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**Diffuse Reflectance Infrared
Fourier Transform Spectra of
Selected Organic Compounds**

Sara H. Harmon
John E. Caton

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DIFFUSE REFLECTANCE INFRARED FOURIER-TRANSFORM SPECTRA OF
SELECTED ORGANIC COMPOUNDS

Sara H. Harmon and John E. Caton

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HIGHLIGHTS

A procedure for determining infrared spectra by the Diffuse Reflectance Infrared Fourier Transform (DRIFT) technique is described. The resulting DRIFT spectra are shown to be essentially identical to conventional transmission spectra. The Appendix includes a library of DRIFT spectra of forty different compounds with each spectra accompanied by a table listing the location and relative intensity of the principal spectral bands between 3800 cm^{-1} and 600 cm^{-1} .

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DIFFUSE REFLECTANCE INFRARED FOURIER TRANSFORM SPECTRA OF SELECTED ORGANIC COMPOUNDS

Sara H. Harmon and John E. Caton

ABSTRACT

Diffuse reflectance infrared spectra of a variety of different organic compounds have been determined. Profiles of the spectra along with the location and relative intensity of the principal bands have been included for each compound studied. In addition both diffuse reflectance and transmittance infrared spectra were obtained for the same samples, and the spectral results were compared. Although some minor variations are observed between a diffuse reflectance spectrum and the corresponding transmittance spectrum, the diffuse reflectance is quite useful and may be a superior technique for the study of many samples because it possesses an inherently higher signal-to-noise response, requires less sample preparation and allows a very wide range of samples (solids, liquids of low volatility, neat sample, or sample diluted in a reflecting medium) to be studied under very similar conditions.

INTRODUCTION

The basic concept of diffuse reflectance spectrometry is not new and it has been widely utilized in the measurement of the ultraviolet, visible, and near-infrared spectra of powders and opaque solutions.¹ For the mid infrared spectral region, however, the measurement of diffuse reflectance spectra for qualitative and quantitative analysis has only recently become a practical technique. This increased utility of diffuse reflectance spectrometry in the mid infrared region has been brought about by two innovations of fairly recent origin: (1) the commercial availability of dependable rapid scanning fourier transform infrared (FTIR) spectrometers; and (2) the introduction of an optical configuration for diffuse reflectance that did not require an integrating sphere.² Following this second innovation the development of

DRIFT² (Diffuse Reflectance Infrared Fourier Transform) Spectrometry has been quite rapid.^{2,3,4,5}

The basic theory for diffuse reflectance by powdered samples was presented by Kubelka and Munk^{6,7} many years ago. More recently, Fuller and Griffiths² have interpreted the Kubelka-Munk theory to relate it to single-beam diffuse reflectance spectra according to the following relationship:

$$\frac{(1-R)^2}{2R} = KC \quad (1)$$

Here R represents the ratio of the single-beam diffuse reflectance spectrum of the sample (R_S) to the single-beam diffuse reflectance spectrum of a reference material or sample medium (R_r), ($R = R_S/R_r$); C represents the sample concentration; and K is a constant which has been related to the molar absorptivity, (ϵ), in Beers Law, ($\epsilon = A/bc$), as it applies to absorbance/transmittance spectrometry.^{1,2} Thus, diffuse reflectance spectral data after transformation according to the Kubelka-Munk relationship (Equation 1) should yield spectra similar to conventional absorption/transmittance spectra [This abbreviated description of the Kubelka-Munk theory has been highly simplified; and although sufficient for the purpose of this document, interested readers may find more rigorous discussions elsewhere.^{1,2,4,6,7}

In this document the mid-infrared DRIFT spectra of approximately forty compounds are presented. DRIFT spectra of some compounds are also compared to the corresponding transmittance spectra. By this comparison it is shown that the signal-to-noise ratio is usually significantly higher for DRIFT spectra relative to transmittance spectra

measured under similar conditions. In addition, the required sample preparations for determining DRIFT spectra is both easier and faster than the sample preparation required for the determination of transmittance spectra. These advantages, coupled with the fact that DRIFT spectrometry allows the spectra of a wide variety of samples ranging from liquids of low volatility to intractable solids to be determined under identical conditions, suggest that the DRIFT technique may be the preferred method of routinely determining mid-infrared spectra of samples associated with fossil fuel energy development and the associated environmental assessments. Therefore, it is hoped that the spectra illustrated herein will demonstrate the overall utility of DRIFT spectrometry as a routine tool and serve as the beginning of a library of DRIFT spectra of organic compounds associated with on-going development of fossil fuel energy sources.

