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The mechanochemical modification of polyolefins using reactive modifier systems.

by

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A thesis submitted for the degree of doctor of philosophy.

The University of Aston in Birmingham.

October 1990.

The University of Aston in Birmingham.

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Summary.

The principal objective of this work was to improve the mechanical properties of glass fibre reinforced polypropylene (PP) composites by the mechanochemical modification of the PP. The modification of the PP was carried out by reactive processing of the PP with a modifier in a Buss Ko-Kneader. Two main types of modifier were evaluated one type based on N-subsituted maleimides the others based on 2-allylamino-4,6-dichloro-1,3,5-triazine (ACCT).

The modification of the PP was carried out in two stages. Firstly the PP was reactively processed with the modifier and a free radical initiator. The objective of this stage was to bind the modifier to the PP. In the second stage the modified PP was reactively processed with the glass fibre. The objective in this stage was to form a chemical bond between the bound modifier and the silane coupling agent on the surface of the glass. Two silane coupling agents were evaluated these had a aliphatic chloro group and an aliphatic amino group respectively available for reaction with the modifier.

The modifiers synthesised for this work had two main functional groups. The first was a double bond for free radical addition to the PP. The second was an organic group chosen for its potential reactivity to the silane coupling agent.

A preliminary investigation was carried out using maleic anhydride (MA) as the modifier, this is reactive to the amino silane coupled glass. Studies of a commercially available system were also carried out for comparison purposes.

During the work it was found that the amino silane coupled glass fibres produced, without any modification being made to the PP, mechanical properties comparable to the commercial system. Further any modification added to the amino silane system failed to improve the mechanical performance and in some cases acted in the opposite fashion. This failure was evident even when a chemical bond between glass fibre and PP could be shown.

In the case of the chloro silane coupled glass fibres the mechanical properties of the composite without modification were poorer than those of the commercial system. It was found that the mechanical properties of these systems could be enhanced by the modifiers, however, no system tested significantly out performed the commercial system.

Of the two modifier systems tested those based on the n-subsituted maleimides were more successful at enhancing mechanical properties than those based on ACCT. This was attributed to the Poor chemical binding of the ACCT based modifiers to the PP.

During the work it was found that several of the modifiers improved the properties of the PP when no glass fibres were present, particularly the % elongation and impact strength. It is possible that these modifiers could be used to improve the impact performance of PP, this may be of particular interest in recycling. These modifiers have only been tested for improving the properties of glass fibre composites. The N-subsituted maleimide based modifiers could be used as compatibleisers for alloys of PP with other polymers. These could function by the formation of the bond with PP via the double bond whilst the group attached to the nitrogen atom could react with the alloying polymer.

Key words: Mechanochemistry, Reactive processing, composites, polypropylene, Maleic anhydride, Glass fibres.

Dedication.

I would like to dedicate this thesis to my father who died suddenly shortly after I began my research at Aston.

Acknowledgements.

I would like to pay tribute to the help and support of Dr Al-Malaika and Professor G Scott and thank them for giving me this opportunity. I would like to thank the remaining staff and technicians for their assistance on occasions too numerous to mention. I would like to thank my friends for their help and encouragement particularly David, Jeremy and Trevor. Finally a very big thank you to my fiancee Jenny without whose help I would not have got this far

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Abbreviations

PP	Polyproplene
ACCT	2-allylamino-4, 6-dichloro-1, 3, 5-triazine
DCP	Di-cumyl peroxide
FGCS1640	Chlorosilane coupled glass fibres
R16E	Aminosilane coupled glass fibres
TS	Tensile strength
EL	Elongation
IM	Impact Strength
FM	Flexural modulus
FS	Flexural strength
HWM25	Unreinforced commercial polypropylene
HW60/GR30	Glass reinforced commercial polypropylene
AACT	2-chloro-4, 6-diallylamino-1, 3, 5-triazine
ABCT	2-allylamino-4-chloro-6-dibutylamino-1, 3, 5-triazine
MFI	Melt flow index
RT	Room temperature
Hr	Hour
MAC	Maleic acid

CHAPTER 1

INTRODUCTION.

1.1 Background.

Thermoplastics have always been used in commodity, engineering and other specialist applications. Their use, however, is limited by their relatively poor mechanical properties and thermal stability when compared with more traditional materials such as metals. The mechanical properties can be improved by the incorporation of reinforcing fibres which can greatly enhance the strength, stiffness and dimensional stability of the thermoplastic. The principal advantages of fibre reinforced thermoplastics are light weight, ease of large scale manufacture (eg injection moulding), low cost and design advantages.

