RESEARCH ARTICLES

GAS CHROMATOGRAPHY- MASS SPECTROMETRY OF SOME VOLATILE METAL β- DIKETONATES

WANNA SRICHUANCHUENSKUL[a], MONGKON RAYANAKORN[b*], SURASAK WATANESK[b], PRASAK THAVORNYUTIKARN[b] AND PISAN KITSAWATPAIBOON[b]

[a] Department of Chemistry, Faculty of Science, Mahasarakham University, Mahasarakham 44000, Thailand.

[b] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

(Received November 21, 1994)

ABSTRACT

A gas chromatographic-mass spectrometric method was investigated for use in the study of the analytical characteristics of some volatile aluminium and chromium β-diketonates employing acetylacetone and trifluoroacetylacetone as ligands. Aluminium and chromium chelates were well separated on a fused silica capillary column of 25 m length and 0.20 mm i.d. Mass spectra, obtained via an electron impact ionization source with a quadrupole mass analyzer under normal operating conditions, yielded the unique base peak pattern corresponding to the loss of one ligand from the molecular ion. Chromium (III) as 1,1,1-trifluoroacetylacetonate complex alone exhibited a pair of chromatographic peaks which were found to produce nearly identical mass spectra, suggesting the existence of the chromium chelate as two geometrical isomers.

INTRODUCTION

Although a conceptual approach to the analysis of metal ions as metal chelates by gas chromatography was first described by Lederer[1] in 1955 and the mass spectrum of chromium acetylaceonate was first reported by McLafferty[2] in 1957, work on metal chelates by a combination of gas chromatography and mass spectrometry (GC-MS) did not appear in the literature until the late 1960's[3] due to difficulties involved in interfacing the two instruments. Early interfacial systems were generally used with packed columns[4] while methods for directly coupling capillary columns have just recently evolved along with concurrent improvements in high-speed turbo-molecular pumps and in capillary column manufacturing technology[5].

* To whom correspondence should be addressed.

In gas chromatographic studies of metal chelates up to the late 1980's, packed columns were generally employed with various detectors including a thermal conductivity detector[6,7], an electron capture detector[6,8-13] and a flame ionization detector[6, 13-19]. One of the pioneering works on chromium and beryllium chelates, reported in 1972, employed a mass spectromer as a GC detector together with a packed GC column[20]; the mass spectrometer had to be extensively modified. Since then, several workers have realized that GC-MS can provide positive corroborative identification for the minute amounts of materials detectable by flame-ionization and/or electron-capture gas chromatography and that this method holds great potential for ultra-trace analysis of metals in a wide variety of materials.

This work is an attempt to establish some GC-MS analytical characteristics of two trivalent metals, namely aluminium (III) and chromium (III) as some volatile metal chelates using pentan-2,4-dione (acetylacetone), H(AA), and 1,1,1-trifluoropentan-2,4-dione (trifluoroacetylacetone), H(TFA), as ligands since their compatibility with GC is already well established[6,13,19]. However, much of the previous work has been based on packed columns. The four metal chelates investigated in this study were aluminium acetylacetonate [$Al(AA)_3$], chromium acetylacetonate [$Cr(AA)_3$], aluminium trifluoroacetylacetonate [$Al(TFA)_3$] and chromium trifluoroacetylacetonate [$Cr(TFA)_3$] employing a capillary GC column and an electron impact ionization source with a quadrupole mass analyzer.

MATERIALS AND METHODS

Chemicals

All chemicals used were of analytical grade. Aluminium(III) nitrate 9-hydrate and chromium(III) nitrate 9-hydrate were obtained from E. Merck (Darmstadt, Germany) while H(AA) and H(TFA)) were obtained from Fluka Chemie A.G. (Buchs, Switzerland).

Preparation of metal chelates

$Al(AA)_3$ and $Cr(AA)_3$ were prepared using a modified Berg and Truemper[21] method in which 10 ml of a 1% w/v metal ion solution and 0.5 g sodium acetate were added together in a suitable separatory funnel and equilibrated with 5 ml of 50% v/v H(AA) in chloroform by mechanical shaking for 1 and 2 hours, respectively. After equilibration, the chloroform exract was removed from the separatory funnel and appropriate dilution with chloroform was made from this extract to yield the concentration of 20 mg/ml for $Al(AA)_3$ and 10 mg/ml for $Cr(AA)_3$. $Al(TFA)_3$ and $Cr(TFA)_3$ were prepared and diluted by a procedure similar to that for the metal acetylacetonates, the buffered metal ion solution being equilibrated with 5 cm^3 of 0.2 M H(TFA) in chloroform. The equilibration time for $Al(TFA)_3$ was 1 hour whilst that for $Cr(TFA)_3$ was 2 hours. The concentrations of these two metal chelates in the diluted solutions ready for GC injections were both 10 $\mu g/\mu l$. The extraction efficiency of each metal chelate and the sample loading capability of the capillary GC column were always taken into consideration in the dilution steps since all these four metal chelates exhibited different degrees of extraction efficiency[22].