EXPERIMENTAL PROCEDURES

All spectra were made on a Digilab FTS-20/C (Digilab, Division of Bio-Rad Laboratories, Cambridge, MA) FTIR spectrometer equipped with a high intensity Globar source, a triglycine sulfate detector, a Model 496 Michelson interferometer with a KBr beamsplitter, and the associated data system. The diffuse reflectance attachment was obtained from Digilab and was a JASCO Model DRA-100.

Samples were prepared by blending 3 mg (or 3 μ l of a liquid) with 300 mg of spectroscopic grade KBr (Harshaw Chemical Co., Solon, OH) in a Wig-L-bug (Crescent Dental Manufacturing Co., Chicago, IL), for 30 seconds. Subsequently, the blended sample was added to a diffuse reflectance sample cup without compression. Spectra were then obtained

by adding 100 to 400 scans at a resolution of 4 cm^{-1} with the sensitivity set to the highest value consistent with avoiding an overload of the analog-to-digital converter. It should be noted here that the samples were leveled in the sample cup by dropping ("bouncing"), the filled cup onto the laboratory bench surface three or four times from a height of 3 to 5 cm. It is important that the method of adding the sample to the cup remain as reproducible as possible because band intensity is quite dependent on the way the sample is packed into the cup.³ However, the "bouncing" method described here has consistently yielded highly reproducible results.

After pressing the sample mixture used for the diffuse reflectance measurements into a pellet transmittance spectra were obtained under the same instrumental conditions.

DRIFT SPECTROMETRY RESULTS

The ratio of a single-beam diffuse reflectance spectra for a given sample to a reference, (300 mg of KBr subjected to the same treatment as the sample mixture), was calculated to develop a reflectance spectrum (R) from which a Kubelka-Munk plot was generated according to the relationship (Equation 1) discussed previously. This Kubelka-Munk plot was then normalized to make the relative intensity of the strongest spectral band between 3800 cm^{-1} and 600 cm^{-1} have a value of one. These normalized plots along with tables listing the relative intensity and the location of the band maxima are assembled in the Appendix.

COMPARISON OF DRIFT AND TRANSMITTANCE SPECTRA

One of the advantages of DRIFT spectrometry is that one can obtain useful data from either a small amount of sample dispersed in a highly reflecting medium or from a neat sample. In Figure 1, the spectrum of pure β -naphthylamine is illustrated for four different sampling techniques: (a) DRIFT spectra of pure 2-aminonaphthalene; (b) DRIFT spectra of a 1% mixture of 2-aminonaphthalene dispersed in KBr and packed in the sample cup by the "bounce" method; (c) DRIFT spectra of the 1%-mixture compressed in the sample cup; and (d) the transmittance spectra of the 1%-mixture after pressing into a disk. These spectra are all quite similar, however, the spectra of the neat sample (Figure 1-1) does show some band splittings arising from the crystallinity of the sample. The grinding step in the preparation of the sample for the other three 2-aminonaphthalene spectra appears to minimize or eliminate any band splittings. The spectra shown in Figure 1-2, -3, and -4 were all made on the same blended sample with the difference between Figure 1-2 and Figure 1-3 being that the sample was compressed in the sample cup for the latter spectrum. Table 1 indicates that this compression tended to increase band intensity with the extent of the increase not entirely uniform.

In addition to the effect of sample compression, band intensities can also vary with the particle size of the sample. In Figure 2, the spectra of a sample of dotriacontane (DTC) blended with KBr in a Wig-L-bug is compared with a neat, blended sample of DTC, and with a neat sample of DTC which received no blending. All three samples were added to the diffuse reflectance sampling cup by the "bounce" method.

Although the information in all three DTC spectra is essentially the same, the quality of the spectrum of the DTC-KBr blend is best. An examination of Table 2 will indicate some small changes in the location of band maxima between the blended sample and the neat samples. The spectra of the two neat DTC samples show no significant differences in location of band maxima; however, band splittings are more evident in the spectra of the sample which received no blending; and the relative intensities of the band maxima have been increased in the blended sample (Table 2) when compared to the unblended sample. The blending of the neat sample probably reduces the particle size thereby increasing the surface area which can be sampled which leads to the increased band intensity. The blending of a pure 2-aminonaphthalene sample also increases band intensity as illustrated in Figure 3. In addition, Figure 3 also compares spectra transformed by the Kubelka-Munk relationship (Equation 1) to the reflectance spectrum before being transformed. As summarized in Table 3 the reflectance spectrum contains the same qualitative information as the Kubelka-Munk spectra; however, the Kubelka-Munk conversion of the spectrum makes two quantitative differences: (1) the signal-to-noise is improved, and (2) the overall spectral envelope is quite closely related to an absorbance spectrum.

