Mark Ravreby,[1] *B.Sc.*

Quantitative Determination of Cocaine and Heroin by Fourier Transform Infrared Spectrophotometry

REFERENCE: Ravreby, M., **"Quantitative Determination of Cocaine and Heroin by Fourier Transform Infrared Spectrophotometry,"** *Journal of Forensic Sciences,* JFSCA, Vol. 32, No. 1, Jan. 1987, pp. 20-37.

ABSTRACT: Cocaine hydrochloride salt (HCl) and heroin HCl were determined quantitatively by choosing a carbonyl absorption peak as the analytical peak and measuring absorbance versus concentration in standard KBr pellets. The effect of various additives and diluents such as starch, sugars, mannitol, caffeine, and procaine was also studied. Methods were devised to correct for interference contributions based on spectral subtraction of the interfering component or subtraction of the interfering spectral contribution based on absorbance ratios with a noninterfering spectral peak. In mixtures containing both the free base and the hydrochloride salt, the most satisfactory method for determining the concentration was by area integration of the two carbonyl peaks.

KEYWORDS: toxicology, cocaine, heroin, spectroscopic analysis, Fourier transform infrared spectrophotometry, quantitative analysis

Infrared spectrophotometry is a powerful analytical technique frequently used for qualitative analysis of drugs in forensic science in corroboration with other analytical methods. However, quantitative determinations of dangerous drugs in forensic science are generally performed by various chromatographic methods such as gas chromatography (GC) and high pressure liquid chromatography (HPLC) [*1-3*], and less frequently by methods based on ultraviolet (UV) or visible spectrophotometry. With the advent of Fourier transform infrared spectrophotometry (FTIR), the potential application of infrared spectrophotometry to quantitative determinations has been greatly expanded but not exploited [*4*]. In the more recent forensic science reviews there is no mention of the quantitative application of FTIR to dangerous drugs [*2,3*].

In the present work, various techniques were studied on heroin and cocaine samples including simple absorbance measurements, corrections for broadband interferences based on a judicious selection of the baseline, corrections for interferences based on absorbance ratios with a noninterfering spectral peak from a given component, spectral subtraction, and area integration.

Received for publication 14 Nov. 1985; revised manuscript received 1 March 1986; accepted for publication 7 March 1986.

[1]Forensic chemist, Criminal Identification Division, National Police Headquarters, Jerusalem, Israel.

Experimental Procedure

Apparatus

The infrared spectra were obtained using an Analect model FX6160 Fourier transform infrared spectrophotometer with a triglycine sulfate (TGS) detector. A Wilks 1/2-in. (12.7-mm) diameter pellet holder was used to prepare the potassium bromide (KBr) pellets. All weighings were performed on a Sartorius model 1702 MP8 electronic analytical balance.

Reagents

Cocaine · HCl was obtained from Merck. Cocaine base was prepared by neutralizing the cocaine · HCl with an excess of a dilute ammonia solution and extracting into chloroform. Heroin · HCl was obtained from Applied Science Laboratories. Heroin base was prepared by gradually neutralizing the heroin · HCl with the stoichiometric equivalent of an aqueous potassium hydroxide solution, filtering and recrystallizing from acetone.

Procedure

Standard stock mixtures were prepared by mixing 10 mg of a given compound with 490 mg of potassium bromide and thoroughly grinding and mixing three times in an agate mortar and pestle. A total of 100 mg of sample plus potassium bromide was always taken to prepare the pellets. Each time a standard stock mixture was diluted with potassium bromide or mixed with another standard stock mixture, it was thoroughly ground and mixed three times before preparing as a pellet. A ram pressure of 7 tons (6350 kg) was applied to prepare the pellets. Spectra were recorded as transmission, absorbance, and baseline corrected absorbance spectra using sixty-four scans. Data for the calibration graphs was always taken from the baseline corrected absorbance spectrum.

Results and Discussion

Cocaine · HCl has two strong carbonyl absorption peaks at $\lambda = 1730.9$ and $\lambda = 1712.8$ cm^{-1}. The spectra recorded as a transmission spectrum, absorbance spectrum, and baseline corrected absorbance spectrum are in Figs. 1, 2, and 3. A plot of absorbance, from the baseline corrected spectra versus concentration at $\lambda = 1730.9$ and $\lambda = 1712.8$ cm^{-1} is in Fig. 4. The results are linear from 0.2 to 1.5 mg at $\lambda = 1712.8$ cm^{-1} and 0.2 to 1.3 mg at $\lambda = 1730.9$ cm^{-1}. The preferred absorption peak for quantitative measurements is at $\lambda = 1730.9$ cm^{-1}, since many substances interfere more strongly at the lower wave number carbonyl peak. Common diluents such as mannitol, lactose, and glucose do not interfere at either of the two carbonyl absorption peaks. Starch has a broadband absorption in this region but its error contribution is reduced to insignificant in the baseline corrected absorbance spectrum by forcing the baseline at $\lambda = 1850$ cm^{-1}.

Procaine · HCl, a common additive in cocaine samples, has an absorbance contribution at $\lambda = 1730.9$ cm^{-1} caused by the shoulder of the carbonyl peak at $\lambda = 1697$ cm^{-1} which could cause an error as large as 2.5% absolute if no corrections are made for it (see Fig. 5). One method of correcting for the procaine · HCl absorbance contribution is to subtract it mathematically from the spectrum, a feature available on many FTIR instruments. An alternate method is to choose absorption peaks of procaine · HCl that are relatively free of contributions from the cocaine · HCl such as at $\lambda = 1697$ and at $\lambda = 3212$ cm^{-1} and plot the absorbance of these peaks versus procaine · HCl concentration. On the same graph, a plot is made of the absorbance at $\lambda = 1730.9$ cm^{-1} versus procaine · HCl concentration as