1.2 Composites.

A composite material can be defined as a macroscopic combination of two or more distinct materials having a recognisable interface between them. Polymer composites, however, are usually used for their physical properties so the definition can be restricted to include only those materials which are reinforced(1).

The two main phases of a composite are the reinforcement (usually fibres or particles) supported in a binder (matrix) material (figure 1.1).

Composite materials result in a compromise of physical properties between reinforcement and matrix. For example, glass fibres have a high tensile strength but low impact strength while PP, a matrix phase, has in comparison to glass a low tensile strength but higher impact strength. A composite of the two has a higher tensile strength than PP but lower than glass alone and the impact strength is higher than glass but lower than PP (figure 1.2).

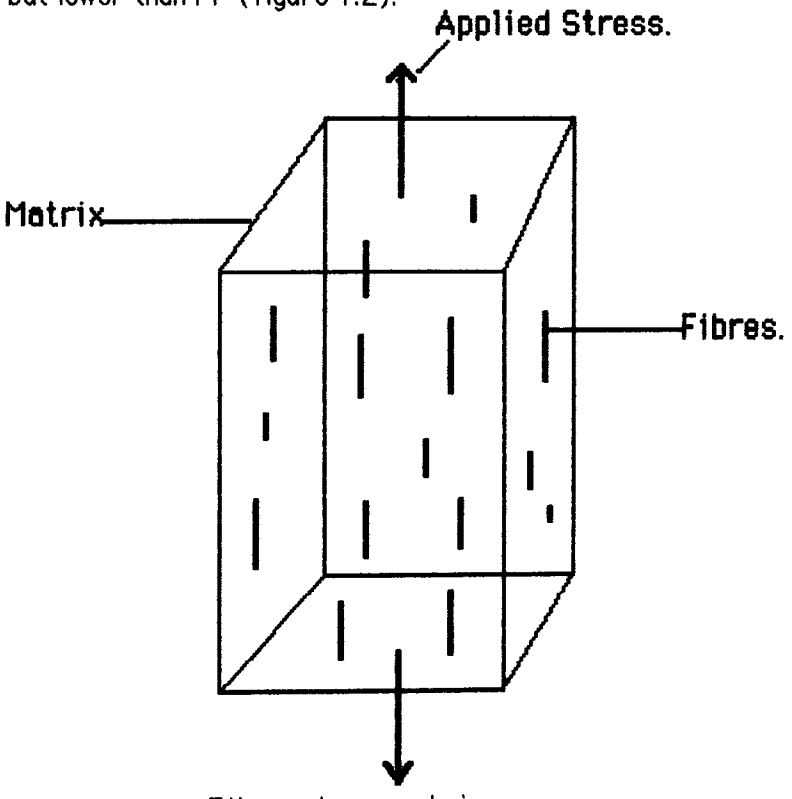


Figure 1.1 Fibres in a matrix.

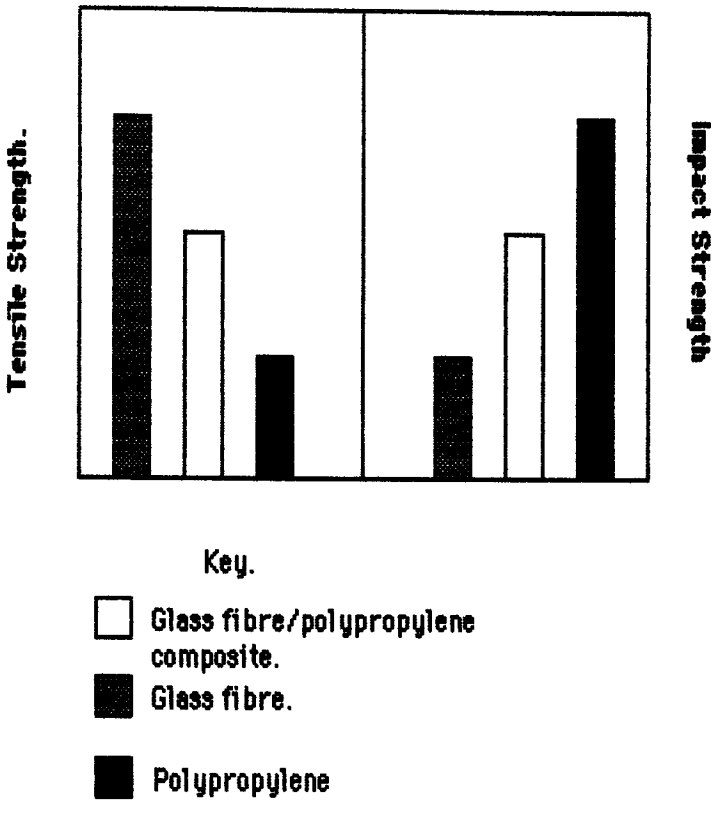


Figure 1.2 Relative properties of composite components and composite.