The previous discussion indicates both advantages and disadvantages of DRIFT spectrometry. The principal disadvantages are the non-uniform variation of band intensity caused by sample compression and particle size. On the advantage side of the ledger are (1) an inherently higher signal-to-noise for a DRIFT spectrum compared to a transmittance spectrum for the same sample; (2) less sample preparation

(pressing sample disks is eliminated); (3) the ability to make spectra of either pure solid samples or dilute samples dispersed in a reflecting medium; and (4) the ability to handle samples ranging from intractable solids to non-volatile liquids in an identical manner. For the study of a wide range of complex samples these advantages tend to favor DRIFT spectrometry relative to conventional transmittance spectrometry especially when the disadvantages caused by matrix variations are minimized by using dilute samples blended in a reflecting medium and added to the sample cup by the "bounce" technique. (See section on Experimental Procedures.) Both the qualitative and quantitative aspects of a DRIFT spectrum and an absorbance spectrum of the same samples pressed into a KBr disk are quite similar. There are a few minor differences in these spectra which may arise from matrix differences between a powdered sample and a compressed disk. Such matrix differences (such as particle size, range of particle sizes, and the assumption of an absolute reflecting medium)² will allow the Kubelka-Munk units (Equation 1) to deviate slightly from absorbance. However, with careful preparation of dilute samples such differences have been observed to be minimal for all the DRIFT spectra included in the Appendix of this document.

Table 1

Comparison of Different DRIFT Spectra and
Transmission Spectrum of β -naphthylamine

Wavenumber, cm ⁻¹	Relative Intensity of Absorption Bands ^a			
	DRIFT Spectra ^b			Transmission spectrum, KBr Disk
	Pure	Blended	Blended and compressed	
3395	0.94	0.37	0.24	0.51
3325	0.88			
3321			0.26	
3318		0.39		0.49
3314	0.88			
3275	0.76			
3260		0.18	0.12	
3211	0.88	0.30	0.21	
3050	0.88	0.33	0.23	0.40
3024	0.65	0.16	0.10	0.30
3009	0.65	0.16	0.10	0.31
1636	1.00		0.33	
1632		0.78	0.57	0.87
1612		0.25	0.16	
1601	0.94	0.54	0.37	0.58
1512	1.00	0.96	0.64	0.83
1470	0.88	0.34	0.22	0.35
1393	0.88	0.22	0.15	0.20
1385	0.88	0.24	0.16	0.24
1377	0.82	0.17	0.10	-
1366	0.88	0.25	0.17	0.26
1283	0.88	0.41	0.29	0.41
1269	0.88	0.28	0.17	0.28
1227	0.88	0.41	0.26	0.35
1184	0.94	0.37	0.24	0.34
868	-	-	0.16	0.15
845	0.94	0.62	0.49	0.52
818	1.00	0.99	0.81	0.88
756	1.00			
743		1.00	1.00	1.00

^aRelative intensity based on most intense absorbance band normalized to value of one.

^bPure indicates DRIFT spectrum of powdered β -naphthylamine. Blended indicates DRIFT spectrum of 3 mg of β -naphthylamine blended with 300 mg of KBr and added to sample cup by "bounce" technique. Blended and compressed indicates DRIFT spectrum of 3 mg of β -naphthylamine blended with 300 mg of KBr and compressed into sample cup.

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Fig. 1. Spectra of 2-aminonaphthalene under different conditions: (1) DRIFT spectrum of 2-aminonaphthalene as supplied; (2) DRIFT spectrum of 3 mg of 2-aminonaphthalene blended with 300 mg of potassium bromide; (3) same as spectrum No. 2 except that the blended sample was compressed into the sample cup; and (4) transmission spectrum of sample used for spectra 2 and 3 after pressing into a disk. The arbitrary units are proportional to absorbance.

Table 2

Comparison of Several DRIFT Spectra of Dotriacontane Obtained
Under Different Sampling Conditions

Wavenumber, cm ⁻¹	Relative Intensity of Absorption Bands ^a		
	Blended with KBr ^b	Pure and Mixed ^c	Pure ^d
2963	-	0.56	-
2955	0.27	0.57	0.88
2930	-	0.60	1.00
2916	1.00	-	-
2907	-	0.57	0.76
2897	-	-	0.78
2872	0.19	0.56	0.95
2853	0.80	0.61	0.95
1474	0.34	0.80	0.94
1462	0.31	0.84	0.94
1365	-	0.28	0.29
729	0.19	0.95	0.94
721	0.14	1.00	0.99

^aRelative intensity based on most intense absorbance band normalized to value of one.