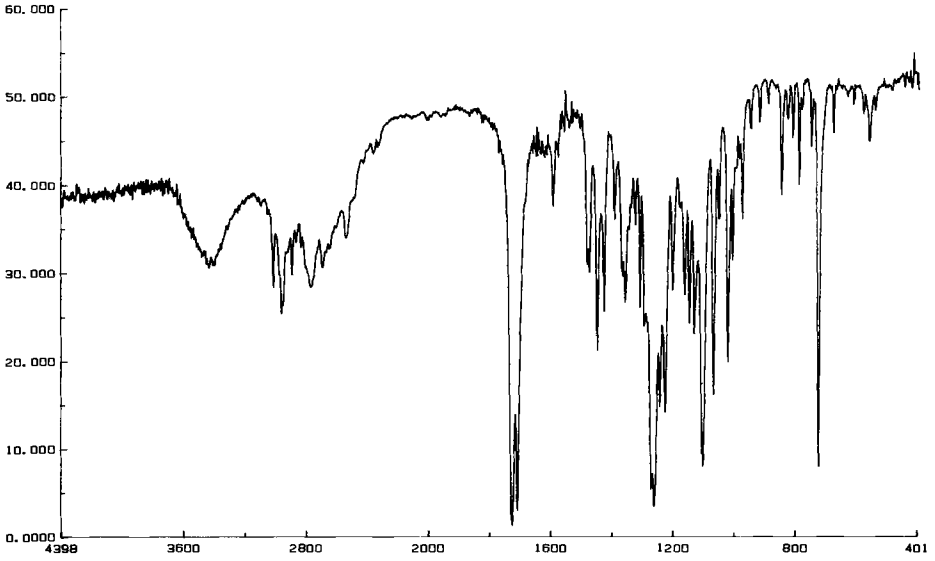

FIG. 1—*Transmission spectrum of cocaine · HCl.*

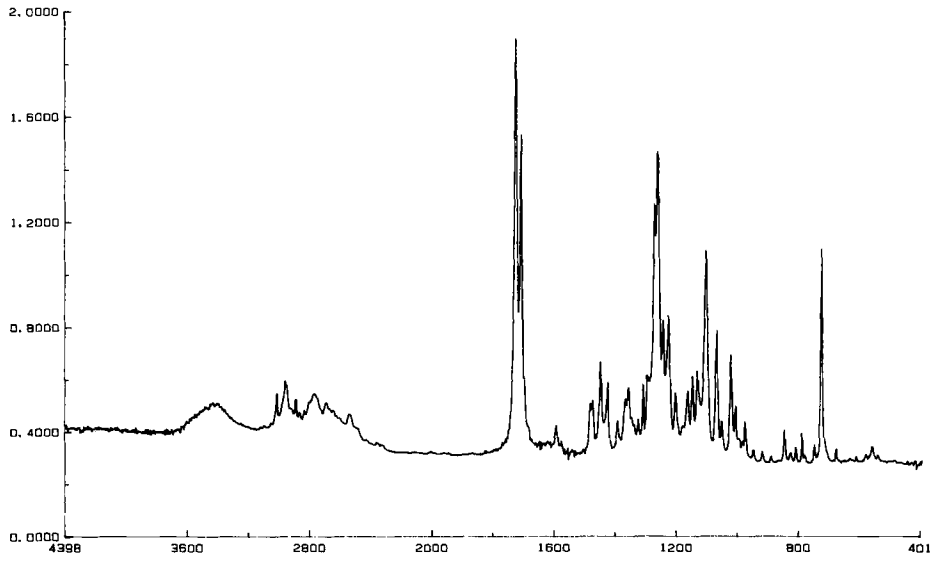

FIG. 2—*Absorbance spectrum of cocaine · HCl.*

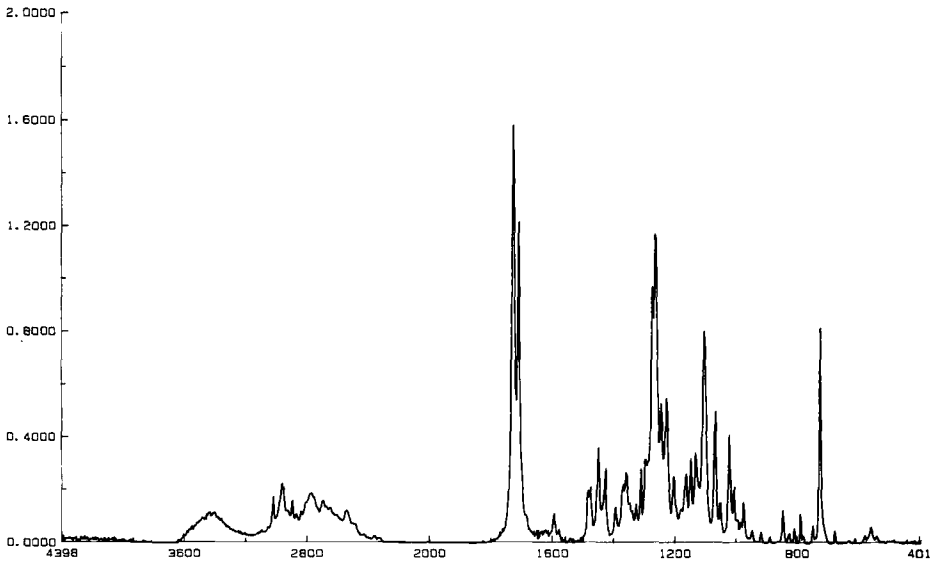

FIG. 3—*Baseline corrected absorbance spectrum of cocaine · HCl.*

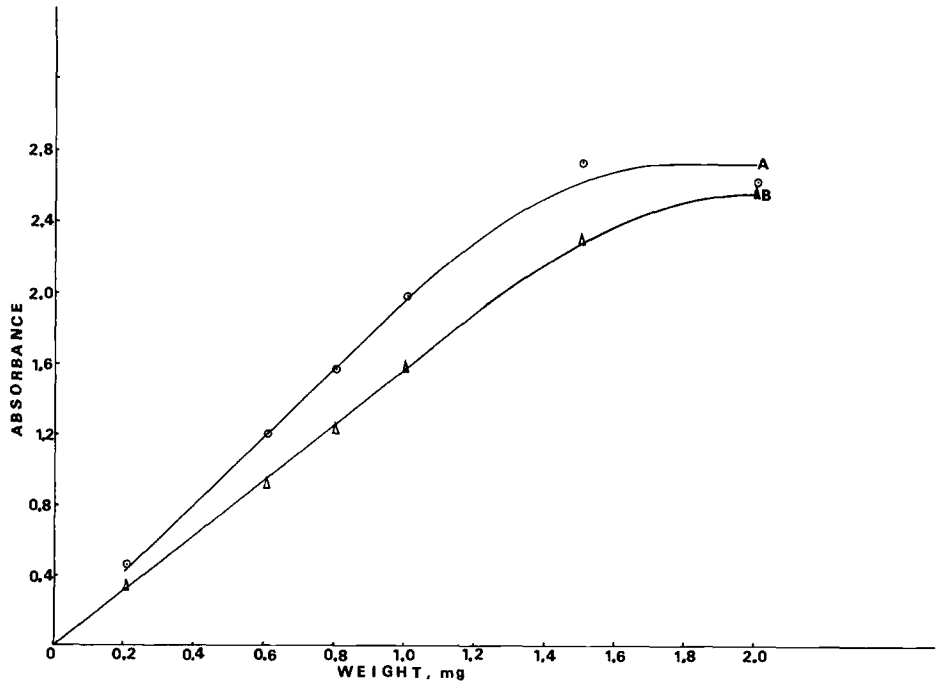

FIG. 4—*Absorbance versus weight of cocaine · HCl at:* a $\lambda = 1730.9\ cm^{-1}$ *and* b $\lambda = 1712.8\ cm^{-1}$.

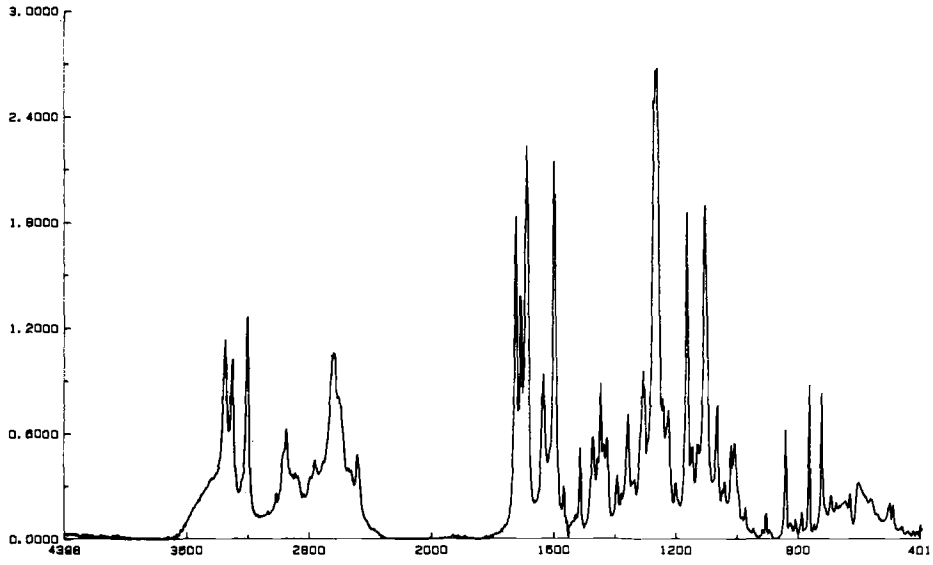

FIG. 5—*Baseline corrected absorbance spectrum of a mixture of cocaine · HCl and procaine · HCl.*

shown in Fig. 6. Since the slope of the line at $\lambda = 1730.9$ cm^{-1} is relatively flat, maximum accuracy of the procaine · HCl concentration is not necessary to provide an adequate correction factor.

A summary of the results obtained from various synthetic cocaine · HCl mixtures are in Table 1. The relative mean value is 99.16% with a standard deviation of ±7.5%.

Mixtures of cocaine · HCl and cocaine base were also investigated. A shift in the carbonyl absorption maxima occurs in cocaine base to $\lambda = 1736.0$ cm^{-1} and $\lambda = 1710.3$ cm^{-1} (see Fig. 7). A plot of absorbance versus concentration at $\lambda = 1736.0$ and $\lambda = 1710.3$ cm^{-1} is in Fig. 8. The results are linear from 0.2 to 1.0 mg. In mixtures containing cocaine · HCl:cocaine base in the ratios of 3:1, 2:1, and 1:1, good quantitative results were obtained from the absorbance values at $\lambda = 1712.8$ cm^{-1}. However, in mixtures containing cocaine base:cocaine · HCl in the ratios of 3:1 and 2:1, unsatisfactory quantitative results were obtained from the absorbance values at $\lambda = 1710.3$ or $\lambda = 1736.0$ cm^{-1} (see Table 2).