Instrumentation

A benchtop gas chromatograph-mass spectrometer (Shimadzu Model QP2000A, Shimadzu Corporation, Kyoto, Japan) with an electron impact ionization source and quadrupole analyzers was used throughout this investigation. The GC-MS was run in the split mode with a Shimadzu CBP-1 column (25 m, 0.20 mm i.d., 0.25 mm film thickness). The operating conditions employed for $Al(AA)_3$ and $Cr(AA)_3$ were : GC injector temperature, 250°C; column temeperature, 170°C; MS ion source temperature, 250°C; helium carrier gas inlet pressure, 0.75 kg/cm^2. Similarly, the conditions for $Al(TFA)_3$ and $Cr(TFA)_3$ were : GC injector temperature, 225°C; column temperature, 150°C; MS ion source temperature: 250°C; helium carrier gas inlet pressure, 0.75 kg/cm^2. The sample volume introduced through the GC inlet system was usually 0.5 μl, corresponding to the concentration of 10 μg/μl for Al(AA)3 and 5 μg/μl for $Cr(AA)_3$, $Al(TFA)_3$ and $Cr(TFA)_3$. The excess chloroform solvent was prevented from entering the MS ion source by setting the solvent cut-off time up to 1.5 minutes. Fragment ions were produced by 70 eV electron ionization in the ion source heated to about 250°C.

RESULTS AND DISCUSSION

Unless otherwise stated, each set of the retention data reported here was based on at least three GC-MS runs which yielded the maximum relative error of 1.77% for $Al(AA)_3$, 0.90% for $Cr(AA)_3$, 1.50% for $Al(TFA)_3$, 1.85% for the first peak of $Cr(TFA)_3$ and 1.72% for the second peak of $Cr(TFA)_3$. The relative errors for mass spectral relative intensities were all well within the 2-3% range.

An injection of a mixture of $Al(AA)_3$ and $Cr(AA)_3$ yielded a total ion chromatogram (TIC) shown in Fig. 1 in which mass chromatograms (MCs) of mass 225 and 250 are also illustrated. It can be seen that an ion mass of 225 appears at the same position of the first peak in the TIC coinciding with the scan numbered 125 at retention time (R.T.) 5.66 minutes and that an ion mass of 250 appears at the same position of the second chromatographic peak at the scan numbered 288 at 11.10 minutes. Fig. 2 shows a TIC obtained from a mixture of $Al(TFA)_3$ and $Cr(TFA)_3$ together with mass chromatograms for mass 333 at 3.30 minutes (Scan No. 54) and mass 358 at 5.40 and 5.80 minutes (Scan Nos. 117 and 129).

Fig. 3 shows the relative intensities of characteristic peaks of the spectrum obtained from Scan No. 125 in Fig. 1 in parallel with those of the reference $Al(AA)_3$ spectrum obtained from the GC-MS library search software which is based on the NBS/NIH/EPA Mass Spectral Data Base containing mass spectra of 43,004 known compounds. Fig. 4 gives the relative intensities of characteristic peaks of the spectrum obtained from Scan No. 288 in Fig. 1 in comparison with those of the reference $Cr(AA)_3$ spectrum. Mass spectral data drawn from the chromatographic peak at R.T. 3.30 minutes (Scan No. 54, Fig. 2) alone are shown in Fig. 5 due to the fact that the library search software does not contain a mass spectrum of any metal chelate with a base peak at the mass-to-charge ratio (m/z) of 333. Furthermore, a detailed spectrum of $Al(TFA)_3$ has not yet become available in commonly used mass spectral compilations. Fig. 6 illustrates the relative intensities of characteristic peaks from