^bBlended with KBr indicates 3 mg of dotriacontane has been blended with 300 mg of KBr.

^cPure and Mixed indicates that DRIFT spectrum of pure dotriacontane was made after the sample had been blended. This blending was likely to yield a more uniform and smaller particle size.

^dPure indicates that a DRIFT spectrum of pure dotriacontane was made on a sample taken directly from the commercial supply.

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Fig. 2. Spectra of dotriacontane under different conditions: (1) DRIFT spectrum of 3 mg of dotriacontane blended with 300 mg of potassium bromide; (2) DRIFT spectrum of dotriacontane as supplied by commercial source; and (3) DRIFT spectrum of pure dotriacontane after blending. The arbitrary units are proportional to absorbance.

Table 3

Comparison of Reflectance Spectra of 2-aminonaphthalene

Wavenumber, cm ⁻¹	Relative Intensity of Absorption Bands		
	Pure ^b	Pure and Mixed ^c	Reflectance ^d
3397	0.94	0.83	1.00
3325	0.88	0.83	0.97
3316	0.88	0.83	0.96
3275	0.76	-	-
3210	0.88	0.77	0.92
3051	0.88	0.73	0.91
3024	0.65	0.53	0.66
3009	0.65	0.53	0.66
1636	1.00	0.97	1.00
1601	0.94	0.93	0.91
1512	1.00	1.00	1.00
1470	0.88	0.87	0.82
1393	0.88	0.80	0.78
1385	0.88	0.83	0.79
1377	0.82	-	-
1366	0.88	0.80	0.81
1283	0.88	0.90	0.77
1269	0.88	0.87	0.81
1227	0.88	0.93	0.81
1184	0.94	0.90	0.87
858	0.94	0.93	0.82
845	0.94	0.93	0.83
822	1.00	0.97	0.95
756	1.00		0.94
745		1.00	

^aRelative intensity based on most intense absorbance band normalized to value of one.

^bPure indicates Kubelka-Munk spectrum of 2-aminonaphthalene as it comes from the commercial supply.

^cPure and Mixed indicates the Kubelka-Munk spectrum of 2-aminonaphthalene that had been blended in a Wig-L-Bug.

^dReflectance indicates the diffuse reflectance spectrum of 2-aminonaphthalene that has not been transformed by the Kubelka-Munk relationship.

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Fig. 3. Spectra of 2-aminonaphthalene under different conditions: (1) DRIFT spectrum of 2-aminonaphthalene after blending; (2) DRIFT spectrum of 2-aminonaphthalene without blending; and (3) DRIFT reflectance spectrum of 2-aminonaphthalene without Kubelka-Munk manipulation.

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APPENDIX: CATALOG OF DRIFT SPECTRA

In this section one will find a library of forty DRIFT spectra. All spectral samples were prepared by dispersing 3 mg of the known into 300 mg of KBr and adding the blended sample to the diffuse reflectance sample cup as described in the Experimental Procedure Section of this document. Both a figure of the DRIFT spectrum and a table listing the location and relative intensity of the principal spectral bands are presented on facing pages. The relative intensity of each band was determined by normalizing all band intensities to the intensity of the strongest band observed after the diffuse reflectance spectrum had been transformed according to the Kubelka-Munk theory (Equation 1 in text).

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Acenaphthene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3055	0.36
3040	0.31
2940	0.34
2920	0.45
2835	0.30
1933	0.16
1790	0.11
1771	0.11
1616	0.20
1601	0.47
1593	0.42
1501	0.17
1470	0.19
1450	0.16
1420	0.36
1369	0.61
1277	0.16
1254	0.09
1211	0.11
1177	0.16
895	0.14
841	0.58
799	1.00

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XACENAPTHE
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 10:10:21

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Acenaphthylene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3063	0.20
3040	0.23
1933	0.08
1825	0.08
1809	0.08
1744	0.08
1558	0.10
1539	0.08
1489	0.23
1477	0.38
1458	0.40
1427	0.60
1389	0.20
1223	0.13
1204	0.15
1177	0.08
1150	0.10
1084	0.10
914	0.08
864	0.20
829	1.00
775	0.73
729	0.78