A probable explanation for these results may be found by examining the qualitative shape of the carbonyl absorption peaks (see Figs. 7 and 9). The carbonyl peaks at 1712.8 and 1710.3 cm^{-1} are clearly asymmetric with a higher slope value at the lower wave number side of the peak maximum. Thus, adding cocaine base to a sample containing predominantly cocaine · HCl would cause a band broadening on the lower wave number side from the maximum of the cocaine · HCl peak with perhaps a shoulder effect. It would also have a significant absorbance additive factor at the peak maximum itself of cocaine · HCl since this is on the side of the lower slope value for cocaine base. The reverse situation is exactly the opposite. Adding cocaine · HCl to a sample containing predominantly cocaine base would primarily cause a peak broadening of the maximum from cocaine base since the higher slope side from the cocaine · HCl peak is being added to the lower slope side of the cocaine base. It would have a less significant absorbance additive factor at the peak maximum of cocaine base since this is on the side of the higher slope value for cocaine · HCl. This is indeed the situation that exists in Fig. 9*b* and *c*.

Further examination of the carbonyl band region shows the presence of additional doublets and shoulders in mixtures of cocaine · HCl and cocaine base (see Fig. 9). In a 1:1

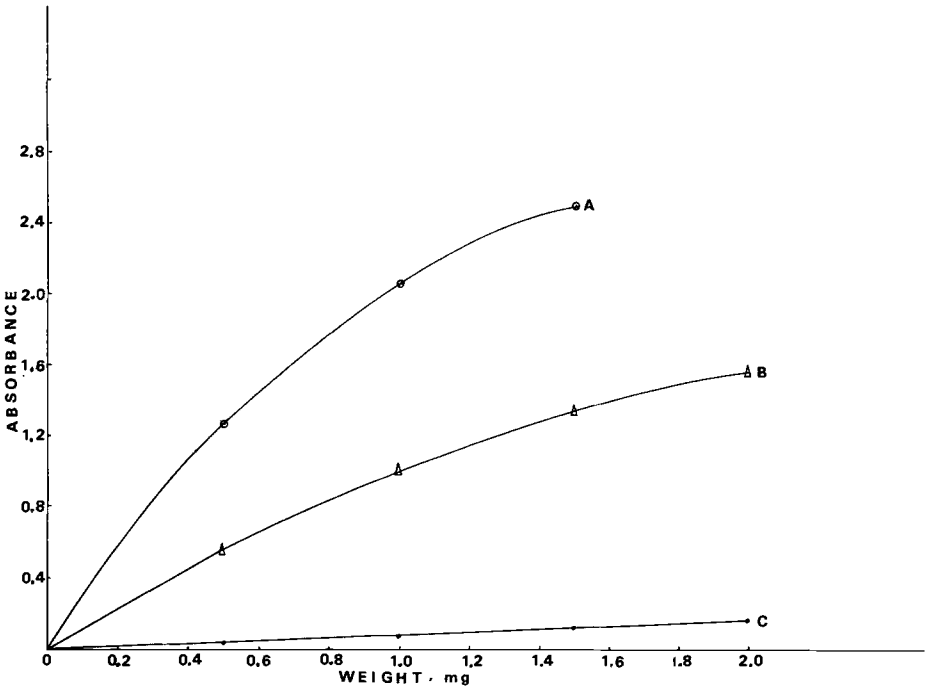

FIG. 6—*Absorbance versus weight of procaine · HCl at:* a $\lambda = 1697$, b $\lambda = 3212$, *and* c $\lambda = 1730.9$ cm^{-1}.

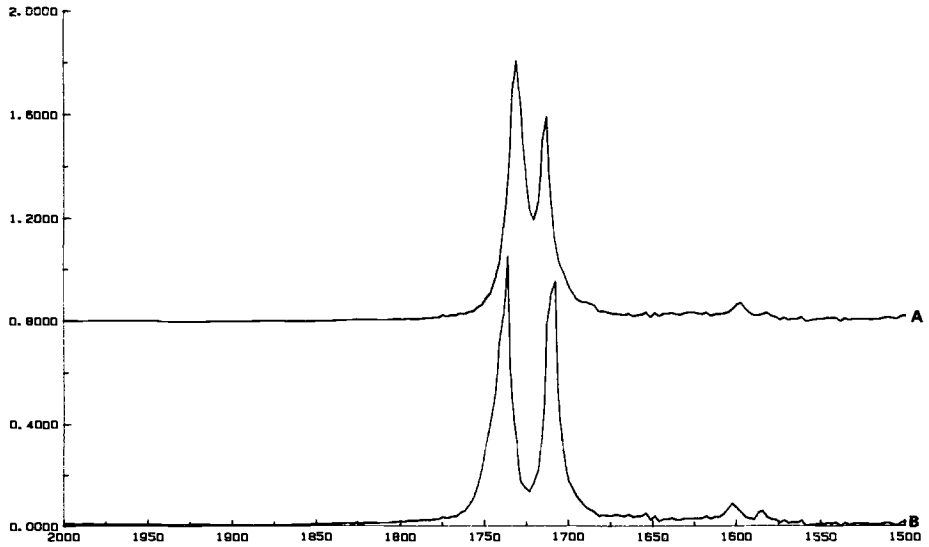

FIG. 7—*Absorbance spectra of carbonyl region for:* a *cocaine · HCl and* b *cocaine base.*

TABLE 1—*Cocaine · HCl determinations by absorbance at* $\lambda = 1730.9\ cm^{-1}$ *in synthetic mixtures.*

No.	Sample	mg Cocaine HCl Found	% Error
1	1.000-mg cocaine · HCl + 1.000-mg mannitol	0.956	−4.4
2	1.000-mg cocaine · HCl + 1.000-mg starch	0.941	−5.9
3	0.800-mg cocaine · HCl + 1.200-mg procaine HCl	0.862	+7.8

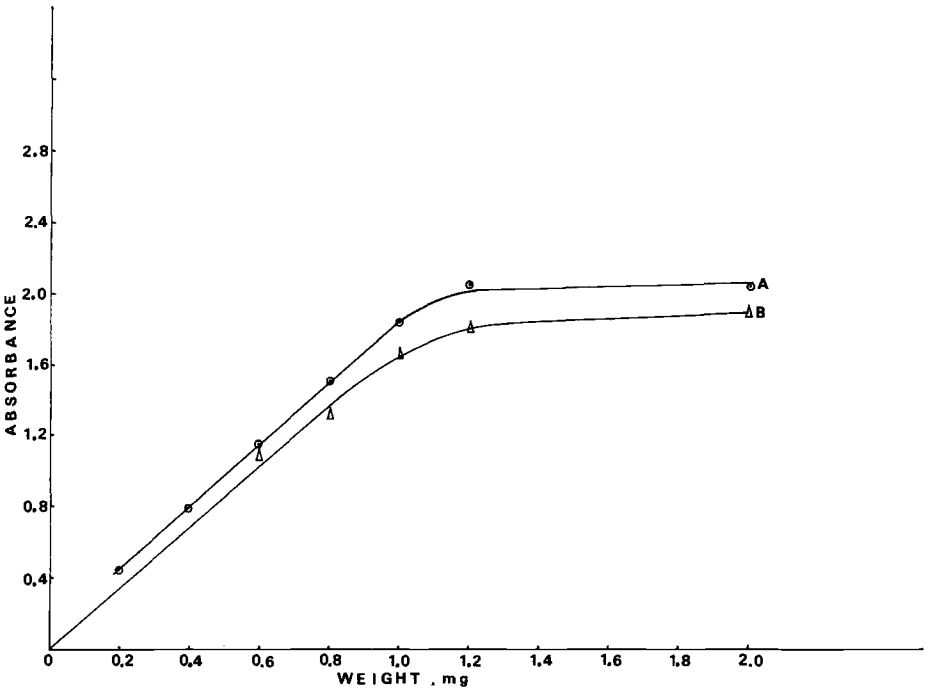

FIG. 8—*Absorbance versus weight of cocaine base at:* a $\lambda = 1736.0$ *and* b $\lambda = 1710.3\ cm^{-1}$.

mixture of cocaine · HCl and cocaine base, a doublet is clearly visible at $\lambda = 1736.0$ and 1730.9 cm^{-1} and a singlet occurs at $\lambda = 1712.8\ cm^{-1}$ (see Fig. 9*a*). In a 2:1 mixture of cocaine base:cocaine · HCl, an absorption maximum occurs at 1736.0 cm^{-1} with a shoulder at 1730.9 cm^{-1} followed by a broad absorption peak with a maximum at 1710.3 cm^{-1} (see Fig. 9*c*). In a 2:1 mixture of cocaine · HCl:cocaine base, two sharp absorption peaks occur at $\lambda = 1730.9$ and $\lambda = 1712.8\ cm^{-1}$ with indications of a shoulder in the region $\lambda = 1710.8\ cm^{-1}$ (see Fig. 9*b*). Attempts to correct the results in mixtures containing predominantly cocaine base by subtracting the cocaine · HCl contribution at $\lambda = 1736.0\ cm^{-1}$ were also unsatisfactory since the slope of the correction factor is not flat. This would require an initial accurate estimate of the cocaine · HCl concentration which is not available since the absorbance of the shoulder at $\lambda = 1730.9\ cm^{-1}$ has a large contribution from the cocaine base peak at $\lambda = 1736.0\ cm^{-1}$.