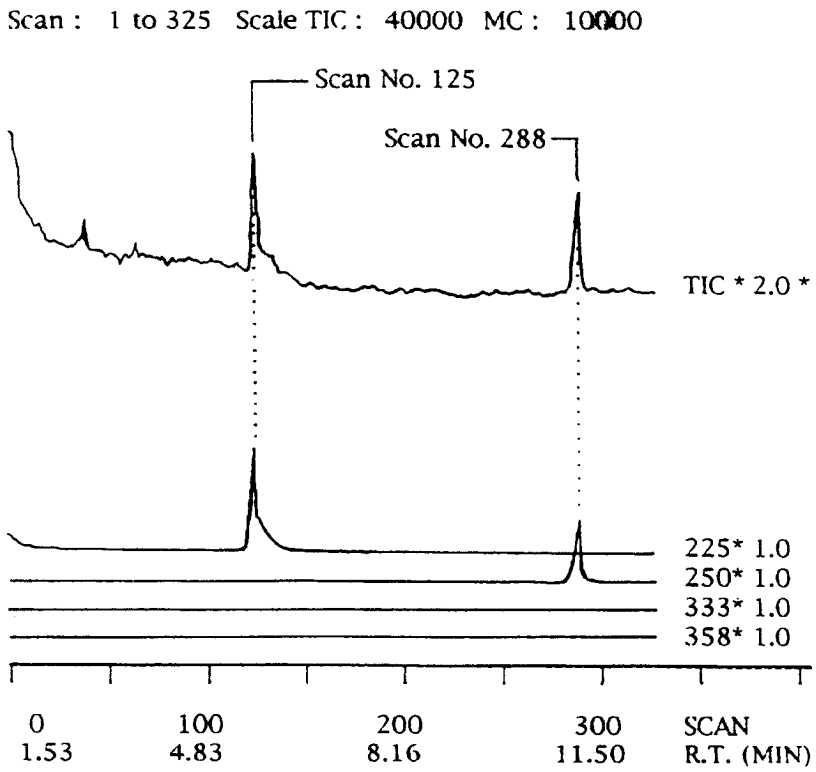

Fig. 1. Total ion chromatogram (TIC) obtained from a mixture of $Al(AA)_3$ (Scan No. 125, R.T. 5.66 min) and $Cr(AA)_3$ (Scan No. 288, R.T. 11.10 min) in comparison with two mass chromatograms (MCs) of mass 225 and 250.

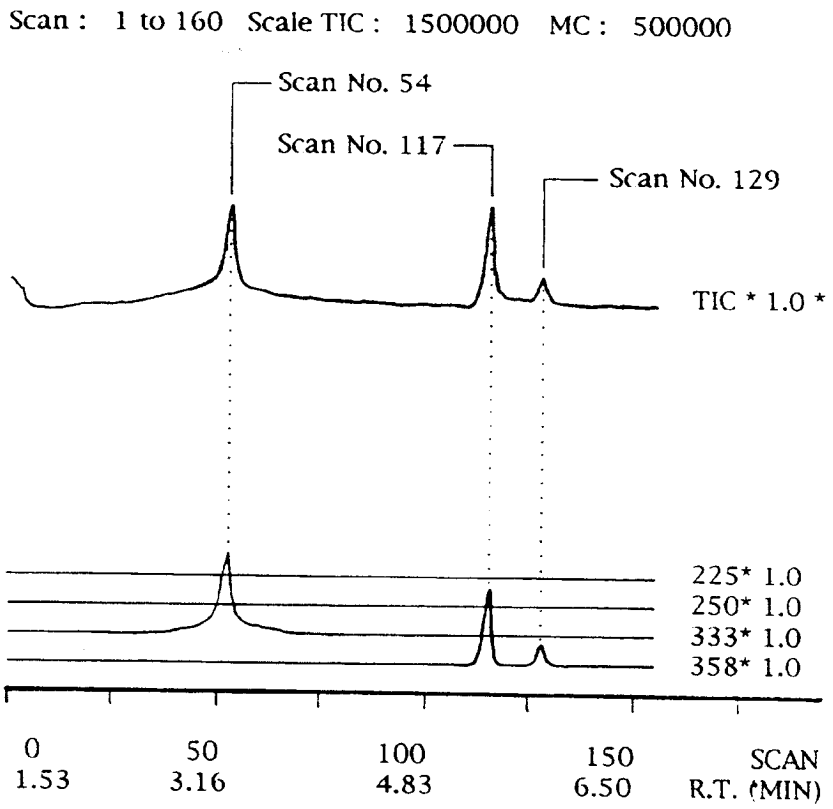

Fig. 2. Total ion chomatogram (TIC) obtained from a mixture of $Al(TFA)_3$ (Scan No. 54, R.T. 3.30 min) and $Cr(TFA)_3$ (Scan Nos. 117, R.T. 5.40 min and 129, R.T. 5.80 min) in comparison with two mass chromatograms (MCs) of mass 333 and 358.

the spectra scanned from positions 117 and 129 together with those of the reference $Cr(TFA)_3$ spectrum from the library search software. All of these spectra exhibited the same base peak at m/z 358.