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XACENAPHTHY
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 10:7:5

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Anthracene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3055	0.25
3021	0.07
1929	0.05
1809	0.05
1786	0.06
1620	0.15
1535	0.14
1450	0.21
1315	0.17
1273	0.15
1169	0.09
1146	0.15
999	0.15
957	0.40
907	0.15
883	1.00
745	0.23
737	0.32
725	0.78
602	0.09

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XANTHRAC
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 10:53:57

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 1,2-benzanthracene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3051	0.20
3032	0.18
3005	0.08
1948	0.04
1925	0.04
1501	0.18
1477	0.11
1412	0.05
1339	0.15
1300	0.09
1277	0.07
1261	0.05
1238	0.14
1227	0.07
1157	0.07
953	0.08
899	0.38
883	0.64
814	0.53
783	0.16
748	1.00
687	0.11

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF 1,2-BENZANTHRACENE IN KBR

PFA=XBAA
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 15:6:7

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Benzo(a)Pyrene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3075	0.13
3051	0.19
3036	0.21
1589	0.06
1562	0.06
1512	0.08
1474	0.09
1416	0.07
1408	0.07
1312	0.10
1246	0.08
1200	0.07
1184	0.11
883	0.31
849	0.24
841	0.40
829	0.34
814	0.10
756	1.00
744	0.47
691	0.63
536	0.07

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XBAP
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 15:3:50

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Benzo(e)pyrene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3078	0.12
3048	0.28
1929	0.07
1921	0.07
1790	0.06
1601	0.21
1589	0.11
1477	0.19
1443	0.24
1412	0.30
1319	0.15
1269	0.07
1204	0.14
1192	0.24
1169	0.08
1153	0.13
899	0.12
826	0.90
772	0.48
745	1.00
710	0.20
644	0.07
571	0.23

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XBEP
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 10:57:21

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Benzo(ghi)Perylene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3048	0.27
1921	0.08
1902	0.05
1794	0.08
1612	0.10
1597	0.10
1512	0.11
1447	0.15
1393	0.14
1339	0.16
1204	0.14
1146	0.23
1130	0.08
895	0.10
845	1.00
814	0.38
768	0.53
752	0.51
648	0.22
544	0.22

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF BENZO(GHI)PERYLENE IN KBR

PFA=XBENZPER
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:25:7

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Chrysene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3051	0.08
1701	0.06
1616	0.06
1593	0.05
1558	0.10
1539	0.05
1516	0.11
1485	0.10
1435	0.14
1300	0.06
1265	0.23
864	0.11
818	1.00
756	0.96
683	0.08
579	0.08

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XCHRYSENE
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:35:6

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Dibenz(a,h)anthracene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3067	0.14
3055	0.14
3048	0.16
3034	0.15
1506	0.21
1454	0.16
1429	0.15
891	0.74
816	1.00
750	0.63
743	0.58
667	0.58
534	0.12

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21333

PFA=XDIBENZAN
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:52:34

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Fluorene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3064	0.06
3041	0.06
1447	0.28
1401	0.07
1312	0.07
1192	0.10
999	0.06
953	0.08
737	1.00
698	0.11
413	0.21

*Relative intensity based on most intense absorbance band normalized to value of one.

SFL=KMPL0T
NSCANS=100
PLM=S

RES=4 DP

12/18/80 11:14:52

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Naphthalene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3048	0.63
3028	0.36
3005	0.28
1956	0.21
1921	0.12
1910	0.14
1844	0.12
1736	0.16
1593	0.76
1566	0.16
1520	0.19
1504	0.64
1389	0.59
1362	0.29
1273	0.52
1246	0.21
1211	0.36
1142	0.26
1123	0.52
1007	0.52
980	0.17
961	0.62
845	0.36
785	1.00

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF NAPHTHALENE IN KBR

PFA=XNAP
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 13:1:47

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Phenanthrene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3055	0.21
1948	0.05
1921	0.05
1890	0.04
1836	0.03
1809	0.04
1612	0.06
1601	0.05
1501	0.13
1454	0.18
1427	0.13
1304	0.13
1242	0.16
1200	0.06
1142	0.23
1092	0.06
1038	0.07
999	0.05
949	0.10
872	0.15
864	0.10
818	0.81
733	1.00
714	0.24