A different approach was tried, namely, area integration of the carbonyl band region from $\lambda = 1680$ to $\lambda = 1780\ cm^{-1}$. This is a standard feature on the FTIR instrument where the

TABLE 2—*Analysis of synthetic mixtures of cocaine HCl and cocaine base by absorbance.*

No.	Sample	mg Cocaine Theoretical as		Uncorrected					Corrected	
		Cocaine · HCl	Cocaine Base	λ = 1736.0 cm^{-1}	λ = 1730.9 cm^{-1}	λ = 1712.8 cm^{-1}	% Error	λ = 1710.3 cm^{-1}	λ = 1736.0 cm^{-1}	λ = 1730.9 cm^{-1}
1	0.600-mg cocaine base + 0.200-mg cocaine · HCl	0.872	0.779	0.700 mg as cocaine base	. . .	0.720 mg as cocaine · HCl	−17.4	0.680 mg as cocaine base	. . .	. . .
2	0.600-mg cocaine base + 0.300-mg cocaine · HCl	0.972	0.868	0.700 mg as cocaine base	. . .	0.800 mg as cocaine · HCl	−17.7	0.760 mg as cocaine base	0.380 mg as cocaine base	0.220 mg as cocaine · HCl
3	0.400-mg cocaine base + 0.400-mg cocaine · HCl	0.848	0.757	0.620 mg as cocaine base	0.600 mg as cocaine · HCl	0.800 mg as cocaine · HCl	−5.7	0.640 mg as cocaine base	0.260 mg as cocaine base	0.420 mg as cocaine · HCl
4	0.300-mg cocaine base + 0.600-mg cocaine · HCl	0.936	0.836	. . .	0.660 mg as cocaine · HCl	0.890 mg as cocaine · HCl	−4.9	. . .	. . .	. . .
5	0.200-mg cocaine base + 0.600-mg cocaine · HCl	0.824	0.736	. . .	0.780 mg as cocaine · HCl	0.800 mg as cocaine · HCl	−2.9	. . .	. . .	. . .

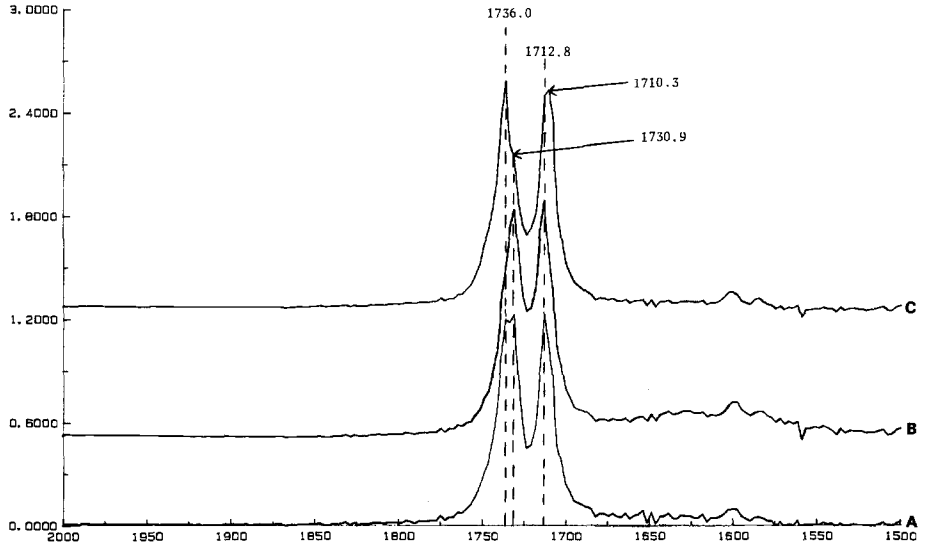

FIG. 9—*Absorbance spectra of carbonyl region of mixtures of cocaine · HCl and cocaine base:* a *1:1 cocaine · HCl:cocaine base,* b *2:1 cocaine · HCl:cocaine base,* c *2:1 cocaine base:cocaine · HCl.*

operator chooses the minimum and maximum wavelength over which the integration is to be performed and a baseline is drawn from the intersection of the cursors with the absorbance spectrum. A plot of net area versus concentration for cocaine · HCl and cocaine base is in Fig. 10. The appropriate calibration curve was chosen based on the wave number of the peak heights indicating that the major component was the free base or the hydrochloride salt. Results are summarized in Table 3. The relative mean value is 100.6% with a standard deviation of ±5.4%.

Heroin · HCl has two strong carbonyl absorption peaks at $\lambda = 1763.0$ and $\lambda = 1736.0$ cm^{-1}. The spectra recorded as a transmission spectrum, absorbance spectrum, and baseline corrected absorbance spectrum are in Figs. 11, 12, and 13. A plot of absorbance, from the baseline corrected spectra versus concentration at $\lambda = 1763.0$ and $\lambda = 1736.0$ cm^{-1}, is in Fig. 14. The results are linear from 0.2 to 2.0 mg at both wave numbers. The preferred wave number for quantitative determinations is at $\lambda = 1763.0$ cm^{-1} since some common additives, diluents, and impurities have a significant absorbance at wave numbers slightly lower than this. There is no significant interference from common diluents such as mannitol, lactose, and glucose or from impurities such as morphine and codeine at $\lambda = 1763.0$ and $\lambda = 1736.0$ cm^{-1}. A judicious selection of the baseline eliminates any significant interference from broadband absorption of starch at $\lambda = 1763.0$ cm^{-1}. Procaine · HCl does not constitute an interference at $\lambda = 1763.0$ cm^{-1} but does have a significant absorbance at $\lambda = 1736.0$ cm^{-1}.

Caffeine, a common additive in heroin samples, has an appreciable absorbance at $\lambda = 1763.0$ cm^{-1} and an even larger absorbance at $\lambda = 1736.0$ cm^{-1} as a result of the shoulder from the carbonyl peak at $\lambda = 1690$ cm^{-1}. It can be corrected based on the absorbance ratio of a caffeine peak relatively free of absorbance interferences from heroin, such as at $\lambda = 1548.2$ cm^{-1}, to the absorbance value at 1763.0 cm^{-1} (see Fig. 15). The slope of the line at $\lambda = 1763.0$ cm^{-1} is flat up to a concentration of 1.7-mg caffeine and then the slope starts to increase rapidly because of the effect of band broadening of the caffeine carbonyl peak at $\lambda = 1690$ cm^{-1}. Over the caffeine concentration range of the relatively flat slope at $\lambda = 1763$

