	45	10	26	9	308>	24	2	31	5	39	6
314>	32	6	32	11	35	6	24	4	322>	19	6	16	7	26	5
328>	23	6	25	5	24	5	19	2	336>	15	5	13	0	15	0
342>	14	4	16	5	12	0	14	2	350>	11	1	12	1	11	6
356>	10	4	9	2	10	2	9	0	364>	10	2	7	2	6	3
370>	8	2	6	2	6	0	6	1	378>	7	2	6	2	3	3
384>	4	3	3	2	4	2	3	0	392>	2	3	2	4	2	3
398>	1	3	1	4	1	2	0	3	406>	1	2	1	2	0	3
412>	1	0	0	2	2	1	0	0	420>	1	0	0	2	0	0
426>	1	0	0	0	1	0	0	0	434>	0	0	0	0	0	0

SUM ODD 124.4 97.3 143.8 106.6 53.3 71.6 103.0
 EV 579.8 457.4 405.2 258.3 184.1 227.8 542.1
 RATIO 0.21451 0.21270 0.35485 0.41291 0.28945 0.31443 0.18998
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.263686

A14006.006 370 PKS W MIN. 1 CNTS. 14-JUN-93 11:09:08 SUM I: 0.5453E+04
 REF NO. 6(CONSOL) N AV MW: 336.2
 ACQUIRED 6- 4-93 15:09:44 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 349.0
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 94 TO 156 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR				U3			U1		RH		RDH	
174>	0	0	0	0	0	0	0	4:	182>	4	0	0	2	3	3
188>	0	0	0	0	0	0	4	3:	196>	5	2	0	0	3	3
202>	12	2	4	2	0	0	6	3:	210>	3	1	2	3	2	3
216>	14	7	7	3	4	5	7	4:	224>	5	2	3	2	4	2
230>	10	9	8	4	7	9	8	6:	238>	5	2	3	5	42	10
244>	18	11	8	7	6	9	7	4:	252>	12	0	10	6	52	24
258>	23	17	12	13	10	9	8	9:	266>	18	8	28	13	54	26
272>	40	15	19	14	92	17	25	10:	280>	27	12	82	22	61	29
286>	46	14	26	23	60	23	45	9:	294>	40	12	86	23	77	30
300>	52	22	29	20	46	17	51	18:	308>	55	16	87	24	80	20
314>	41	22	56	0	54	14	51	17:	322>	57	18	78	25	68	23
328>	48	22	56	19	53	23	45	17:	336>	59	21	65	35	46	20
342>	41	17	41	18	45	0	49	16:	350>	52	20	45	23	41	15
356>	39	0	41	0	44	13	39	13:	364>	39	18	37	16	32	14
370>	32	12	31	14	32	13	35	10:	378>	31	12	32	12	25	10
384>	24	17	24	0	20	20	20	18:	392>	12	23	21	18	14	20
398>	9	21	9	17	13	20	8	17:	406>	10	17	11	15	7	13
412>	9	13	7	15	11	12	9	12:	420>	7	14	0	15	9	9
426>	10	7	11	9	9	6	12	6:	434>	9	9	6	9	9	7
440>	7	5	10	7	5	8	8	4:	448>	9	7	5	5	8	5
454>	7	6	6	6	5	5	5	4:	462>	5	6	5	4	4	4
468>	5	4	4	4	4	4	4	3:	476>	3	4	3	3	4	3
482>	4	2	5	3	4	2	2	3:	490>	2	4	2	3	2	3
496>	3	4	2	4	2	3	3	1:	504>	3	2	2	2	2	2
510>	2	2	2	2	3	0	3	1:	518>	2	2	2	1	2	1
524>	1	2	2	2	2	1	1	1:	532>	2	3	5	1	2	1
538>	2	1	2	1	1	0	2	1:	546>	1	0	2	1	1	0
552>	2	1	2	0	2	0	1	0:	560>	1	1	0	1	0	0
566>	2	1	1	0	0	0	2	0:	574>	0	0	0	0	0	0
580>	0	0	0	0	0	0	0	0:	588>	0	0	0	0	0	0
594>	0	0	0	0	0	0	0	0:	602>	0	0	0	0	0	0
608>	0	0	0	0	0	0	0	0:	616>	0	0	0	0	0	0
622>	0	0	0	0	0	0	0	0:	630>	0	0	0	0	0	0
636>	0	0	0	0	0	0	0	0:	644>	0	0	0	0	0	0
650>	0	0	0	0	0	0	0	0:	658>	0	0	0	0	0	0
664>	0	0	0	0	0	0	0	0:	672>	0	0	0	0	0	0
678>	0	0	0	0	0	0	0	0:	686>	0	0	0	0	0	0
692>	0	0	0	0	0	0	0	0:	700>	0	0	0	0	0	0
706>	0	0	0	0	0	0	0	0:	714>	0	0	0	0	0	0
720>	0	0	0	0	0	0	0	0:	728>	0	0	0	0	0	0
734>	0	0	0	0	0	0	0	0:	742>	0	0	0	0	0	0
748>	0	0	0	0	0	0	0	0:	756>	0	0	0	0	0	0
762>	0	0	0	0	0	0	0	0:	770>	0	0	0	0	0	3
776>	2	1	0	0	0	0	0	0:	784>	0	0	0	0	0	0

SUM ODD 257.2 206.2 232.5 211.5 235.1 287.4 300.5
 EV 502.8 427.1 533.1 462.6 479.3 622.1 653.4
 RATIO 0.51152 0.48276 0.43620 0.45730 0.49052 0.46194 0.45984
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.470166