In Figs. 3-6, $[M]^{+\cdot}$, $[M-L]^+$ and SI refer to the molecular ion, fragment ion after the loss of one ligand and similarity index, respectively. The GC-MS system employed in this work enables manual matching of mass spectra to be reduced or virtually eliminated by computerizing the comparison process. For a perfect match, SI = 100, while SI = 0 if no peaks are in common. For the SI calculation described here, a value of 80 or more indicates a good match[23].

From the mass spectral data shown in Figs. 3 and 4, it is possible to assign chromatographic peaks at R.T. 5.66 and 11.10 minutes (Scan Nos. 125 and 288) in Fig. 1 as $Al(AA)_3$ and $Cr(AA)_3$ with SI = 81 and 75, respectively . This assignment is also acceptable in terms of elution order expected for $Al(AA)_3$ with a molecular weight (MW) of 324 and $Cr(AA)_3$ (MW = 349) on a non-polar column such as CBP-1. $Al(AA)_3$ exhibits a base peak at m/z 225, corresponding to $[M-L]^+$ or $[Al(AA)_2]^+$, and $[M]^{+\cdot}$ at m/z 324 with intensity less than 10% of the base peak, as can be seen in Fig. 3. Peaks at m/z 226 $[(M-L)+1]^+$ and at m/z 325 $[M+1]^{+\cdot}$ could be attributed to the contributions from the ^{13}C isotope of carbon since $Al(AA)_3$ or $(CH_3COCHCOCH_3)_3Al$ contains 15 carbon atoms and the natural abundance of ^{13}C isotope is approximately 1.12% of that of ^{12}C. Similarly, in Fig. 4, $Cr(AA)_3$ or $(CH_3COCHCOCH_3)_3Cr$ is shown to give a base peak at m/z 250, corresponding to $[Cr(AA)_2]^+$, $[M]^{+\cdot}$ at m/z 349, $[(M-L)+1]^+$at m/z 251 and $[M+1]^{+\cdot}$ at m/z 350. It is noticeable that the $[M]^{+\cdot}$ peak of $Cr(AA)_3$ is somewhat more intense than that of $Al(AA)_3$, indicating that fragmentation from $[M]^{+\cdot}$ was more facile in $Al(AA)_3$ than in $Cr(AA)_3$.

A quick inspection of Fig. 2 suggests that chromatographic peaks at R.T. 3.30, 5.40 and 5.80 minutes (Scan Nos. 54, 117 and 129) could produce mass spectra with major fragment ions at m/z 333, 358 and 358, respectively. Although reference mass spectral data of $Al(TFA)_3$ or $(CH_3COCHCOCF_3)_3Al$ is not readily available, it is chromatographically reasonable to assign the first chromatographic peak at Scan No. 54 as $Al(TFA)_3$ because its MW is 486 while that of $Cr(TFA)_3$ or $(CH_3COCHCOCF_3)_3Cr$ is 511. Fig. 5 reveals that the fragment at m/z 333 is not only a major ion; it is in fact the base peak, most likely to have resulted from the loss of one ligand from the molecular ion of $Al(AA)_3$ to become $[Al(TFA)_2]^+$. As for the assignment of $Cr(TFA)_3$, Fig. 2 seems to pose a problem at first glance because a mass chromatogram showing mass 358 is indicated for both chromatographic peaks at R.T. 5.40 and 5.80 minutes (Scan Nos. 117 and 129). On further inspection of Fig. 6, it would be realized that the mass spectra data scanned from these last two chromatographic peaks are hardly different and they match well with the reference $Cr(TFA)_3$ spectral data through the computerized search. The last peak in Fig. 2 which might be mistakenly identified as an impurity peak was found to have the highest SI (91) in comparison with the reference $Cr(TFA)_3$. Trial comparison of mass spectral data from Scan Nos. 117 and 129 with a mass range from 358 (base peak) to 513 $[M+2]^{+\cdot}$ (instead of a mass range from 50 onwards) with the reference $Cr(TFA)_3$ via the computerized library search software still yielded a high value of SI. A decrease of only 1-2 units of the SI value in such a trial search indicates that real characteristic peaks of $Cr(TFA)_3$ can be taken from the base peak upwards.