1.3 Theory of short fibre reinforcement of thermoplastics.

The simplest theory to explain the reinforcement of thermoplastics by high modulus inorganic fibres is the "Law of mixtures"[2,3], more complex analysis based on elasticity theory have also been attempted[4,5]. The law of mixtures in its simplest form assumes that the composite consists of uniaxially aligned fibres of uniform length, with perfect fibre-matrix bonding and with the applied stress being in the same direction as the fibre alignment (see Figure 1.1). The mechanical properties such as tensile strength may then be estimated by the relative proportions of the two components in the composite[2].

$$\sigma_c = \sigma_f \cdot v_f + \sigma_m \cdot v_m \qquad --(1).$$

Where

σ_c = Tensile strength of composite.
σ_f = Tensile strength of fibre.
σ_m = Tensile strength of matrix.
v_f = Volume fraction of fibre.
v_m = Volume fraction of matrix.

In order to account for the fibre orientation an additional factor must be added to equation (1) this is the fibre orientation factor (n). In injection moulded fibre reinforced thermoplastics the fibres are aligned in all directions (the orientation of the fibres is dependent on mould design and moulding conditions). The values of n lie between 0-1. When the fibre is in line with the applied stress then n=1, if it is perpendicular to the applied stress then n=0[2,3].

$$\sigma_c = n \cdot \sigma_f \cdot v_f + \sigma_m \cdot v_m \qquad --(2).$$

Where

n= fibre orientation factor.

In order to account for the variety of fibre lengths present in a composite the critical fibre length factor (L_c) is used[2]. Fibres improve the strength of a composite by transfer of stresses from the fibre to the ductile matrix, the length of fibre determines the amount of stress that is transferred. Any fibre shorter than the critical fibre length gives incomplete stress transfer and fibre pull-out from the matrix. The critical fibre length L_c is given by Equation 3[2].

$$L_c = \frac{\sigma_f \cdot d}{2\tau} \qquad --(3).$$

Where

d = Fibre diameter.
τ = interfacial shear strength.

The interfacial shear strength factor (τ) is introduced to account for the incomplete fibre matrix bonding. Putting Equation (3) into Equation (2) gives[6,7]:

$$\sigma_c = n \cdot \sigma_f \cdot v_f \cdot \frac{(1-Lc)}{2L} + \sigma_m \cdot v_m$$

Where

L = Actual fibre length.
Lc = Critical fibre length.

For E type glass fibres in polypropylene L_c has been shown to be 1.78mm with an aspect ratio (L_c/d) of 140[6].

1.4 The matrix polymer.

The matrix polymer used in this work is PP. There are considerable cost advantages in enhancing the properties of this low cost cheap commodity thermoplastic. In figure 1.3 the relative cost per unit volume for several common thermoplastics are shown[7]. It is clear from this that PP is far cheaper than the more common engineering plastics. Polypropylene is semi-crystalline and nonpolar with a melting point in the range 160-165'C. It is resistant to many chemicals including strong acids and bases. In spite of its apparent favourable properties, PP is not used in engineering applications because of its low stiffness, strength and heat distortion temperature (figure 1.4)[7]. In an attempt to improve these properties fillers and reinforcing fibres have been added to PP[8-14] which allow it to be competitive on a cost-peformance basis with engineering plastics such as nylon, ABS and polycarbonate[7].