A14006.007 539 PKS W MIN. 1 CNTS. 14-JUN-93 11:09:54 SUM I: 0.6090E+04
 REF NO. 6(CONSOL) N AV MW: 405.5
 ACQUIRED 6- 4-93 15:21:37 CHAN.#8 0- 8191; 6 MS/CHAN. WT AV MW: 426.2
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 161 TU 239 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		RDH	
160>	0	0	0	0	0	0	0	0	0: 168>	0	0	0	0	0	2
174>	0	0	0	0	0	0	0	0	0: 182>	3	0	0	2	2	0
188>	0	0	0	0	3	0	0	3	3: 196>	3	2	2	3	0	3
202>	7	2	2	0	2	2	4	2	2: 210>	2	2	3	3	0	2
216>	5	3	5	2	3	2	4	4	4: 224>	4	2	4	2	3	2
230>	5	3	3	4	4	3	4	3	3: 238>	3	2	3	0	8	4
244>	5	4	4	3	4	0	6	3	3: 252>	4	3	5	4	10	7
258>	6	3	5	3	3	2	3	4	4: 266>	6	3	8	5	8	6
272>	6	3	6	7	36	10	9	5	5: 280>	8	7	11	12	10	10
286>	6	5	4	5	38	0	18	8	8: 294>	12	10	18	10	11	10
300>	18	9	11	4	26	16	20	11	11: 308>	20	13	19	15	12	9
314>	11	0	55	16	33	17	25	16	16: 322>	22	14	20	14	28	11
328>	13	13	46	20	0	42	24	22	22: 336>	26	15	23	21	31	19
342>	30	16	47	22	39	25	36	21	350>	47	17	35	23	28	20
356>	37	29	41	32	36	24	31	26	364>	38	24	31	25	25	0
370>	47	27	44	28	44	26	29	20	378>	38	19	31	28	28	36
384>	27	37	39	25	34	25	32	18	392>	34	30	29	22	36	24
398>	30	33	33	29	30	20	31	28	406>	30	27	23	29	19	35
412>	28	0	43	23	29	24	25	17	420>	31	21	28	27	24	20
426>	36	20	31	23	23	16	23	27	434>	23	18	25	26	23	21
440>	26	21	25	14	20	20	23	21	448>	19	23	17	18	21	18
454>	19	16	20	18	15	19	22	13	462>	20	17	15	11	18	17
468>	15	15	14	15	16	15	14	16	476>	15	15	13	14	11	18
482>	12	11	14	10	12	12	13	11	490>	15	11	13	10	11	10
496>	13	11	11	9	10	9	9	11	504>	10	10	7	11	9	8
510>	10	7	8	9	8	7	10	7	518>	9	10	7	7	9	6
524>	8	8	8	7	7	7	8	11	532>	9	6	6	8	5	7
538>	8	6	4	7	6	5	6	5	546>	5	6	7	6	6	6
552>	7	5	6	6	5	3	6	4	560>	5	6	5	4	6	4
566>	5	2	6	3	5	5	4	4	574>	4	4	4	4	4	3
580>	3	4	3	5	2	5	3	3	588>	4	3	3	3	3	3
594>	5	3	3	3	3	3	3	0	602>	4	3	3	4	3	2
608>	2	4	2	3	2	2	3	3	616>	2	3	2	2	3	1
622>	2	3	2	3	2	1	3	2	630>	3	2	2	2	2	3
636>	2	2	1	2	2	1	2	2	644>	1	1	1	3	1	2
650>	2	1	2	0	3	1	2	2	658>	1	1	2	2	1	1
664>	1	2	1	1	1	1	2	1	672>	1	1	1	1	1	2
678>	1	1	1	1	1	1	1	1	686>	0	0	1	1	1	1
692>	1	1	1	1	0	2	0	0	700>	2	1	0	1	1	1
706>	1	0	1	0	1	1	1	0	714>	1	0	0	1	1	0
720>	1	0	1	1	0	0	0	0	728>	1	0	0	0	0	0
734>	0	0	0	0	0	0	0	0	742>	0	0	0	1	0	0
748>	0	0	0	0	0	1	0	0	756>	0	0	0	0	0	0
762>	0	0	0	1	0	0	0	0	770>	0	0	0	7	8	2
776>	0	0	0	0	0	0	0	0	784>	0	0	0	0	0	0

SUM ODD 329.4 364.5 373.7 354.5 349.3 391.4 359.3
 EV 463.1 554.5 509.7 456.7 486.4 428.5 432.0
 RATIO 0.71122 0.65743 0.73318 0.77623 0.71809 0.91337 0.83161
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.757161