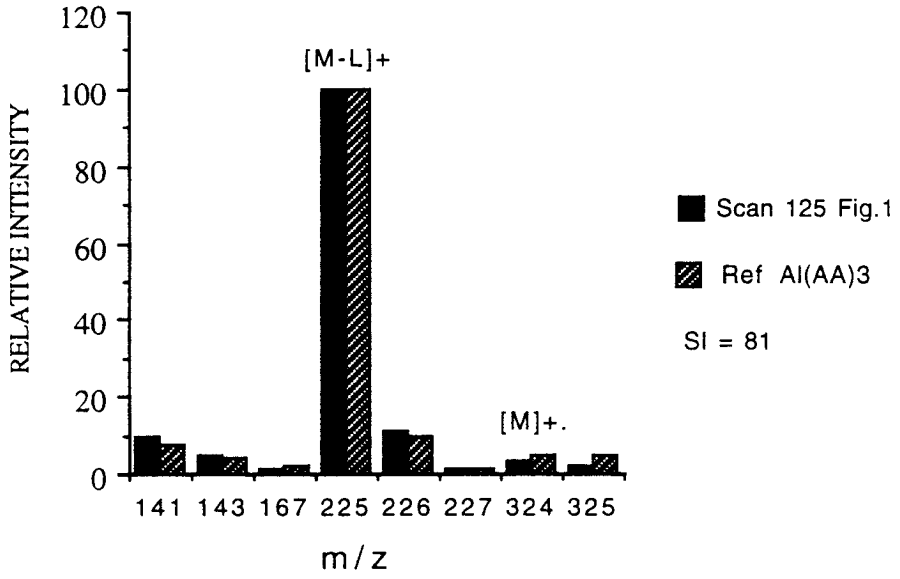

Fig. 3. Relative intensities of characteristic peaks of the mass spectrum obtained from Scan No. 125 (R.T. 5.66 min) in Fig. 1 in comparison with those of the reference $Al(AA)_3$ spectrum.

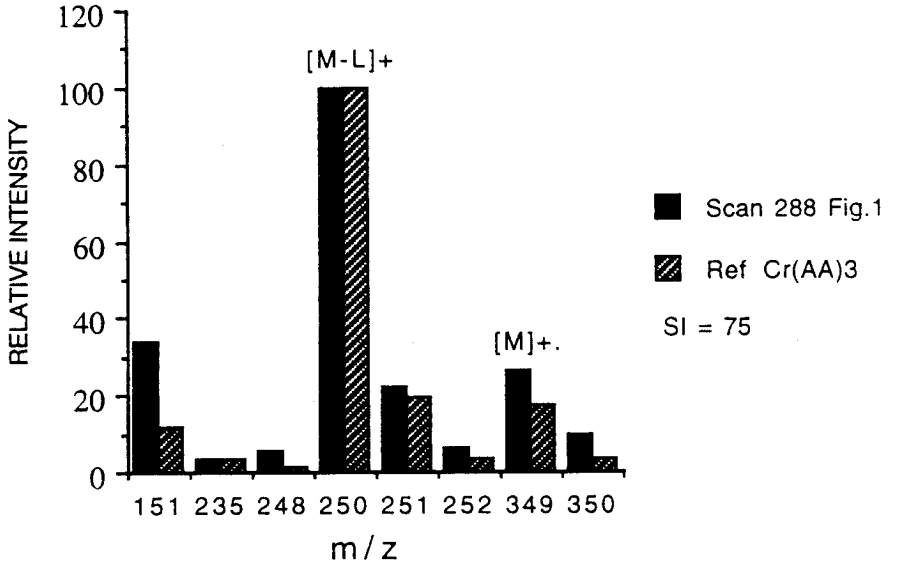

Fig. 4. Relative intensities of characteristic peaks of the mass spectrum obtained from Scan No. 288 (R.T. 11.10 min) in Fig. 1 in comparison with those of the reference $Cr(AA)_3$ spectrum.