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21326

PFA=XPHENANTH
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 13:48:0

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Pyrene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3048	0.16
3028	0.12
1933	0.06
1921	0.07
1871	0.04
1802	0.08
1763	0.05
1601	0.10
1485	0.07
1466	0.05
1450	0.07
1435	0.15
1404	0.05
1312	0.05
1242	0.11
1184	0.29
964	0.05
841	1.00
822	0.12
748	0.32
710	0.97

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XPYRENE
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 13:57:16

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Catechol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3453	1.00
3325	0.79
3051	0.27
1620	0.44
1601	0.29
1516	0.77
1470	0.73
1366	0.89
1281	0.81
1258	0.84
1242	0.74
1188	0.73
1165	0.34
1096	0.76
1042	0.49
849	0.33
772	0.53
756	0.67
741	0.54
633	0.30

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21340

PFA=XCATECHOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:27:43

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 3-Methyl Catechol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3472	0.51
3368	0.71
3032	0.09
1628	0.38
1593	0.30
1504	0.57
1481	1.00
1366	0.68
1323	0.67
1281	0.97
1242	0.61
1196	0.72
1153	0.37
1080	0.39
1018	0.47
945	0.55
829	0.39
772	0.51
764	0.76
729	0.73
637	0.36

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=X3MCA1
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:30:9

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 4-Methyl Catechol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3283	1.00
3036	0.29
1605	0.39
1520	0.80
1458	0.35
1377	0.45
1358	0.44
1335	0.33
1288	0.90
1265	0.58
1204	0.54
1196	0.56
1150	0.27
1111	0.56
945	0.30
864	0.18
853	0.10
802	0.50
783	0.39
586	0.30

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF 4-METHYL CATECHOL IN KBR

PFA=X4MCAT
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:32:51

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of m-Cresol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3337	1.00
3040	0.23
2978	0.13
2951	0.14
2920	0.19
2859	0.10
1616	0.28
1589	0.55
1493	0.41
1462	0.31
1440	0.21
1339	0.17
1281	0.36
1265	0.35
1246	0.30
1157	0.42
926	0.24
775	0.33
733	0.15
691	0.29

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21335

PFA=XMCRE SOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:41:39

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of o-Cresol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3352	0.43
3032	0.27
2967	0.18
2951	0.22
2859	0.14
1593	0.53
1504	0.55
1493	0.59
1466	0.71
1346	0.33
1327	0.37
1242	0.73
1207	0.55
1177	0.53
1107	0.67
845	0.45
752	1.00
714	0.29

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21334

PFA=XOCRESOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:45:33

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of p-Cresol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3325	1.00
3287	0.93
3271	0.79
3032	0.28
3024	0.29
2920	0.26
1612	0.22
1601	0.29
1512	0.95
1462	0.23
1435	0.24
1362	0.20
1238	0.57
1173	0.30
1103	0.19
841	0.19
818	0.39
741	0.24

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21337

PFA=XPCRESOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:39:42

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 4,6-Dinitro-o-cresol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3561	0.02
3098	0.05
2967	0.02
2936	0.02
1609	0.45
1570	0.35
1555	0.83
1501	0.19
1454	0.21
1420	0.13
1358	0.49
1342	1.00
1304	0.31
1285	0.28
1258	0.32
1215	0.07
1180	0.09
1099	0.12
934	0.04
907	0.04
783	0.12
748	0.07
706	0.07

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=XDINITCRE
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:49:48

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Guaiacol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3518	1.00
3051	0.22
3005	0.19
2957	0.29
2843	0.29
1612	0.27
1597	0.49
1504	0.90
1470	0.53
1458	0.41
1443	0.49
1362	0.37
1304	0.26
1258	0.76
1223	0.63
1173	0.38
1157	0.24
1111	0.55
1042	0.47
1022	0.47
918	0.12
833	0.16
745	0.50

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21330

K/M SPECTRA OF GUAIACOL IN KBR

PFA=XGUAIACOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:57:7

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Hydroquinone

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3256	0.98
3233	1.00
3032	0.48
2859	0.16
2851	0.16
2716	0.15
2608	0.11
2465	0.08
1856	0.08
1516	0.91
1477	0.92
1354	0.37
1258	0.48
1242	0.62
1223	0.74
1211	0.85
1192	0.71
1096	0.27
826	0.55
760	0.67
702	0.26
613	0.29

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21329

K/M SPECTRA OF HYDROQUINONE IN KBR

PFA=XHYDQUIN
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:59:31

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 3 Hydroxy-Benzo(a)pyrene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3260	0.23
1506	0.25
1498	0.43
1261	0.21
1250	0.30
876	0.25
870	0.32
829	0.40
822	1.00
748	0.47
737	0.93
691	0.42
673	0.26
669	0.20