A14000.008 623 PMS W MIN. 1 CNTS. 14-JUN-93 11:10:46 SUM I: 0.4741E+04
 REF NO. 6(CONSOL) N AV MW: 476.9
 ACQUIRED 6- 4-93 15:33:31 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 501.1
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 244 TO 305 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% FG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		ROH	
174>	0	0	2	0	0	0	0	0	0: 182>	0	0	0	0	0	0
188>	0	0	0	0	0	0	0	0	0: 196>	0	2	0	0	0	0
202>	3	2	0	0	0	0	0	0	0: 210>	0	0	0	0	0	0
216>	0	0	0	0	0	0	2	2	3: 224>	0	0	0	0	0	0
230>	3	0	3	0	0	3	2	2	2: 238>	2	2	0	3	3	2
244>	2	1	0	3	2	2	3	2	2: 252>	2	0	3	2	3	2
258>	3	1	1	3	0	3	2	1	1: 266>	0	0	3	2	2	3
272>	0	2	2	2	4	3	2	3	3: 280>	2	2	3	3	2	3
286>	2	2	0	3	3	4	3	2	2: 294>	4	3	3	3	2	3
300>	4	3	2	2	4	4	5	2	2: 308>	3	3	3	2	3	2
314>	4	5	8	5	4	3	4	3	3: 322>	4	0	4	3	9	2
328>	5	4	10	6	4	4	6	4	4: 336>	2	3	3	5	14	5
342>	7	7	8	9	7	6	4	4	4: 350>	25	8	7	6	12	10
356>	11	9	10	9	8	6	5	5	5: 364>	28	9	15	10	12	11
370>	15	9	14	10	22	11	11	15	5: 378>	20	11	24	11	18	14
384>	16	11	12	9	13	11	23	13	3: 392>	19	19	22	19	16	18
398>	21	15	19	7	17	13	25	19	4: 406>	15	28	16	20	20	17
412>	17	18	28	12	20	14	19	23	4: 420>	23	24	24	15	23	17
426>	16	18	20	22	15	23	24	20	4: 434>	23	26	18	21	21	23
440>	18	17	18	18	23	18	26	23	4: 448>	22	24	20	22	23	20
454>	16	21	20	19	19	22	20	23	4: 462>	21	24	21	20	20	19
468>	19	18	18	19	20	19	19	22	4: 476>	22	19	16	20	20	17
482>	15	20	18	17	17	18	19	20	4: 490>	18	16	17	19	15	17
496>	17	15	18	16	17	15	19	17	4: 504>	16	19	14	16	14	17
510>	16	16	12	16	16	14	14	16	4: 518>	13	16	12	14	14	13
524>	13	16	13	14	14	12	14	12	4: 532>	14	14	10	11	12	12
538>	13	8	13	9	12	12	12	9	4: 546>	11	10	11	9	10	13
552>	8	11	10	10	11	10	10	10	4: 560>	9	9	10	9	8	10
566>	10	9	8	9	9	9	7	9	4: 574>	7	9	9	6	9	8
580>	7	7	9	6	8	6	8	6	4: 588>	8	6	6	7	6	8
594>	6	6	7	7	7	6	5	8	4: 602>	5	5	7	6	6	7
608>	6	7	5	7	5	6	6	6	4: 616>	5	6	4	6	4	5
622>	5	3	5	5	5	5	4	4	4: 630>	4	5	4	5	4	5
636>	5	4	3	5	4	4	4	4	4: 644>	3	4	3	4	4	5
650>	3	4	3	4	3	4	3	3	4: 658>	4	3	0	6	2	3
664>	3	2	3	3	3	4	3	2	4: 672>	3	3	3	2	2	3
678>	2	3	3	3	3	3	2	2	4: 686>	3	2	2	3	2	3
692>	2	2	2	2	2	2	3	3	4: 700>	2	2	3	2	2	2
706>	2	2	2	1	2	2	3	2	4: 714>	2	2	1	2	1	2
720>	1	2	1	2	3	1	1	1	4: 728>	2	1	2	1	2	1
734>	1	2	1	2	1	1	2	1	4: 742>	1	1	2	1	2	1
748>	2	2	1	1	1	1	2	1	4: 756>	2	1	1	1	1	1
762>	1	1	1	2	1	1	1	1	4: 770>	1	1	1	1	2	1
776>	1	1	0	2	1	1	1	1	4: 784>	1	1	1	1	1	1
790>	0	1	0	1	0	1	1	1	4: 798>	1	0	1	0	2	0
804>	0	1	0	1	1	1	0	0	4: 812>	1	1	0	1	0	1
818>	1	0	0	2	0	1	0	0	4: 826>	0	0	1	0	0	0
832>	2	0	1	1	0	0	0	0	4: 840>	0	1	1	0	0	0
846>	0	0	0	0	1	0	1	0	4: 854>	1	0	1	0	0	0
860>	0	1	0	1	0	0	0	1	4: 868>	0	0	0	0	1	0
874>	0	0	0	1	0	0	0	0	4: 882>	0	0	0	1	0	0
888>	0	0	0	0	0	0	0	0	4: 896>	0	0	1	0	0	0

A14006.008 623 FKS W MIN. 1 CNTS. 14-JUN-93 11:11:26 SUM I: 0.4741E+04
 REF NO. 6(CONSOL) N AV MW: 476.9
 ACQUIRED 6- 4-93 15:33:31 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 501.1
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 244 TO 305 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
902>	1	0	0	0	1	0	0	0	0: 910>	0	0	0	0	0	0
916>	0	0	0	0	0	1	0	0	0: 924>	0	0	0	0	0	0
930>	0	1	0	0	0	0	0	0	0: 938>	0	0	0	0	0	0

SUM ODD	312.7	309.1	312.8	328.9	343.7	316.6	326.7
EV	326.8	335.7	333.9	348.8	372.2	334.4	351.1
RATIO	0.95686	0.92089	0.93662	0.94301	0.92350	0.94684	0.93034

OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.936575

A14006.009 795 PKS W MIN. 1 CNTS. 14-JUN-93 11:11:52 SUM I: 0.5848E+04
 REF NO. 6(CONSOL) N AV MW: 541.6
 ACQUIRED 6- 4-93 15:45:25 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 572.6
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 310 TO 399 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS	0	1	2	3	4	5
			AR		U3		U2			U1		RH		RUH	
48>	0	0	0	0	0	0	0	0	56>	0	5	0	0	0	0
62>	0	0	0	0	0	0	0	3	70>	0	0	0	0	0	0
76>	0	0	0	0	0	0	0	0	84>	0	0	0	0	0	0
90>	0	0	0	0	0	0	0	0	98>	0	0	0	0	0	0
104>	0	0	0	0	0	0	0	0	112>	0	0	0	0	0	0
118>	0	0	0	0	0	0	0	0	126>	0	0	0	0	0	0
132>	0	0	0	0	0	0	0	0	140>	0	0	0	0	0	0
146>	0	0	0	0	0	0	0	0	154>	0	0	0	0	0	0
160>	0	0	0	0	0	0	0	0	168>	0	0	0	0	0	0
174>	0	0	0	0	0	0	0	0	182>	0	0	0	0	0	0
188>	0	0	0	0	2	0	0	0	196>	0	0	0	0	0	0
202>	0	0	0	0	0	0	0	0	210>	0	0	0	0	0	0
216>	0	2	2	0	0	0	0	0	224>	3	0	0	0	0	0
230>	0	2	2	0	3	2	0	0	238>	0	2	2	2	0	0
244>	0	0	0	4	2	2	0	0	252>	0	3	2	3	3	2
258>	2	0	0	3	2	2	2	0	266>	2	2	3	2	3	3
272>	2	0	2	0	4	2	2	0	280>	0	3	3	2	0	3
286>	2	2	2	1	2	2	2	2	294>	3	2	2	0	0	3
300>	1	3	1	2	2	0	3	4	308>	2	2	0	3	3	3
314>	2	4	3	2	2	2	2	3	322>	2	2	2	2	3	0
328>	4	3	4	4	3	2	3	4	336>	2	1	3	3	4	3
342>	3	4	3	4	3	2	3	6	350>	4	3	3	4	2	4
356>	5	2	3	2	4	2	3	3	364>	8	5	5	4	5	4
370>	4	3	4	3	11	6	6	3	378>	7	7	9	7	5	5
384>	5	3	5	3	11	7	12	12	392>	7	6	9	8	6	7
398>	8	8	0	15	10	11	16	13	406>	11	11	7	9	6	7
412>	8	9	19	23	13	11	14	12	420>	13	8	11	7	27	14
426>	13	9	20	17	17	18	14	16	434>	11	12	13	11	25	24
440>	17	16	22	16	19	18	17	15	448>	23	20	15	16	20	23
454>	24	22	22	21	20	19	16	17	462>	20	17	25	22	21	22
468>	26	24	23	23	19	23	23	20	476>	23	19	25	25	28	24
482>	23	26	21	25	18	22	22	25	490>	21	20	23	23	26	25
496>	25	23	24	23	22	19	20	21	504>	22	23	23	23	24	21
510>	23	22	22	25	22	20	22	18	518>	21	21	21	21	25	22
524>	22	20	20	21	24	19	20	22	532>	20	20	19	22	20	19
538>	20	23	18	20	18	20	19	20	546>	20	17	22	20	20	18
552>	19	19	19	18	17	18	17	19	560>	20	18	16	19	16	17
566>	16	18	18	17	16	17	15	17	574>	16	17	18	16	16	17
580>	17	15	17	14	15	16	16	14	588>	16	14	15	16	13	14
594>	13	15	14	12	14	13	14	13	602>	13	13	13	15	11	13
608>	13	11	14	9	13	13	13	12	616>	12	11	11	11	12	10
622>	11	11	10	10	11	11	9	12	630>	11	10	11	10	10	9
636>	10	12	8	10	8	10	8	12	644>	7	11	8	9	8	8
650>	9	7	9	7	11	7	8	8	658>	9	8	9	7	9	8
664>	11	6	7	8	7	7	7	7	672>	7	7	7	7	7	6
678>	7	6	6	8	6	7	7	5	686>	7	6	6	6	6	5
692>	6	6	7	4	6	5	5	5	700>	7	4	6	6	5	5
706>	5	5	6	4	4	5	3	4	714>	5	6	5	4	5	4
720>	5	4	5	5	4	4	5	4	728>	4	5	3	5	4	3
734>	5	3	4	5	3	4	5	4	742>	4	4	4	4	4	2
748>	5	3	4	3	4	4	3	3	756>	3	5	4	2	3	3
762>	3	3	3	4	2	3	3	3	770>	3	3	3	3	3	3