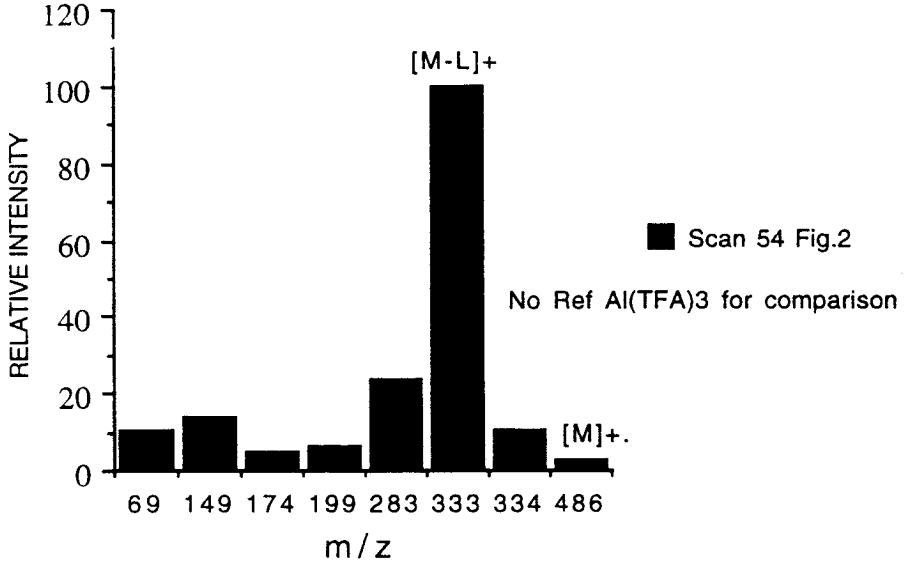

Fig. 5. Relative intensities of characteristic peaks of the mass spectrum obtained from Scan No. 54 (R.T. 3.30 min) in Fig. 2.

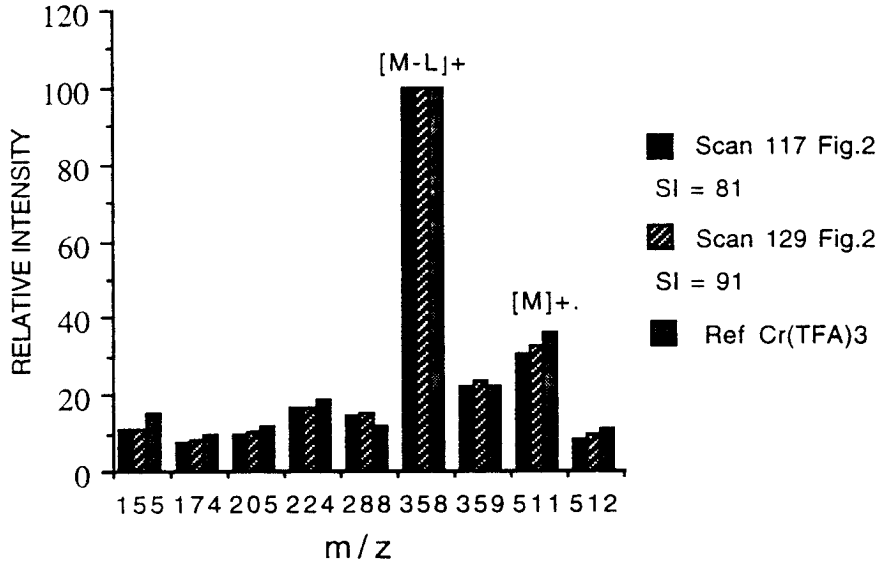

Fig. 6. Relative intensities of characteristic peaks of the mass spectra obtained from Scan Nos. 117 (R.T. 5.40 min) and 129 (R.T. 5.80 min) in Fig. 2 in comparison with those of the reference $Cr(TFA)_3$ spectrum.

This is valid because as the mass of an ion fragment increases, there are fewer compounds that could have given rise to such a fragment[23]. Similar findings were obtained when computerized mass spectral search for the afore-mentioned metal chelates was made on the basis of a mass range from the base peak upwards.

Regarding the assignment of the last two peaks in Fig. 2 as $Cr(TFA)_3$, it is still possible to postulate, according to the "like dissolves like" rule in chromatography, that the peak at R.T. 5.40 minutes is an isomer of $Cr(TFA)_3$ which is less preferentially retained by a non-polar stationary phase such as CBP-1 and that the peak at R.T. 5.80 minutes is the more non-polar isomer of $Cr(TFA)_3$. Between the *facial* and *meridional* isomers of $Cr(TFA)_3$, the *facial* isomer would be expected to be more polar because the trifluoromethyl groups are all on the same side of the molecule whereas in the *meridional* isomer, one of the trifluoromethyl groups is reversed[24-26]. It should be noted that strong-field d^3 and d^6 octahedral complexes (such as Cr(III) and Co(III) complexes, respectively) are generally inert[27]; inert complexes of this type can therefore exhibit geometrical isomers. Such isomers are not observable for $Al(TFA)_3$, a complex of a *p* block element, which is relatively more labile than $Cr(TFA)_3$. It may then be stated that in Fig. 2, the chromatographic peaks at R.T. 5.40 and 5.80 minutes could well be the *facial* and *meridional* isomer of $Cr(TFA)_3$, respectively. The area ratio of the *facial* isomer peak to that of the *meridional* isomer peak was found to be 3.90 : 1 or about 4 : 1, which agrees with the early work of Sievers and Sadlowski [24] and Mugo and Orians[26].