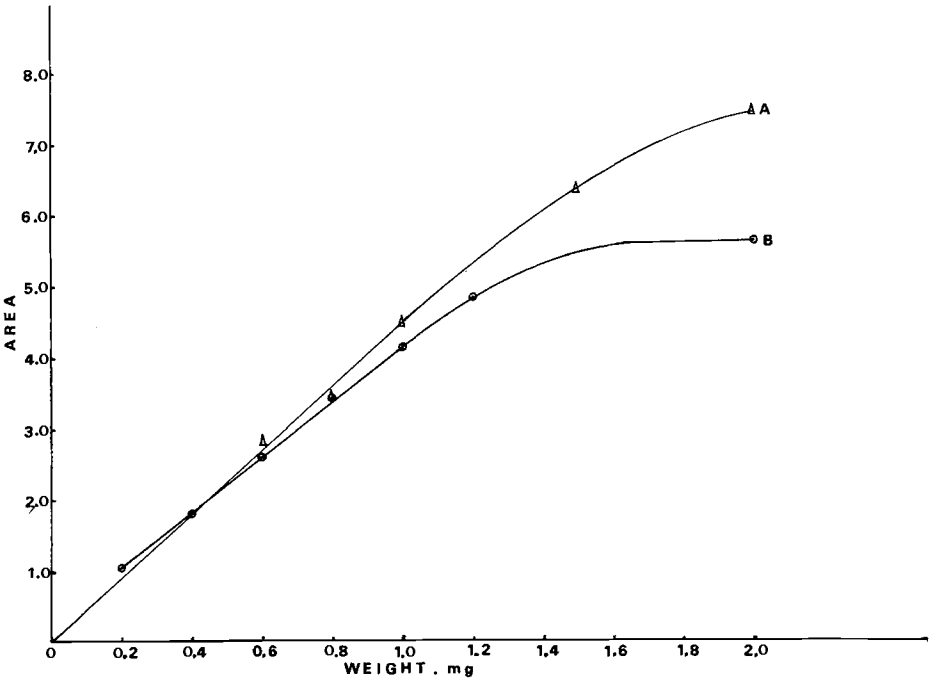

FIG. 10—*Area from* $\lambda = 1680$ *to* $1780\ cm^{-1}$ *versus weight for:* a *cocaine · HCl and* b *cocaine base.*

TABLE 3—*Analysis of synthetic mixtures of cocaine base and cocaine · HCl by area integration from* $\lambda = 1680$ *to* $1780\ cm^{-1}$.

No.	Sample	% Cocaine Found	% Cocaine Theoretical	% Error
1	0.600-mg cocaine base + 0.200-mg cocaine · HCl	0.832 mg as cocaine base	0.779 mg as cocaine base	+6.8
2	0.600-mg cocaine base + 0.300-mg cocaine · HCl	0.900 mg as cocaine base	0.868 mg as cocaine base	+3.7
3	0.400-mg cocaine base + 0.400-mg cocaine · HCl	0.837 mg as cocaine · HCl	0.848 mg as cocaine · HCl	−1.3
4	0.300-mg cocaine base + 0.600-mg cocaine · HCl	0.866 mg as cocaine · HCl	0.936 mg as cocaine · HCl	−7.5
5	0.200-mg cocaine base + 0.600-mg cocaine · HCl	0.835 mg as cocaine · HCl	0.824 mg as cocaine · HCl	+1.3

cm^{-1} an approximate estimate of the caffeine concentration from the absorbance value at $\lambda = 1548.2\ cm^{-1}$ provides an adequate correction factor. In a four-component mixture containing heroin · HCl, caffeine, starch, and lactose (see Fig. 16) and only requiring a correction factor as a result of the caffeine, very good results were obtained (see Table 4).

Acetylcodeine and o^6-monoacetylmorphine both have a very strong absorbance peak near $\lambda = 1736.0\ cm^{-1}$ with a much weaker absorbance at $\lambda = 1763.0\ cm^{-1}$ because of a shoulder effect. Acetylcodeine has an absorbance at $\lambda = 1763.0\ cm^{-1}$ ranging from 0.03 to 0.05 when present in concentrations ranging from 0.5 to 1.5 mg of acetylcodeine in a 100-mg KBr pel-