A14006.009 795 PPS W MIN. 1 CNIS. 14-JUN-93 11:12:32 SUM 1: 0.5848E+04
 REF NO. 6(CONSUL) N AV MW: 541.6
 ACQUIRED 6- 4-93 15:45:25 CHAN.#8 0- 8191 6 MS/CHAN. WT AV MW: 572.6
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 310 TO 399 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AK		U3		U2			U1		RH		RUH	
776>	2	3	3	2	3	3	2	4: 784>	1	3	2	3	2	2	2
790>	2	2	3	2	0	4	1	2: 798>	2	2	2	3	2	2	2
804>	2	2	2	2	2	3	2	1: 812>	2	2	2	2	2	2	2
818>	2	1	3	1	2	2	2	1: 826>	2	1	2	2	1	1	1
832>	2	3	1	2	1	2	2	1: 840>	2	1	2	1	2	2	2
846>	2	1	2	2	1	1	2	1: 854>	2	1	1	1	1	1	2
860>	1	2	1	1	2	1	1	1: 868>	1	2	1	1	1	1	1
874>	1	1	2	1	2	1	1	1: 882>	1	1	1	1	1	1	1
898>	1	1	1	2	1	1	2	1: 896>	1	1	1	1	1	1	1
902>	1	0	1	0	1	0	2	0: 910>	1	1	1	1	1	1	1
916>	1	0	1	1	1	1	1	1: 924>	1	1	1	1	2	0	0
930>	1	1	1	1	0	1	0	1: 938>	1	1	1	1	1	0	0
944>	0	1	0	1	0	1	0	1: 952>	1	1	1	1	1	1	1
958>	0	0	2	0	1	0	1	0: 966>	1	0	1	1	1	0	0
972>	1	0	0	1	1	0	0	0: 980>	1	0	1	1	1	0	0
986>	1	0	1	1	0	0	1	0: 994>	0	1	0	1	0	0	0
1000>	0	0	1	1	0	1	0	1:1008>	0	1	0	0	0	0	0
1014>	0	0	0	1	0	0	0	1:1022>	0	1	0	1	0	0	1
1028>	1	0	0	0	0	1	0	0:1036>	1	0	1	0	0	0	1
1042>	0	1	0	0	0	0	0	0:1050>	0	0	0	0	1	0	0
1056>	0	0	0	0	0	0	0	0:1064>	0	0	0	0	0	0	0
1070>	0	0	0	0	0	0	0	0:1078>	0	0	1	0	0	0	0
1084>	0	0	1	0	0	0	0	0:1092>	0	0	0	0	0	0	0
1098>	0	0	0	0	0	0	0	0:1106>	0	0	0	0	0	0	0
1112>	0	0	0	0	0	0	0	0:1120>	0	0	0	0	0	0	0
1126>	0	0	0	0	0	0	0	0:1134>	0	0	0	0	0	0	0
1140>	0	0	0	0	0	0	0	0:1148>	0	0	0	0	0	0	0

SUM ODD 395.1 418.1 401.8 396.3 395.6 398.5 403.1
 EV 418.6 415.4 409.5 396.9 409.7 403.9 429.5
 RATIO 0.94404 1.00644 0.98113 0.99868 0.96561 0.98668 0.93853
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.974035