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF 3-HYDROXY BENZO(A)PYRENE IN KBR

PFA=X30HBAP
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:17:59

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of β -Naphthol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3291	0.72
3055	0.42
1632	0.71
1601	0.63
1585	0.37
1512	0.62
1470	0.68
1454	0.34
1408	0.55
1381	0.33
1362	0.25
1323	0.24
1281	0.71
1242	0.52
1219	1.00
1173	0.64
1119	0.29
961	0.53
907	0.52
880	0.29
845	0.78
818	0.86
752	0.36
741	0.79

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21341

K/M SPECTRA OF 2-NAPHTHOL IN KBR

PFA=X2NAPHTHOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:21:57

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of p-nitrophenol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3329	1.00
3121	0.23
3086	0.32
2438	0.13
1612	0.44
1589	0.78
1516	0.62
1501	0.92
1493	0.65
1450	0.17
1435	0.17
1346	0.57
1327	0.78
1288	0.75
1219	0.62
1169	0.45
1115	0.61
868	0.23
853	0.58
756	0.34
694	0.17
637	0.30
629	0.33

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21320

K/M SPECTRA OF P-NITROPHENOL IN KBR

PFA=XPNITPHEN
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 14:33:39

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Phenol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3205	1.00
3048	0.81
3021	0.73
2839	0.41
2723	0.39
2604	0.32
2484	0.22
1597	0.63
1501	0.64
1474	0.75
1388	0.41
1373	0.51
1234	0.63
1169	0.39
1153	0.36
1072	0.36
887	0.25
821	0.32
810	0.41
752	0.59
691	0.58

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21321

PFA=XPHENOL
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 14:23:33

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Resorcinol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3206	1.00
2886	0.39
2654	0.39
2646	0.39
2523	0.28
1609	0.94
1504	0.50
1493	1.00
1408	0.50
1381	0.67
1312	0.61
1296	0.72
1285	0.56
1169	0.72
1153	0.94
964	0.78
845	0.50
775	0.83
741	0.67
683	0.56
544	0.61

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF EXC RESORCINOL IN KBR

PFA=XEXGRES
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 13:59:54

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 4 Ethyl Resorcinol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3302	1.00
3240	0.65
2970	0.28
2916	0.11
2851	0.09
1624	0.35
1612	0.25
1528	0.39
1458	0.59
1427	0.15
1308	0.34
1292	0.60
1246	0.16
1227	0.17
1188	0.24
1165	0.34
1111	0.61
976	0.95
841	0.23
810	0.16
779	0.07
741	0.10
721	0.12

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF 4-ETHYL RESORCINOL IN KBR

PFA=X4ERES
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 14:21:25

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 2 Methyl Resorcinol

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3333	1.00
3040	0.13
2970	0.12
2920	0.13
1624	0.34
1601	0.39
1524	0.18
1470	0.69
1381	0.46
1281	0.46
1219	0.20
1169	0.32
1061	0.69
918	0.23
775	0.43
714	0.17
687	0.21

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF 2-METHYL RESORCINOL IN KBR

PFA=X2MRES
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 14:19:4

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Acridine

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
1620	0.04
1555	0.05
1516	0.17
1462	0.05
1142	0.06
961	0.08
922	0.10
911	0.09
860	0.12
814	0.03
795	0.10
737	1.00
617	0.06
602	0.08
478	0.05
467	0.05

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 82-8954

K/M SPECTRA OF ACRIDINE IN KBR

SFL-KMPL01
NSCANS=100
PLM=5

RES=4 DP

12/19/80 9:58:51

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Aniline

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3433	0.29
3356	0.59
3213	0.23
3086	0.14
3071	0.20
3036	0.40
3009	0.19
1929	0.05
1620	0.69
1601	1.00
1501	0.93
1466	0.25
1312	0.14
1277	0.34
1177	0.21
1153	0.08
1026	0.08
995	0.11
883	0.13
752	0.46
694	0.44

*Relative intensity based on most intense absorbance band normalized to value of one.