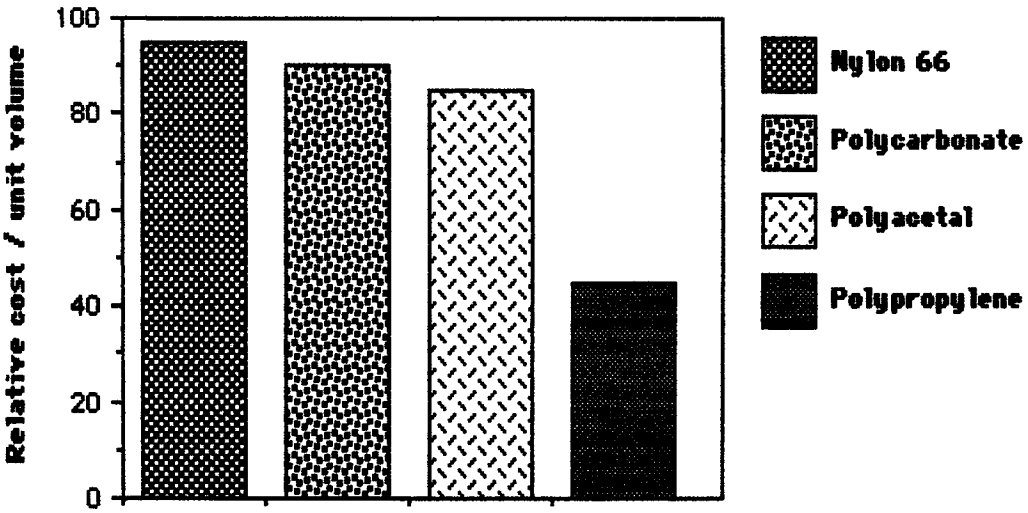


Figure 1.3 The relative cost per unit volume for some common thermoplastics.

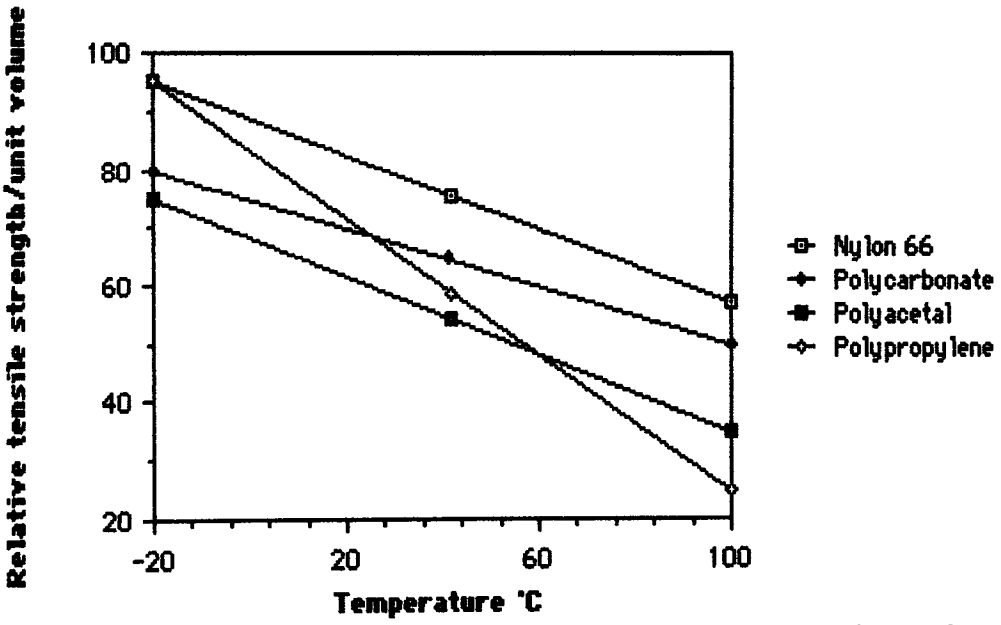


Figure 1.4 The relative tensile strength per unit volume for some common thermoplastics.

1.5 Chemical modification of Polypropylene.

To enhance the mechanical properties of PP composites it is necessary to increase the interfacial shear strength between the matrix and fibre. Due to the relatively inert chemical nature of PP it is necessary to chemically modify the PP, this can be achieved by chemically grafting groups reactive towards functional groups present on the glass surface.

Maleic anhydride (MA) has been grafted to polyethylene and PP to promote wettability[15], adhesion to give functionality for cross linking and to promote compatibility with other polymers and fillers[16,17].

A variety of methods have been employed to achieve grafting, these include using free radical addition in organic solutions of maleic anhydride and PP[18-20], vapour phase graft polymerisations[21], chemically by heating with degraded polymer in an inert atmosphere[22-25], mechanochemically with or without free radical initiator[26-42] and by using radiation techniques[43]. Solvent extracts and IR spectra have shown that grafting is achieved[16].