414006.010 860 PPS W MIN. 1 UNIT. 14-JUN-93 11:13:15 SUM 1: 0.53588+04
 REF NO. 6(CONSUL) N AV MW: 576.3
 ACQUIRED 6-4-93 15:57:19 CHAN.#5 0-81911 6 MS/CHAN. WT AV MW: 613.6
 MAG. REL. TIME: 9999 MS, 12 SCANS/SPECTRM. 408 TO 462 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% P.G. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2				U1		RH		ROH
43>	0	0	0	0	0	0	0	0	0: 56>	7	5	0	0	0	0
62>	0	0	0	0	0	0	4	0	0: 70>	6	0	0	0	0	0
74>	0	0	0	0	0	0	0	0	0: 84>	0	0	0	0	0	0
90>	0	0	0	0	0	0	0	0	0: 98>	0	0	0	0	0	0
104>	0	0	0	0	5	0	0	0	0: 112>	0	0	0	0	0	0
118>	0	0	0	0	2	0	3	0	0: 126>	0	0	0	0	0	0
132>	0	0	0	0	3	0	0	0	0: 140>	0	0	0	0	0	0
146>	0	0	0	0	0	0	0	0	0: 154>	0	2	0	0	3	0
160>	0	0	0	0	0	0	0	0	0: 168>	0	0	0	0	0	0
174>	2	0	0	0	0	0	0	0	0: 182>	0	0	0	0	2	0
188>	0	0	0	0	0	0	3	0	0: 196>	2	1	2	0	0	0
202>	3	0	2	0	0	0	0	0	0: 210>	3	0	0	0	3	0
216>	3	0	3	0	0	0	3	1	1: 224>	0	3	2	0	3	0
230>	0	0	0	0	3	0	4	2	2: 238>	3	2	0	3	1	2
244>	3	3	3	2	0	4	0	3	3: 252>	3	0	4	2	3	2
258>	3	0	2	2	4	2	3	0	0: 266>	4	1	2	4	2	3
272>	3	2	4	2	3	2	2	2	2: 280>	2	3	3	3	3	2
286>	3	0	3	2	3	2	3	0	0: 294>	4	3	2	2	3	2
300>	3	2	2	3	3	4	3	2	2: 308>	3	2	2	2	2	3
314>	3	2	3	2	3	3	3	3	3: 322>	3	2	2	2	3	2
328>	2	3	4	3	2	3	2	2	2: 336>	3	2	3	2	4	2
342>	3	3	3	3	3	3	1	2	3: 350>	4	3	2	4	2	3
356>	4	3	3	3	3	2	2	3	3: 364>	3	3	3	2	3	3
370>	3	2	3	2	2	2	2	3	3: 378>	3	4	3	3	4	2
384>	3	2	3	2	3	3	4	3	3: 392>	3	3	3	3	3	3
398>	4	3	4	3	3	4	5	2	2: 406>	5	3	4	2	3	3
412>	3	3	5	5	4	5	3	4	4: 420>	4	2	4	2	10	0
426>	7	4	8	6	6	4	4	4	4: 434>	2	4	5	3	11	8
440>	8	7	7	5	5	5	5	4	4: 448>	14	7	0	12	8	11
454>	9	9	7	6	6	5	4	7	7: 462>	0	18	13	14	11	10
468>	12	5	10	5	13	9	14	14	14: 476>	10	15	15	13	12	11
482>	9	9	8	6	14	11	23	16	16: 490>	17	16	13	16	13	11
496>	12	10	18	15	15	13	22	19	19: 504>	21	19	13	17	12	10
510>	12	11	23	18	18	19	19	22	22: 518>	18	16	14	15	16	15
524>	16	14	19	19	23	17	22	18	18: 532>	19	17	18	12	21	15
538>	20	17	23	18	21	21	21	21	21: 546>	18	16	18	16	16	17
552>	21	18	22	20	21	18	22	17	17: 560>	15	17	17	17	19	16
566>	20	20	21	22	18	19	20	14	14: 574>	17	12	19	18	20	17
580>	22	18	20	19	17	18	17	16	16: 588>	17	14	16	17	20	17
594>	18	20	18	18	16	14	16	14	14: 602>	16	15	17	15	17	14
608>	18	17	17	14	15	12	17	11	11: 616>	16	14	17	13	19	15
622>	17	13	16	14	12	12	13	14	14: 630>	12	14	14	13	16	15
636>	11	15	11	11	13	14	12	13	13: 644>	13	15	13	10	12	12
650>	13	10	12	10	11	12	11	11	11: 658>	11	10	11	13	10	12
664>	10	12	10	10	11	10	10	10	10: 672>	10	9	11	11	9	10
678>	10	8	8	10	8	12	7	8	8: 686>	12	7	9	10	9	8
692>	9	7	8	8	8	9	8	9	9: 700>	7	7	7	9	6	6
706>	8	7	7	8	7	6	8	7	7: 714>	6	7	8	6	6	7
720>	7	6	8	6	7	7	6	6	6: 728>	6	6	6	5	5	6
734>	5	5	6	6	6	6	4	6	6: 742>	5	6	5	6	5	4
748>	6	2	7	4	5	5	4	5	5: 756>	5	5	6	3	6	3
762>	5	4	5	4	5	4	4	4	4: 770>	3	5	3	5	3	4

A14006.010 860 FKS W MIN. 1 CNTS. 14-JUN-93 11:13:52 SUM 1: 0.5356E+04
 REF NO. 6(CONSOL) N AV MW: 576.3
 ACQUIRED 6-4-93 15:57:19 CHAN.#5 0- 81911 6 MS/CHAN. WT AV MW: 613.6
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 408 TO 468 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PU. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AK		U3		U2				U1		KH		KUH
776>	4	3	3	4	5	3	3	4	: 784>	3	4	3	3	4	3
790>	4	4	2	4	3	3	5	2	: 798>	5	3	2	4	2	3
804>	3	3	3	4	2	2	3	3	: 812>	3	3	2	3	2	3
818>	2	3	3	1	3	2	3	2	: 826>	2	3	2	2	3	2
832>	2	3	3	2	3	2	2	2	: 840>	2	2	1	3	2	3
846>	2	2	2	2	1	2	2	2	: 854>	1	3	1	2	2	2
860>	2	1	2	1	2	1	2	2	: 868>	2	2	2	1	1	2
874>	3	1	1	1	2	1	2	1	: 882>	2	1	2	1	2	1
888>	1	1	1	1	2	0	2	1	: 896>	2	1	1	1	2	0
902>	1	1	1	1	1	1	2	1	: 910>	0	2	1	1	2	1
916>	0	2	1	1	1	0	0	2	: 924>	0	2	1	1	1	1
930>	1	0	1	1	1	1	1	1	: 938>	1	0	2	0	1	1
944>	1	1	1	1	1	0	1	1	: 952>	1	1	1	0	1	0
958>	1	1	0	0	2	0	0	0	: 966>	2	0	0	2	0	1
972>	1	0	1	1	1	0	1	0	: 980>	0	1	1	1	1	1
986>	0	1	0	1	0	1	1	0	: 994>	1	0	0	2	0	0
1000>	1	0	0	1	0	1	1	0	: 1008>	1	0	0	0	0	0
1014>	0	1	0	0	0	1	0	0	: 1022>	0	0	1	0	0	0
1028>	0	1	0	1	1	0	1	0	: 1036>	0	0	1	0	1	0
1042>	1	0	0	1	0	1	0	1	: 1050>	0	0	0	0	0	0
1056>	0	0	0	1	0	0	0	0	: 1064>	1	0	0	0	0	0
1070>	1	0	1	0	0	0	0	0	: 1078>	0	1	0	0	0	0
1084>	0	0	0	0	0	0	0	0	: 1092>	1	0	0	0	0	0
1098>	0	0	0	0	1	0	1	0	: 1106>	0	0	0	1	0	0
1112>	1	0	0	1	0	0	0	0	: 1120>	0	0	0	0	0	0
1126>	0	0	1	0	0	0	0	0	: 1134>	0	0	0	0	0	0
1140>	0	0	0	0	0	0	0	0	: 1148>	0	0	0	0	0	0
1154>	0	0	0	0	0	0	0	0	: 1162>	1	0	0	0	0	0
1168>	0	0	0	0	0	0	0	0	: 1176>	0	0	0	0	0	0
1182>	0	0	0	0	0	0	0	0	: 1190>	0	0	0	0	0	0