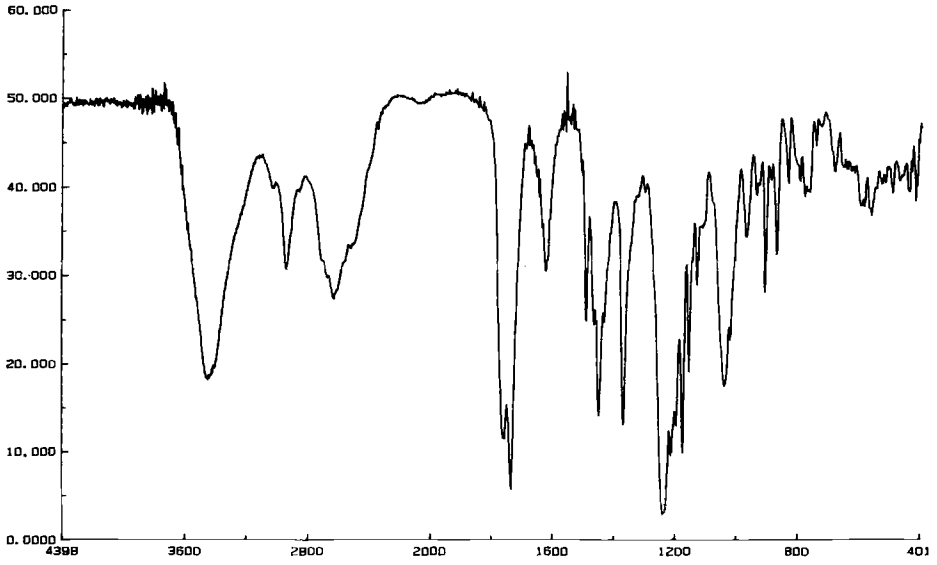

FIG. 11—*Transmission spectrum of heroin · HCl.*

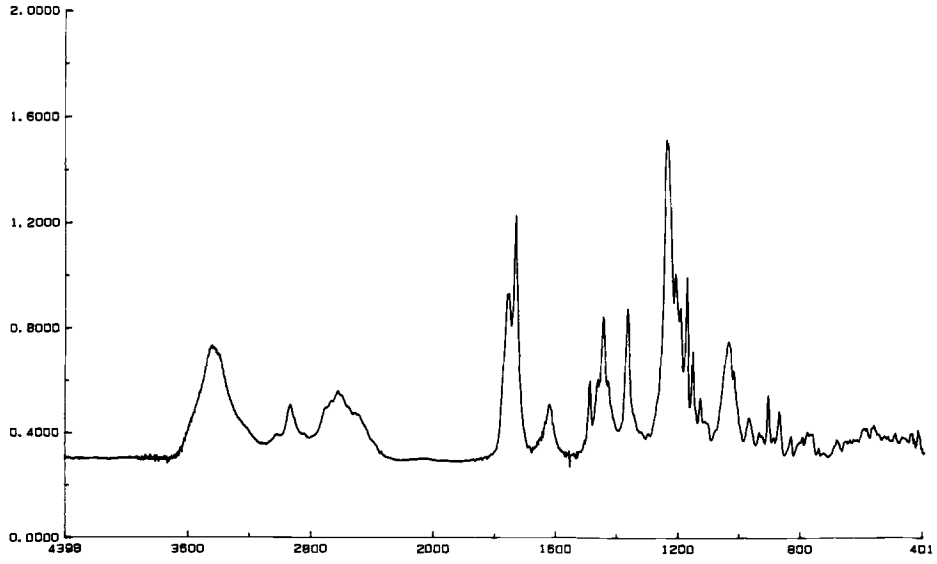

FIG. 12—*Absorbance spectrum of heroin · HCl.*

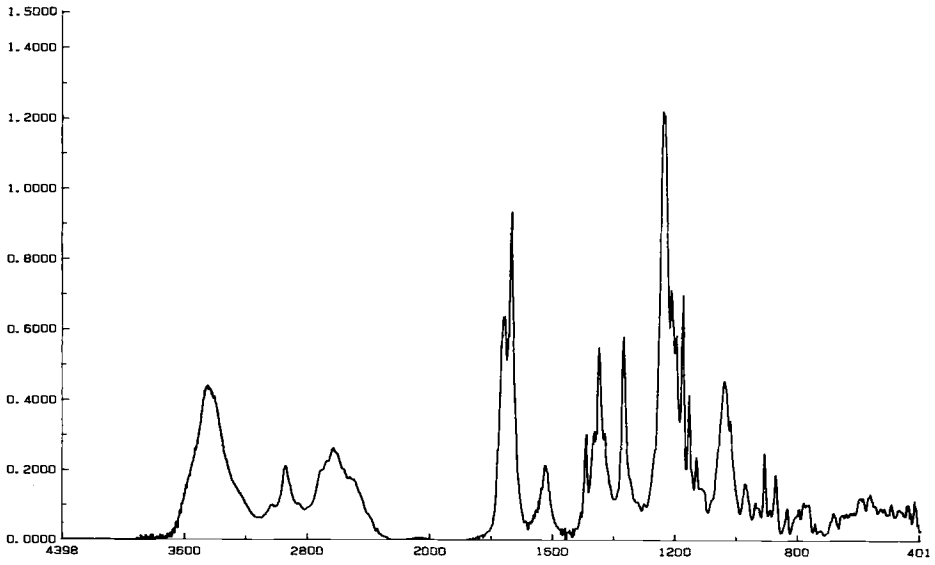

FIG. 13—*Baseline corrected absorbance spectrum of heroin · HCl.*

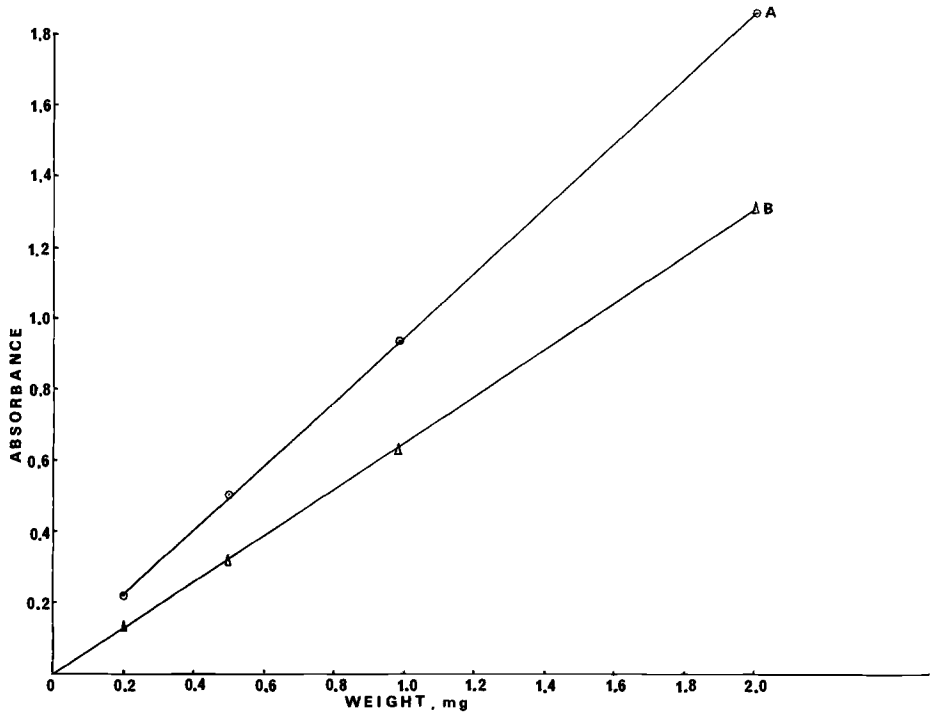

FIG. 14—*Absorbance versus weight of heroin · HCl at:* a $\lambda = 1736.0$ *and* b $\lambda = 1763.0\ cm^{-1}$.

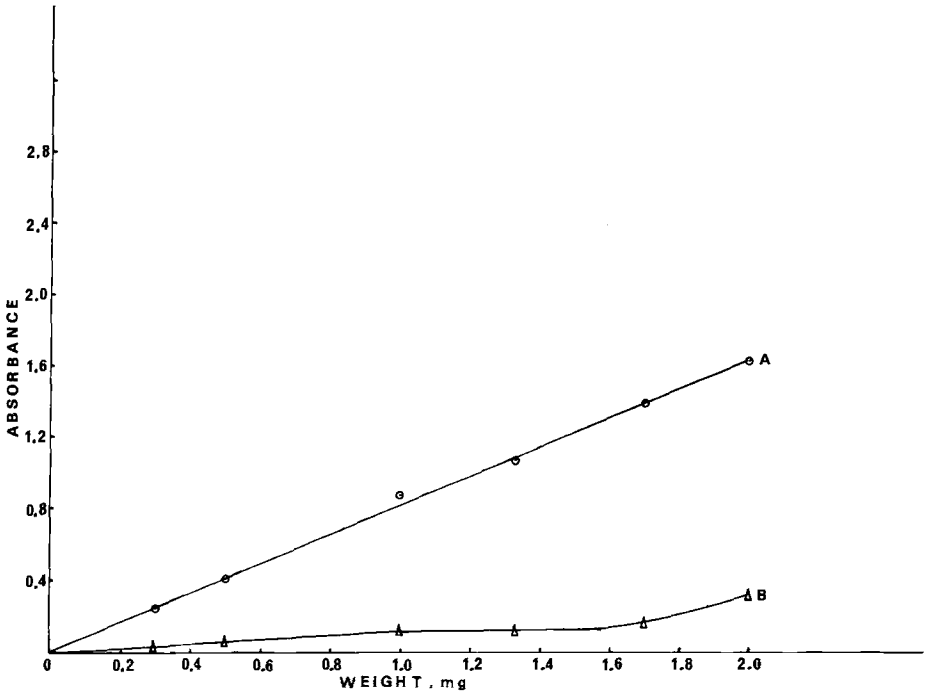

FIG. 15—*Absorbance versus weight of caffeine at:* a $\lambda = 1548.2$ *and* b $\lambda = 1763\ cm^{-1}$.

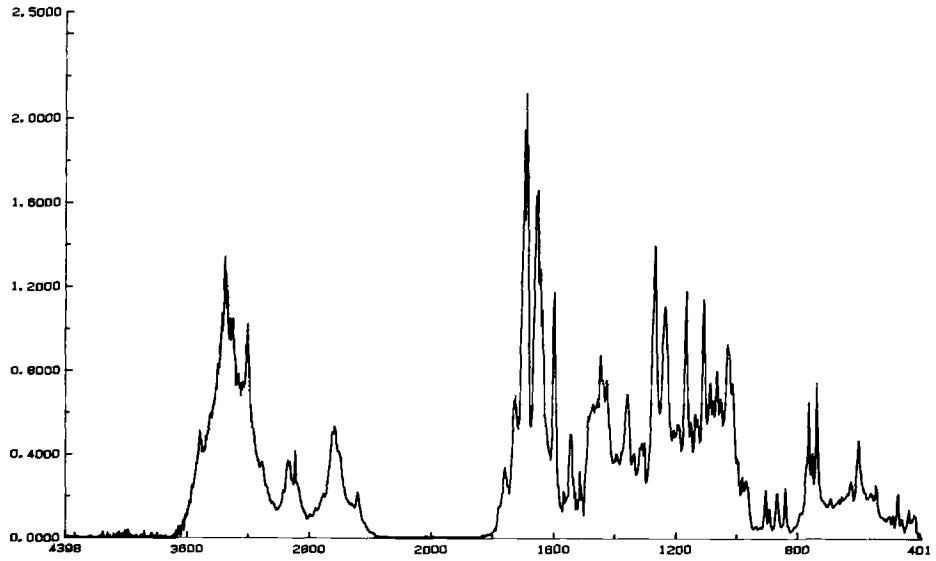

FIG. 16—*Baseline corrected absorbance spectrum of a mixture containing 25% each heroin · HCl, caffeine, starch, and lactose.*

TABLE 4—*Heroin · HCl determinations by absorbance at* $\lambda = 1763.0\ cm^{-1}$ *in synthetic mixtures.*

No.	Sample	mg Heroin HCl Found	% Error
1	1.000-mg heroin · HCl + 1.000-mg caffeine	1.040	+4.0
2	0.667-mg heroin · HCl + 1.333-mg caffeine	0.682	+2.4
3	0.500-mg heroin · HCl + 0.500-mg caffeine + 1.000-mg procaine · HCl	0.479	−4.0
4	0.400-mg heroin · HCl + 1.600-mg lactose	0.426	+6.5
5	1.000-mg heroin · HCl + 1.000-mg starch	1.006	+0.6
6	0.800-mg heroin · HCl + 0.600-mg caffeine + 0.600-mg lactose	0.828	+3.5
7	0.500-mg heroin · HCl + 0.500-mg caffeine + 0.500-mg procaine HCl + 0.500-mg lactose	0.498	−0.4
8	1.200-mg heroin · HCl + 0.400-mg procaine · HCl + 0.400-mg starch	1.215	+1.3
9	1.000-mg heroin · HCl + 1.000-mg o^6-monoacetylmorphine	0.961	−3.9
10	1.000-mg heroin · HCl + 1.000-mg acetylcodeine	0.987	−1.3

let. This can be corrected for by subtracting the heroin spectrum from the mixture and then measuring the absorbance at $\lambda = 1733.4$ or $\lambda = 1237.1\ cm^{-1}$ to give an approximate estimate of the acetylcodeine concentration. The absorbance ratio at $\lambda = 1763.0\ cm^{-1}$ to either of the above two peaks can then be used to determine the appropriate correction factor to be subtracted from the mixture at $\lambda = 1763.0\ cm^{-1}$. In a similar manner, corrections can be made for absorbance contributions at $\lambda = 1763.0\ cm^{-1}$ as a result of o^6-monoacetylmorphine, using the absorbance values at $\lambda = 1733.4$ or $\lambda = 1242.3\ cm^{-1}$ to estimate the o^6-monoacetylmorphine concentration on the spectrum obtained after subtracting the heroin. Table 4 summarizes the results of various synthetic mixtures containing heroin · HCl. The relative mean value is 100.9% with a standard deviation of ±3.4%.