In Fig. 6, the relative intensities of the fragment at 512, corresponding to $[M+1]^{+\cdot}$, and the fragment at m/z 359, corresponding to $[(M-L)+1]^+$ can be seen to be quite high due to the contribution from the ^{53}Cr isotope with natural abundance as high as approximately 11% of the ^{52}Cr isotope together with the contribution from the ^{13}C isotope from the 15 carbon atoms in $Cr(TFA)_3$. In a detailed mass spectrum of $Cr(TFA)_3$, fragment ions at m/z 509, corrsponding to $[M-2]^{+\cdot}$ and at m/z 356, corresponding to $[(M-L)-2]^+$, should also be present but their relative intensities would be minimal compared to the first eight peaks because the natural abundance of ^{50}Cr is only 5% of that of ^{52}Cr. The contribution from ^{54}Cr would be even hardly noticeable since its abundance is only 2.8% of ^{52}Cr. Although such isotopic peaks of metal chelates are not usually included in the first 8 or 10 major peaks, their presence would be quite helpful in identification[28], particularly when reference mass spectra are not readily available. Trial GC-MS runs of the metal concentrations at nanogram levels did not pose any problem in mass spectral indentification of the metal chelates since the high signal-to-noise ratio was achieved in the reconstructed TIC of $Cr(TFA)_3$ but a more thorough investigation would be required to establish the exact detection limit for each of the metals studied. Regarding the choice of ligand for extraction of metals in a real sample, H(TFA) should clearly be a better choice than H(AA), mainly because the more volatile $Al(TFA)_3$ and $Cr(TFA)_3$ give higher sensitivity than the corresponding acetylacetonates[22] even though both ligands require a similar procedure for complex formation and extraction. The GC-MS method should soon become a method of choice for trace metal analysis *inter alia* as there already exists a wide range of the benchtop GC-MS instruments at affordable prices with the mass range up to 800 and sensitivity at picogram levels[29].

CONCLUSIONS

The GC-MS investigation of four aluminium and chromium β-diketonates in this study reveals that all metal β-diketonates could be conveniently chromatographed with abundant resolution using a non-polar fused silica capillary GC column. The metal trifluoroacetylacetonates required milder conditions than the metal acetylacetonates due to their relatively higher volatility. In all of the four metal chelates investigated, the base peak and hence the most diagnostic peak occurred from the loss of one ligand from the molecular ion. The molecular ion peaks all appeared to be intense enough to be included as major peaks, indicating the thermal stability of these metal chelates under the conditions employed. The base peak, the molecular ion and isotopic peaks around both the base peak and the molecular ion peak are characteristic peaks, especially when the metal of interest has more than one isotope and the number of carbon atoms is high. Ions other than these appeared to be hardly indicative as far as metal chelates are concerned. Under the GC-MS conditions employed, $Cr(TFA)_3$ alone exhibited two well-separated chromatographic peaks which could be identified as the *facial* and *meridional* isomers of $Cr(TFA)_3$ with an area ratio of 4:1. This GC-MS method offers low detection limits. It holds promise for the determination of aluminium, chromium and possibly other metals which can be chromatographed as metal chelates since various metal chelates have different GC retention times and the intensity measurements are made in a mass range where the contributions from background are very small.

ACKNOWLEDGEMENTS

The authors would like to express their sincere thanks to Dr. Colin Simpson of Birkbeck College, University of London, for his suggestions concerning the initial approach to the GC-MS work and also to Dr. Robert Molloy of Chiang Mai University for his helpful contribution.

REFERENCES

1. Lederer, M. (1955). *Nature*, **176**, 462-471.
2. McLafferty, F,W. (1957). *Appl. Spectr.*, **11**, 148-151; Litzow, M.R. and Spalding, T.R. (1973). *Mass Spectrometry of Inorganic and Organometallic Compounds*. Elsevier, Amsterdam. p. 563.
3. Booker, J.L., Isenhour, T.L., and Sievers, R.E. (1969). *Anal. Chem.*, **41**, 1705-1707.
4. Simpson, C.F. (1972). *Gas Chromatography-Mass Spectrometry Interfacial Systems, CRC Review of Analytical Chemistry*. CRC Press, Cleveland.
5. White, F.A. and Wood, G.M. (1986). *Mass Spectrometry: Applications in Science and Engineering*. John Wiley & Sons, New York. p. 215.
6. Moshier, R.W. and Sievers, R.E. (1965). *Gas Chromatography of Metal Chelates*. Pergamon Press, Oxford.
7. Morie, G.P. and Sweet, T. (1966). *Anal. Chim. Acta.*, **34**, 314-321.
8. Lee, M.-L. and Burrell, D.C. (1973). *Anal. Chim. Acta.*, **66**, 245-250.
9. Ahmad, M. and Aziz, A. (1978). *J. Chromatogr.*, **152**, 542-545.
10. Hansen, L.C., Scribner, W.G., Gilbert, T.W. and Sievers, R.E. (1971). *Anal. Chem.*, **43**, 349-353.
11. Genty, C., Houin, C., Malherbe, P. and Schott, R. (1971). *Anal. Chem.*, **43**, 235-240.