SUM ODD 326.5 350.9 344.4 348.8 361.2 353.3 328.4
 EV 387.2 391.0 381.1 393.6 386.6 354.0 382.4
 RATIO 0.84330 0.89746 0.90379 0.89631 0.93437 0.99786 0.85867
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.901954

A14006.011 642 PKS W MIN. 1 CNTS. 14-JUN-93 11:14:36 SUM I: 0.2082E+04
 REF NO. 6(CONSOL) N AV MW: 519.1
 ACQUIRED 6- 4-93 16:09:13 CHAN.#5 0- 81911 6 MS/CHAN. WT AV MW: 575.8
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 474 TO 501 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN: 86.00% PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AR		U3		U2			U1		RH		RDH	
42>	0	0	0	0	0	0	0	0	0: 56>	13	0	0	0	0	0
62>	0	0	0	0	0	0	3	0	0: 70>	7	0	0	0	0	0
76>	0	0	0	0	0	0	5	0	0: 84>	0	0	0	0	0	0
90>	0	0	0	0	5	0	7	0	0: 98>	5	0	0	0	0	0
104>	0	0	0	0	9	0	4	0	0: 112>	0	0	0	0	0	0
118>	0	0	4	0	11	0	0	0	0: 126>	0	0	0	0	0	0
132>	3	0	5	0	5	0	0	0	0: 140>	0	0	0	0	3	0
146>	5	0	4	0	2	0	0	0	0: 154>	0	0	0	0	3	2
160>	4	0	3	0	0	0	0	0	0: 168>	0	0	2	0	3	1
174>	0	0	0	0	0	0	0	0	0: 182>	3	0	3	0	2	0
188>	0	0	0	0	0	0	2	0	0: 196>	3	2	4	0	0	0
202>	0	0	0	0	0	0	4	0	0: 210>	3	0	3	0	0	0
216>	3	0	0	0	4	1	3	0	0: 224>	3	0	3	0	0	0
230>	0	0	4	1	3	3	0	0	0: 238>	3	1	0	0	3	0
244>	3	0	3	0	3	2	2	0	0: 252>	3	0	3	1	3	2
258>	3	2	3	2	3	0	0	0	0: 266>	3	0	3	2	4	2
272>	3	2	2	0	2	1	2	0	0: 280>	3	2	2	3	3	2
286>	3	0	3	2	2	2	1	0	0: 294>	0	2	2	2	3	1
300>	2	0	2	2	2	0	2	0	0: 308>	4	2	3	1	3	2
314>	2	3	2	2	2	2	3	1	1: 322>	3	0	2	2	2	0
328>	3	2	3	2	2	2	3	2	2: 336>	3	2	0	2	2	0
342>	3	1	2	2	2	2	1	0	0: 350>	3	2	1	1	2	1
356>	2	0	3	2	2	2	2	0	0: 364>	2	1	3	2	2	1
370>	2	2	3	1	0	2	0	3	3: 378>	0	2	2	1	2	1
384>	2	2	0	2	2	2	2	2	2: 392>	3	1	2	2	2	1
398>	2	2	2	2	2	0	2	2	2: 406>	2	2	2	2	1	1
412>	2	1	0	3	0	2	1	1	1: 420>	2	2	2	1	0	2
426>	1	3	2	2	2	2	2	2	2: 434>	0	3	2	1	2	3
440>	2	3	2	2	2	2	2	2	2: 448>	2	3	1	2	2	2
454>	2	3	1	2	2	2	3	1	1: 462>	2	3	2	3	2	4
468>	1	3	3	1	2	2	3	3	3: 476>	2	3	3	4	2	3
482>	2	3	2	2	3	4	3	6	6: 490>	5	4	3	4	2	3
496>	2	3	3	3	6	3	4	6	6: 504>	5	4	4	3	3	3
510>	2	4	5	8	6	6	4	5	5: 518>	5	5	4	2	3	7
524>	5	6	6	7	8	6	6	6	6: 532>	4	4	3	2	4	8
538>	7	7	9	8	7	6	6	5	5: 546>	0	7	4	7	7	7
552>	8	9	8	9	6	7	4	5	5: 560>	4	6	6	9	8	11
566>	9	8	8	8	6	6	4	6	6: 574>	5	8	6	7	11	9
580>	9	7	8	6	5	5	7	6	6: 588>	0	12	5	10	8	10
594>	8	9	6	6	4	6	5	7	7: 602>	5	9	7	9	6	9
608>	6	7	5	6	4	7	4	7	7: 616>	6	9	7	7	7	4
622>	6	5	5	6	5	6	6	8	8: 630>	6	7	7	7	5	6
636>	4	7	3	5	4	6	6	7	7: 644>	7	4	8	4	4	4
650>	4	5	4	4	5	5	6	5	5: 658>	6	5	5	4	5	3
664>	3	5	4	5	4	5	4	6	6: 672>	4	5	3	4	2	4
678>	3	4	5	3	5	3	4	3	3: 686>	4	2	3	3	4	3
692>	4	3	2	4	4	3	3	3	3: 700>	4	2	2	2	4	3
706>	2	4	3	3	3	3	2	3	3: 714>	2	3	2	2	2	2
720>	3	3	2	3	3	2	3	1	1: 728>	3	1	3	2	2	2
734>	3	2	2	3	1	2	2	2	2: 742>	1	2	1	2	0	3
748>	1	3	2	1	2	2	1	2	2: 756>	1	1	2	2	1	2
762>	1	1	2	1	1	2	1	1	1: 770>	1	1	1	1	2	1