Mixtures of heroin · HCl and heroin base were also investigated. A shift in the carbonyl doublet occurs in heroin base to $\lambda = 1756.6$ and $\lambda = 1728.3\ cm^{-1}$. A plot of absorbance versus heroin base concentration at $\lambda = 1756.6$ and $\lambda = 1728.3\ cm^{-1}$ is illustrated in Fig. 17. The results are linear from 0.2 to 1.5 mg. A close examination of the carbonyl region of pure heroin · HCl and pure heroin base reveals that the main doublet is further resolved into additional doublets or shoulders or both (see Fig. 18). In pure heroin · HCl, a doublet occurs at $\lambda = 1764.3$ and $\lambda = 1759.1\ cm^{-1}$ followed by a singlet at $\lambda = 1736.0\ cm^{-1}$. In pure heroin base, an absorbance maximum occurs at $\lambda = 1756.6\ cm^{-1}$ with a pronounced shoulder at $\lambda = 1763.0\ cm^{-1}$ and a singlet at $\lambda = 1728.3\ cm^{-1}$.

Synthetic mixtures were prepared containing heroin · HCl:heroin base in the ratios of 3:1, 2:1, and 1:1 and heroin base:heroin · HCl in the ratios of 3:1 and 2:1. A close examination of the main carbonyl doublet reveals additional doublets and shoulders in these mixtures (see Fig. 19). In a 2:1 mixture of heroin base:heroin · HCl, a doublet occurs at $\lambda = 1764.3$ and $\lambda = 1759.1\ cm^{-1}$. An additional peak maximum occurs at $\lambda = 1731.8\ cm^{-1}$ with a shoulder at $\lambda = 1738.6\ cm^{-1}$ (see Fig. 19*a*). In a 1:1 mixture of heroin · HCl:heroin base, similar doublets and shoulders exist (see Fig. 19*b*). In a 2:1 mixture of heroin · HCl:heroin base, a doublet also occurs at $\lambda = 1764.3$ and $\lambda = 1759.1\ cm^{-1}$ followed by a peak maximum at $\lambda = 1736.0\ cm^{-1}$ with a shoulder at $\lambda = 1731.5\ cm^{-1}$ (see Fig. 19*c*). In all three mixtures, the maximum absorbance of the higher wave number main carbonyl doublet is at $1759.1\ cm^{-1}$. The best quantitative results based on absorbance values at a given wavelength were those obtained at $\lambda = 1759.1\ cm^{-1}$ (see Table 5). The relative mean value is 100.4% with a standard deviation of ±5.2%. Attempting to determine the individual heroin base and heroin · HCl content by subtracting absorbance contributions of one to the other did not appear to be a feasible approach.

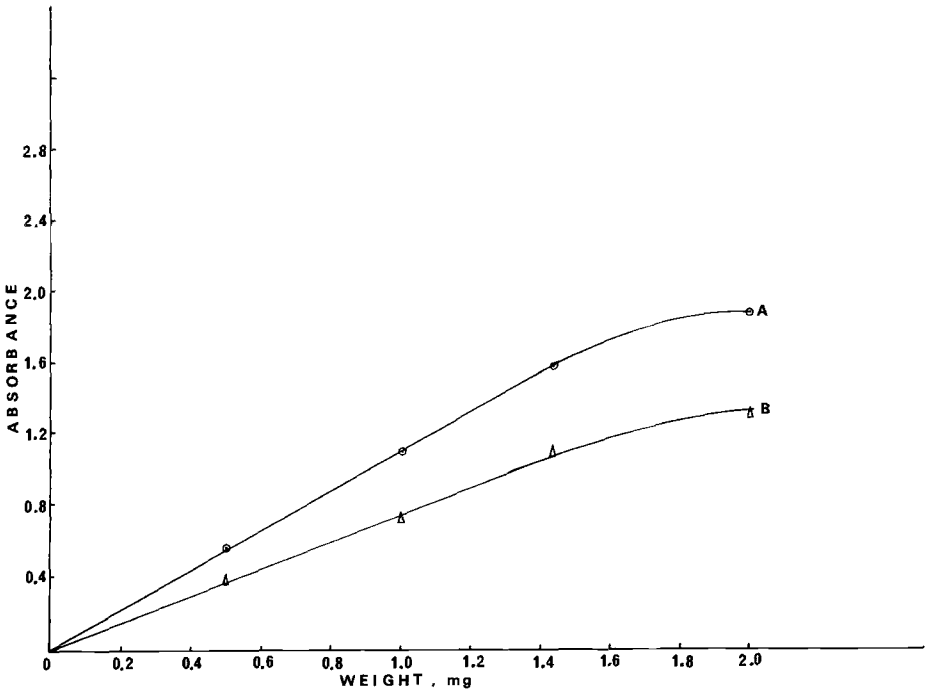

FIG. 17—*Absorbance versus weight of heroin base at:* a $\lambda = 1728.3$ *and* b $\lambda = 1756.6\ cm^{-1}$.

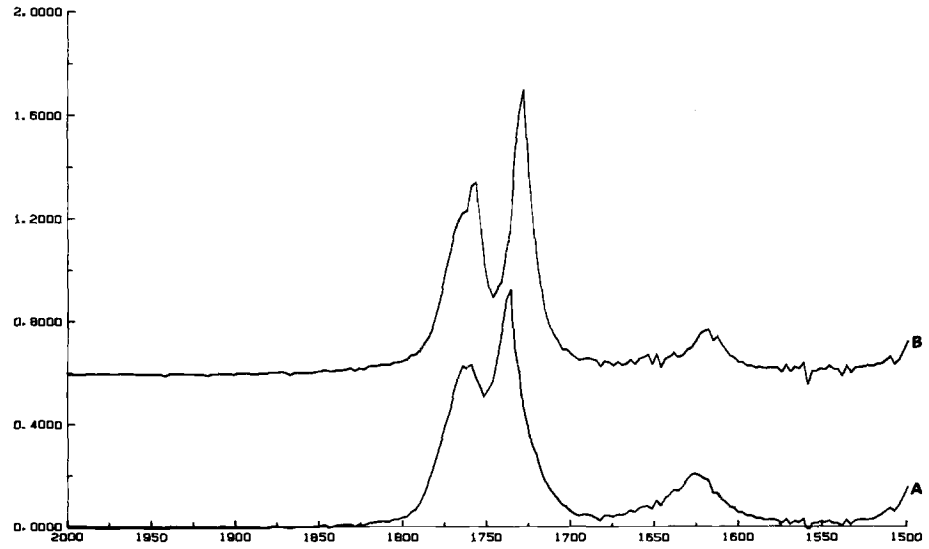

FIG. 18—*Absorbance spectra of carbonyl region for:* a *heroin · HCl, and* b *heroin base.*