12. Gosink, T. (1975). *Anal. Chem.*, **47**, 165-168.
13. Belcher, R., Martin, R.J., Stephen, W.I., Henderson, D.E., Kamalizad, A. and Uden, P.C. (1973). *Anal. Chem.*, **45**, 1197-1203.
14. Hawn, G.G., Talley, C.P. and Brown, A. (1981). *Anal. Chim. Acta.*, **127**, 223-226.
15. Dilli, S. and Patsalides, E. (1979). *J. Chromatogr.*, **176**, 305-318.
16. Radecki, A., Halkiewicz, J., Grzybowski, J. and Lamparczyk, H. (1978). *J. Chromatogr.*, **151**, 259-262.
17. Krupcik, J., Garaj, J., Holotik, S., Oktavec, D. and Kosik, M. (1975). *J. Chromatogr.*, **112**, 189-196.
18. Masaryk, J., Krupcik, J., Garaj, J. and Kosik, M. (1975). *J. Chromatogr.*, **115**, 256-258.
19. Cardwell, T.J. and Lorman, T.H. (1986). *J. Chem. Educ.*, **63**, 90-91.
20. Wolf, W.R., Taylor, M.L., Hughes, B.M., Tiernan, T.O. and Sievers, R.E. (1972). *Anal. Chem.*, **44**, 616-618.
21. Berg, E.W. and Truemper, J.T. (1960). *J. Phys. Chem.*, **64**, 487-490.
22. Srichuanchuenskul, W. (1994). Ph.D. Thesis, Chiang Mai University.
23. Karasek, F.W. and Clement, R.E. (1988). *Basic Gas Chromatography-Mass Spectromeyry: Principles and Techniques.* Elsevier, Amsterdam. p. 107.
24. Sievers, R.E. and Sadlowski, J.E. (1978). *Science*, **201**, 217-223.
25. Hawn, G.G., Talley, C.P. and Brown, A. (1981). *Anal. Chim. Acta.*, **127**, 223-226.
26. Mugo, R.K. and Orians, K.J. (1993). *Anal. Chim. Acta.*, **271**, 1-9.
27. Shriver, D.F., Atkins, P.W. and Longford, C.H. (1994). Inorganic Chemistry, 2nd ed., Oxford University Press, Oxford. p. 266.
28. Aggarwal, S.K., Kinter, M., Willis, M.R., Savory, J. and Herold, D.A. (1989). *Anal. Chim. Acta.*, **224**, 83-95.
29. Wach, F. (1994). *Anal. Chem.*, **66**, 927A-930A.

บทคัดย่อ

ได้ทำการศึกษาวิธีการแก๊สโครมาโทกราฟี-แมสสเปกโทรเมตรี ในการหาลักษณะเฉพาะเชิงวิเคราะห์ของอะลูมิเนียมและโครเมียมในรูปของบีตา-ไดคีโทเนตที่ระเหยได้บางตัว โดยใช้อะเซทิลอะซีโทนและไทรฟลูออโรอะเซทิลอะซีโทนเป็นลิแกนด์ ทั้งอะลูมิเนียมและโครเมียมคีเลตแยกกันได้ดีเมื่อใช้ฟิวซ์ซิลิกาแคพิลารีคอลัมน์ยาว 25 เมตร เส้นผ่าศูนย์กลางภายใน 0.20 มิลลิเมตร แมสสเปกตรัมทั้งหมดที่ได้จากแหล่งกำเนิดไอออนแบบอิเล็กตรอนอิมแพคท์พร้อมกับควาดรูโพลแมสแอนาไลเซอร์ ภายใต้ภาวะการใช้งานปกติ ให้เบสพีคที่มีรูปแบบเฉพาะตัวที่มีค่าเท่ากับโมเลกุลาร์ไอออนที่สูญเสียลิแกนด์ไปหนึ่งตัว โครเมียม (III) ในรูปของ 1,1,1-ไทรฟลูออโรอะเซทิลอะซีโทเนต ให้ 2 โครมาโทกราฟิกพีค โดยพีคทั้งคู่ทำให้ได้แมสสเปกตรัมที่เหมือนกันแทบทุกประการ ซึ่งบ่งบอกว่าโครเมียมคีเลตตัวนี้มีไอโซเมอร์ทางเรขาคณิตอยู่ 2 ไอโซเมอร์