A14006.011 642 PKS W MIN. 1 CNTS. 14-JUN-93 11:15:12 SUM I: 0.2082E+04
 REF NO. 6(CONSOL) N AV MW: 519.1
 ACQUIRED 6- 4-93 16:09:13 CHAN.#8 0- 8191: 6 MS/CHAN. WT AV MW: 575.8
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 474 TO 501 DEG. C SF= 0
 ABSOLUTE INTENSITIES C13XN, 86.00% PG. 2

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
776>	1	2	1	1	1	1	1	1	1: 784>	1	1	1	2	1	1
790>	1	1	1	1	1	0	1	1	1: 798>	0	2	1	2	0	2
804>	0	1	1	1	0	1	1	1	1: 812>	1	0	1	1	1	1
818>	1	1	1	0	1	0	1	1	1: 826>	1	1		0	1	1
832>	1	1	0	0	1	0	1	1	1: 840>	0	0	1	1	1	0
846>	0	0	0	0	0	0	0	0	0: 854>	2	0	0	0	0	1
860>	0	0	1	0	0	0	0	0	0: 868>	0	0	0	0	0	0
874>	1	0	0	1	0	0	0	0	0: 882>	0	0	1	0	0	0
888>	0	0	0	0	0	0	0	0	0: 896>	0	0	0	0	0	0
902>	0	0	0	0	0	0	0	0	0: 910>	0	0	0	0	0	0
916>	0	0	0	1	0	0	0	0	0: 924>	0	0	0	0	0	0
930>	0	0	0	0	0	0	0	0	0: 938>	0	0	0	0	0	0
SUM ODD	135.6	135.5	132.3	122.7					137.7	129.5	142.1				
EV	151.1	150.9	162.2	150.5					160.1	141.4	146.2				
RATIO	0.89734	0.89784	0.81551	0.81525					0.85982	0.91602	0.97155				
OVERALL RATIO OF ODD TO EVEN MASS PEAKS	0.880356														

A14006.SUM 1166 PKS W MIN. 1 CNTS. 14-JUN-93 11:15:53 SUM I: 0.4291E+05
 REF NO. 6(CONSOL) 0-11 N AV MW: 401.6
 ACQUIRED 6- 4-93 16:09:13 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 473.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 DEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC PG. 1

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AK		U3		U2				U1	KH		KOH	
48>	0	0	0	16	0	0	0	14:	56>	58	49	20	0	0	0
62>	0	0	0	0	0	0	25	24:	70>	41	25	0	0	0	0
76>	0	0	0	0	16	0	29	27:	84>	39	21	19	0	0	21
90>	12	0	13	0	31	0	30	15:	98>	28	14	9	8	0	0
104>	0	0	12	12	48	8	24	7:	112>	17	13	11	0	0	10
118>	11	6	17	18	56	11	17	11:	126>	18	17	17	0	14	15
132>	22	15	27	12	40	11	12	11:	140>	7	12	32	10	22	23
146>	66	23	39	19	32	11	20	15:	154>	19	13	46	18	39	34
160>	85	37	40	22	35	12	39	34:	168>	182	24	65	40	156	54
174>	103	47	69	18	104	16	150	91:	182>	499	40	111	79	384	77
188>	148	42	104	22	191	29	286	119:	196>	487	70	167	64	398	84
202>	943	71	370	42	272	67	632	126:	210>	433	71	284	64	338	51
216>	888	101	523	67	424	170	728	143:	224>	421	72	338	66	387	65
230>	506	129	543	91	601	171	713	131:	238>	348	75	296	115	845	120
244>	571	114	461	95	473	163	463	129:	252>	315	60	304	103	612	188
258>	494	151	426	132	454	122	376	101:	266>	313	66	335	109	504	145
272>	473	113	386	0	756	133	381	92:	280>	286	93	485	149	433	145
286>	401	91	323	126	465	154	280	110:	294>	264	101	435	125	410	140
300>	340	116	289	128	348	132	294	117:	308>	289	112	390	134	362	112
314>	240	117	387	140	341	121	281	117:	322>	283	124	337	130	345	115
328>	262	98	356	156	332	120	269	124:	336>	271	114	253	0	344	174
342>	213	0	299	144	291	127	253	115:	350>	363	141	250	156	244	122
356>	298	125	274	140	250	133	215	115:	364>	325	136	249	182	169	0
370>	314	128	260	149	281	137	211	112:	378>	252	177	272	144	204	178
384>	155	134	234	173	203	168	244	205:	392>	183	179	217	191	200	154
398>	231	147	211	207	172	185	240	176:	406>	215	143	197	170	175	162
412>	174	181	216	229	174	180	169	189:	420>	194	173	168	166	228	196
426>	161	185	194	201	183	197	170	169:	434>	186	170	152	171	220	197
440>	182	179	189	156	199	151	182	160:	448>	229	186	175	142	201	190
454>	193	181	178	174	161	161	156	176:	462>	186	202	208	185	176	169
468>	192	171	173	159	176	172	189	182:	476>	183	168	189	190	187	170
482>	174	171	150	158	157	160	204	183:	490>	182	167	169	172	161	164
496>	174	152	190	160	171	151	175	183:	504>	178	181	152	158	159	144
510>	153	154	186	172	169	164	161	173:	518>	153	152	149	146	163	149
524>	157	145	160	171	176	150	161	158:	532>	171	150	133	131	165	136
538>	166	156	164	134	155	157	154	143:	546>	147	129	153	140	140	151
552>	153	155	154	142	145	128	129	135:	560>	128	131	136	136	142	141
566>	137	140	142	132	128	122	124	119:	574>	126	114	138	130	133	134
580>	136	124	128	117	116	120	118	113:	588>	122	106	123	116	122	120
594>	118	121	114	111	101	100	110	100:	602>	109	106	112	106	112	104
608>	111	100	107	86	101	90	106	98:	616>	101	95	96	91	95	84
622>	95	80	94	77	87	89	87	90:	630>	85	95	87	86	87	81
636>	87	78	70	78	77	81	77	87:	644>	73	91	74	63	75	71
650>	77	69	67	67	69	74	66	66:	658>	69	67	68	67	65	62
664>	70	63	63	65	62	57	65	63:	672>	57	55	62	54	53	58
678>	53	54	50	62	50	62	42	50:	686>	59	44	49	51	51	51
692>	46	48	55	46	50	44	49	45:	700>	45	43	43	49	34	45
706>	43	42	43	46	39	40	34	41:	714>	38	38	40	36	37	41
720>	36	36	41	37	36	34	40	27:	728>	38	33	34	29	35	36
734>	35	29	30	40	26	33	27	29:	742>	30	30	31	31	28	25
748>	35	20	32	24	27	28	24	26:	756>	26	31	26	23	23	24
762>	26	23	26	20	28	22	21	25:	770>	22	24	22	23	36	38