SFL=ANILINE
NSCANS=100
PLM=S

RES=4 DP

10/29/81 10:38:6

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Carbazole

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3423	0.10
1601	0.04
1493	0.03
1459	0.10
1451	0.32
1335	0.07
1327	0.12
1242	0.08
930	0.04
857	0.03
756	0.13
749	0.90
725	1.00
575	0.15
567	0.05

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 82-8958

K/M SPECTRA OF CARBAZOLE IN KBR

SFL=KMPL0T
NSCANS=100
PLM=S

RES=4 DP

12/19/88 10:45:8

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 6-Aminochrysene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3445	0.05
3368	0.10
3051	0.08
1628	0.35
1612	0.21
1593	0.21
1574	0.10
1528	0.13
1489	0.17
1443	0.37
1423	0.12
1385	0.16
1300	0.06
1265	0.10
1242	0.21
1231	0.11
856	0.12
845	0.16
810	0.38
756	1.00
741	0.12
683	0.09
556	0.12

*Relative intensity based on most intense absorbance band normalized to value of one.

K/M SPECTRA OF 6-AMINOCHRYSENE IN KBR

PFA=X6AMCHRY
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 10:46:46

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of 1-Aminopyrene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3337	0.13
3217	0.11
3040	0.23
1624	0.35
1601	0.35
1547	0.13
1512	0.66
1485	0.37
1462	0.14
1435	0.30
1420	0.13
1377	0.11
1335	0.15
1315	0.20
1273	0.39
1238	0.27
1192	0.15
1134	0.21
833	1.00
818	0.31
756	0.34
714	0.49
675	0.25

*Relative intensity based on most intense absorbance band normalized to value of one.

PFA=X1AMPYRENE
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 10:49:24

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of β -Naphthylamine

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3395	0.57
3321	0.54
3210	0.39
3051	0.37
3024	0.17
1632	0.85
1601	0.59
1512	1.00
1470	0.33
1447	0.15
1385	0.22
1366	0.24
1281	0.41
1269	0.26
1227	0.39
1184	0.35
1123	0.15
957	0.24
883	0.35
856	0.87
845	0.55
818	0.87
745	0.89
714	0.35
640	0.22
621	0.24

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21319

K/M SPECTRA OF B-NAPHTHYLAMINE IN KBR

PFA=XBNAPAMINE
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 15:8:45

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Aniline Hydrochloride

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
2914	0.40
2901	0.43
2870	0.40
2824	0.40
2594	0.27
2576	0.25
2016	0.13
1992	0.12
1601	0.16
1576	0.18
1558	0.20
1520	0.20
1516	0.19
1495	0.72
1463	0.19
745	1.00
689	0.33

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 82-8956

SFL=XANILHCL
NSCANS=100
PLM=S

RES=4 DP

10/29/81 10:40:16

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Palmitic Acid

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3024	0.13
2986	0.13
2963	0.29
2955	0.36
2916	1.00
2851	0.71
2677	0.11
2654	0.11
1701	0.53
1474	0.14
1462	0.18
1431	0.13
1412	0.12
1312	0.17
1296	0.21
1273	0.12
1250	0.09
1227	0.09
1204	0.08
1188	0.09
941	0.14
729	0.09
721	0.11

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21327

K/M SPECTRA OF PALMITIC ACID IN KBR

PFA=XPALMITIC
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 13:4:52

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Pyridine Hydrochloride

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3059	0.84
2938	0.58
2810	0.55
2677	0.47
1635	0.42
1603	0.68
1528	0.82
1481	0.63
1332	0.13
1247	0.24
1240	0.21
1055	0.32
995	0.18
916	0.18
881	0.24
835	0.16
756	1.00
731	0.16
683	0.68

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 82-8955

SFL=XPYHCL
NSCANS=100
PLM=5

RES=4 DF

10/29/81 10:43:0

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Dotriacontane

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
2955	0.27
2916	1.00
2874	0.19
2851	0.80
1474	0.34
1462	0.31
729	0.19
721	0.14

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 81-21331

K/M SPECTRA OF N-DOTTRIACONTANE IN KBR

PFA=XDOT
NSCANS=100
FCT=SC

RES=4 DP

11/4/81 12:55:28

Principal Bands Between 4000 and 500 cm^{-1}
in the DRIFT Spectrum of Dibenzothiophene

<u>Band Location (cm^{-1})</u>	<u>Relative Intensity*</u>
3068	0.13
3052	0.13
1586	0.15
1439	0.21
1428	0.38
1416	0.18
1312	0.18
1231	0.23
1134	0.13
1073	0.18
1026	0.15
768	0.18
745	1.00
710	0.21
702	0.26

*Relative intensity based on most intense absorbance band normalized to value of one.

ORNL-DWG 82-8957

K/M SPECTRA OF DIBENZOTHIOPHENE

SFL=KMPL0T
NSCANS=100
PLM=S

RES=4 DP

12/19/80 12:44:30

1

2

3

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