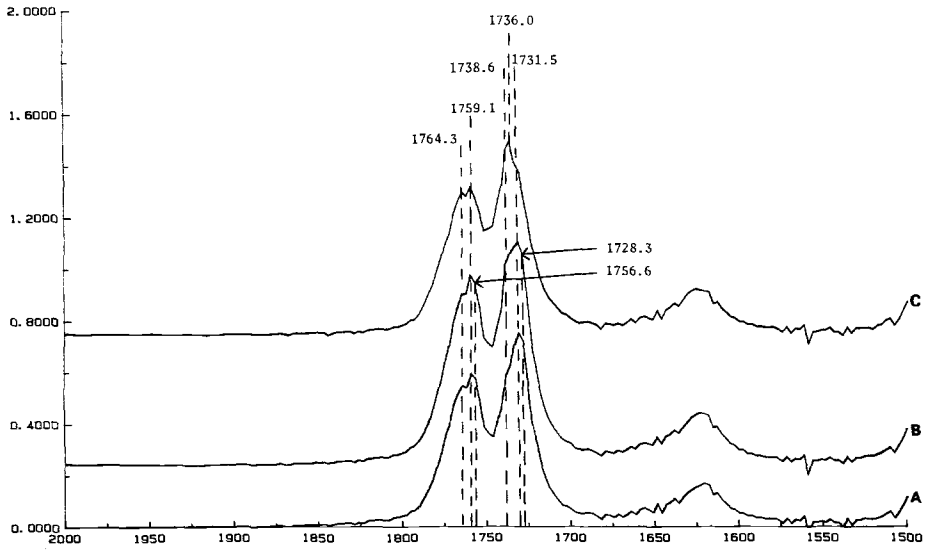

FIG. 19—*Absorbance spectra of carbonyl region of mixtures of heroin · HCl and heroin base:* a *2:1 heroin base:heroin · HCl,* b *1:1 heroin · HCl:heroin base, and* c *2:1 heroin · HCl:heroin base.*

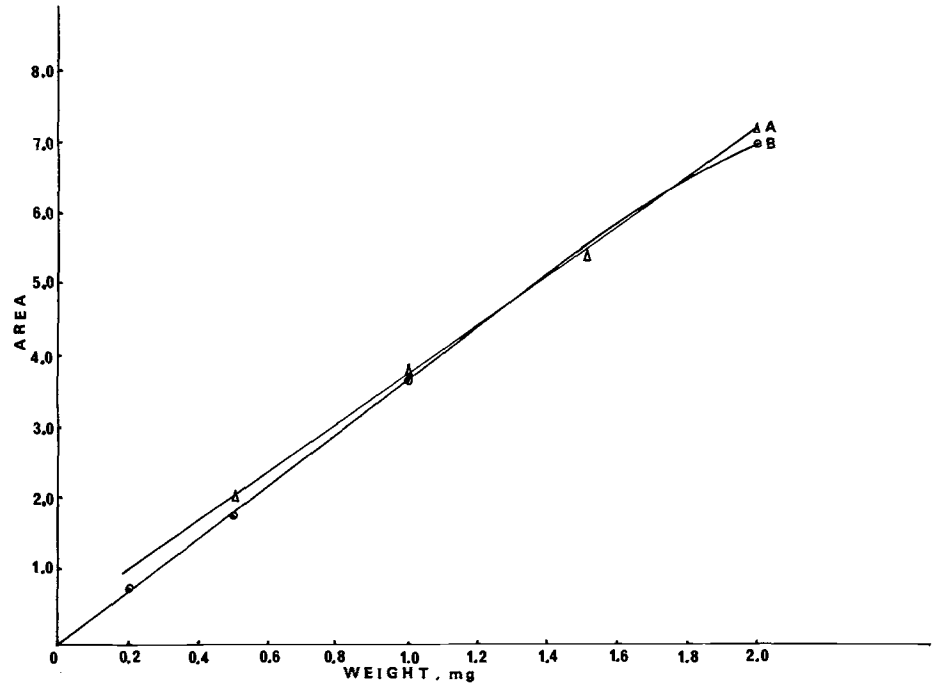

FIG. 20—*Area from* $\lambda = 1675$ *to* $1825\ cm^{-1}$ *versus weight for:* a *heroin base and* b *heroin · HCl.*

TABLE 5—*Analysis of synthetic mixtures of heroin HCl and heroin base by absorbance.*

No.	Sample	mg Heroin Theoretical as		1764.3 cm^{-1}	% Error	1759.1 cm^{-1}	% Error	1756.6 cm^{-1}	1736.6 cm^{-1}	1728.3 cm^{-1}
		Heroin · HCl	Heroin Base							
1	0.600-mg heroin base + 0.200-mg heroin · HCl	0.859 mg	0.782 mg	0.740 mg as heroin · HCl	−13.9	0.850 mg as heroin · HCl	−1.0	0.710 mg as heroin base	. . .	0.650 mg as heroin base
2	0.600-mg heroin base + 0.300-mg heroin · HCl	0.959 mg	0.873 mg	0.830 mg as heroin · HCl	−13.5	0.940 mg as heroin · HCl	−2.0	0.750 mg as heroin base	. . .	0.680 mg as heroin base
3	0.500-mg heroin base + 0.500-mg heroin · HCl	1.050 mg	0.955 mg	1.000 mg as heroin · HCl	−4.8	1.150 mg as heroin · HCl	+9.5	. . .	. . .	. . .
4	0.300-mg heroin base + 0.600-mg heroin · HCl	0.930 mg	0.846 mg	0.830 mg as heroin · HCl	−10.7	0.900 mg as heroin · HCl	−3.2	. . .	0.750 mg as heroin · HCl	. . .
5	0.200-mg heroin base + 0.600-mg heroin · HCl	0.819 mg	0.746 mg	0.760 mg as heroin · HCl	−7.2	0.830 mg as heroin · HCl	+1.3	. . .	0.710 mg as heroin · HCl	. . .

TABLE 6—*Analysis of synthetic mixtures of heroin base and heroin · HCl by area integration from* $\lambda = 1675$ *to* $1825\ cm^{-1}$.

No.	Sample	% Heroin Found	% Heroin Theoretical	% Error
1	0.600-mg heroin base + 0.200-mg heroin · HCl	0.753 mg as heroin base	0.782 mg as heroin base	−3.7
2	0.600-mg heroin base + 0.300 mg heroin · HCl	0.853 mg as heroin base	0.873 mg as heroin base	−2.3
3	0.500-mg heroin base + 0.500-mg heroin · HCl	1.044 mg as heroin base	0.955 mg as heroin base	+9.3
4	0.300-mg heroin base + 0.600-mg heroin · HCl	0.881 mg as heroin HCl	0.930 mg as heroin · HCl	−5.3
5	0.200-mg heroin base + 0.600-mg heroin · HCl	0.800 mg as heroin HCl	0.819 mg as heroin · HCl	−2.3

Net area integration was calculated from $\lambda = 1675$ to $\lambda = 1825\ cm^{-1}$ on the mixture of heroin · HCl and heroin base. Calibration graphs of area versus concentration for heroin · HCl and heroin base are in Fig. 20. If an absorbance maximum occurred at $\lambda = 1736\ cm^{-1}$, the heroin · HCl calibration curve was used. If an absorbance maximum occurred at $\lambda = 1731$ or $\lambda = 1728\ cm^{-1}$, the heroin base calibration curve was used. Results are summarized in Table 6. The relative mean value is 99.14% with a standard deviation of ±5.8%.

Calibration curves are stable for at least a period of several months. If the infrared source is changed or any modifications are made in the electronic circuitry of the instrument to accommodate various accessories, the calibration curves should be rechecked as they might change. The average time for a quantitative determination is approximately 20 min.

Conclusions

Cocaine and heroin concentration can be determined quantitatively by measuring the intensity of the absorbance of the carbonyl peaks. Broadband absorbance interferences can sometimes be corrected for by a judicious selection of the baseline. Spectral interferences can be corrected for based on absorbance ratios with a noninterfering spectral line or alternatively by spectral subtraction of the interfering component. In mixtures containing the free base and the hydrochloride salt, the preferred method for quantitative determination is by net area integration of the carbonyl peaks.

Acknowledgments

The author wishes to express his appreciation to Dr. Arie Frank for technical assistance.

References

[*1*] Gough, T. A. and Baker, P. B., "Identification of Major Drugs of Abuse using Chromatography," *Journal of Chromatographic Science*, Vol. 20, July 1982, pp. 289-329.

[*2*] Bretell, T. A. and Saferstein, R., "Forensic Science," *Analytical Chemistry*, Vol. 57, No. 5, April 1985, pp. 175R-186R.

[*3*] Bretell, T. A. and Saferstein, R., "Forensic Science," *Analytical Chemistry*, Vol. 55, No. 5, April 1983, pp. 19R-31R.

[*4*] Mcdonald, R. S., "Review: Infrared Spectrometry," *Analytical Chemistry*, Vol. 54, No. 8, July 1982, pp. 1250-1275.

Address requests for reprints or additional information to
Mark Ravreby
Criminal Identification Division
National Police Headquarters
Jerusalem, Israel