A14006.SUM 1166 PKS W MIN. 1 CNTS. 14-JUN-93 11:16:31 SUM I: 0.4281E+05
 REF NO. 6(CONSOL) 0-11 N AV MW: 401.6
 ACQUIRED 6- 4-93 16:09:13 CHAN.#S 0- 8191; 6 MS/CHAN. WT AV MW: 470.4
 MAG. RET. TIME: 9999 MS, 12 SCANS/SPECTRM. 30 TO 501 NEG. C SF= 1
 INTENSITIES NORMALIZED TO 100000. C13XN, 86.00XC P

MASS	0	1	2	3	4	5	6	7	MASS>	0	1	2	3	4	5
			AK		U3		U2					RH		ROH	
776>	52	11	25	19	22	19	20	22	784>	16	22	13	23	17	19
790>	21	17	21	15	21	18	16	20	798>	17	18	18	13	18	14
804>	18	15	16	14	19	13	16	15	812>	12	16	13	16	15	13
818>	15	14	14	15	15	14	11	15	826>	13	11	13	12	11	15
832>	15	10	14	14	12	12	12	9	840>	13	11	13	9	12	11
846>	11	10	11	10	11	9	13	9	854>	12	7	12	8	11	8
860>	9	14	5	14	5	11	7	9	868>	7	14	6	11	9	9
874>	8	8	8	9	10	7	10	7	882>	7	9	9	5	8	7
888>	8	7	8	5	8	10	4	9	896>	6	8	9	6	7	6
902>	8	5	6	8	4	10	5	7	910>	7	6	7	6	5	7
916>	5	6	7	7	6	3	8	3	924>	7	5	5	6	4	5
930>	7	5	5	6	6	3	4	3	938>	6	4	2	6	5	3
944>	4	5	7	3	8	4	4	6	952>	4	6	3	4	6	1
958>	6	5	3	5	5	3	6	5	966>	3	4	4	5	3	5
972>	3	5	2	6	3	4	4	5	980>	3	5	2	5	3	3
986>	4	3	3	4	2	2	5	3	994>	4	2	5	3	2	5
1000>	2	4	4	3	2	5	3	2	1008>	4	2	4	2	4	2
1014>	0	4	1	5	2	2	2	4	1022>	2	2	4	4	2	4
1028>	2	3	2	3	2	3	3	2	1036>	4	1	3	1	4	2
1042>	2	0	7	1	3	1	3	3	1050>	2	3	1	2	2	3
1056>	1	3	1	3	1	3	1	4	1064>	0	3	2	1	3	2
1070>	2	2	3	0	3	2	1	2	1078>	3	1	3	1	2	2
1084>	1	3	1	2	1	0	3	0	1092>	3	1	0	3	1	2
1098>	2	2	2	0	2	1	3	0	1106>	4	1	1	2	2	1
1112>	1	3	0	3	1	2	2	0	1120>	3	1	1	0	0	4
1126>	1	1	0	3	2	0	1	3	1134>	0	3	2	2	1	0
1140>	3	0	0	2	1	1	1	0	1148>	2	1	2	2	1	0
1154>	3	0	2	1	2	0	3	0	1162>	0	4	0	2	0	2
1168>	1	0	2	0	2	0	1	1	1176>	2	0	2	1	1	0
1182>	1	0	0	0	2	1	0	0	1190>	2	1	2	1	0	0
1196>	2	0	0	2	0	2	1	0	1204>	0	0	0	0	3	1
1210>	0	2	0	0	0	0	0	0	1218>	0	2	0	0	0	3
1224>	0	0	2	1	0	1	0	1	1232>	0	0	2	2	0	0
1238>	0	0	2	0	1	0	3	0	1246>	1	0	1	1	0	0
1252>	2	0	0	0	2	0	1	0	1260>	0	2	0	0	2	0
1266>	0	0	0	0	0	0	0	0	1274>	0	2	0	0	0	0
1280>	2	0	1	0	0	0	0	2	1288>	0	0	0	0	2	0
1294>	1	0	0	0	0	0	0	0	1302>	2	0	1	0	0	0
1308>	0	0	2	0	0	0	0	0	1316>	0	0	0	0	0	0
1322>	0	0	0	0	0	0	0	0	1330>	0	0	0	0	2	0
1336>	0	0	0	0	0	0	0	0	1344>	0	0	0	0	2	0
1350>	0	0	0	0	0	0	0	0	1358>	0	0	0	0	0	0
1364>	0	0	1	0	0	0	0	0	1372>	0	0	0	0	0	0

SUM ODD 4829.6 4974.6 5132.9 5286.3 4918.8 4913.7 5156.9
 EV 9980.7 8864.5 9266.9 9226.7 9064.5 8093.5 9684.3
 RATIO 0.48390 0.56118 0.55390 0.57294 0.54265 0.60711 0.53251
 OVERALL RATIO OF ODD TO EVEN MASS PEAKS 0.548650

**DATE
FILMED**

6 129/94

END