The improved adhesion in such modified PP has been attributed to dispersional and hydrogen bond forms introduced by the MA[15,44]. Maleimides and bismaleimides have been grafted to PP in similar ways to change properties and cross link the polymer[45-50].

1.6. Glass fibres.

A commercial process for the manufacture of continuous glass fibres was first demonstrated in 1931 by the Owens Illinois glass company. Glass is an amorphous material obtained by cooling from the melt at such a rate that no crystals are formed. Chemically, glass is mainly composed of a silica (Quartz) network to which other chemicals are added to decrease the viscosity and melting point of the silica to aid its processing into glass. There are four main grades of glass used commercially to form continuous fibres, these are high alkali A-glass, electrical grade E-glass, chemically resistant E-glass (ECR-glass) and high strength S-glass. The principle physical properties of these are shown in Table 1.1.[51]

1.7 Fibre sizing.

Within the composite industry the term sizing has come to mean any surface coating applied to a reinforcement to protect it from damage during processing, aid in processing, or improve the mechanical properties of the composite[52]. Other terms used synonymously for sizing include finishing agent, tenside (applied to Inorphil fibres) and coupling agent. Coupling agents are an important part of fibre sizing and are dealt with in Section 1.7.1 The principle functions of the sizing are to protect the fibre

during all stages of handling and improve the physical properties of the final composite. The use of sizing is a compromise of requirements, for example, for the cutting of a continuous filament into short fibre lengths a number of filaments are joined together by means of a binding agent, this binding agent can, however, prevent the homogenisation of the fibres during compounding and injection moulding[52].

Table 1.1 Principle physical properties of glass fibre grades[32].

Glass Fibre.	Specific Gravity.	Tensile strength MPa	Tensile modulus GPa	Thermal expansion coefficient 10^{-6}/K	Dielectric constant.
E	2.58	3450	72.5	5.0	6.3
A	2.50	3040	69.0	8.6	6.9
ECR	2.62	3625	72.5	5.0	6.5
S	2.48	4590	86.0	5.6	5.1

1.7.1 Silane coupling agents.

Coupling agents can be defined as materials that improve the chemical resistance (especially to water) of the bond across an interface[53]. When glass fibres were first used for reinforcement in organic resins it was found that initially the strength to weight ratio was very good, but that this declined rapidly on exposure to moisture. It was found that an interface material was needed to enhance the bonding between the inorganic glass and the organic matrix. Organofunctional silicones being made up of an organic function and inorganic silicone were tested in this role. The silane coupling agents used in this work have the general structure shown in Figure 1.5 and are bonded to the glass via the hydroxyl groups on the surface of the glass[54], (see Figure 1.6). The organic end of the silane can be any chemical group, chosen for its reactivity with the matrix polymer.

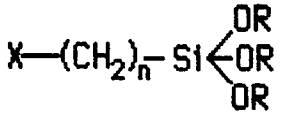


Figure 1.5 General structure of a silane coupling agent.

Prior to coupling the three alkoxy groups are hydrolysed in a weakly acidified water[55,56]. The resulting silanol can then bind to receptive surfaces[57,58]. The silanol condensation reaction is reversible and drying causes condensation of adjacent silanol groups (figure 1.6)[59-61]. This is an idealised picture of the bonding of silane to glass with the result being a monolayer of the silane. Coupling agents have been shown to form 3-dimensional polysiloxane networks through hydrolysis and condensation of adjacent hydroxyl groups. In the case of 3-aminopropyltriethoxy silane it has been shown that this forms a polymeric network with only occasional attachments to the glass surface[62,63].

1.8 The nature of bonding through silane coupling agents.

A number of mechanisms for the bonding of silane coupling agents to the matrix polymer have been proposed.

1.8.1 Bonding by chemical reaction.

Thermoplastics may be generally classified as reactive and nonreactive. Reactive thermoplastics contain organic functional groups such as amides, carboxyl, halide, or hydroxyl. The polyolefins, such as polyethylene and PP, are classified as nonreactive since they contain no reactive functional groups. The concept of bonding by chemical reaction is the simplest and simply involves the formation of a chemical bond between the reactive end of the silane (X) (figure 1.5) and some functional group on the polymer[64] (figure 1.7). This concept is usually associated with the reactive thermoplastics, however, some coupling agents are known to react with the nonreactive thermoplastics, for example, vinylsilanes which are known to react with polyethylene during injection moulding[65].

1.8.2 Bonding by solution compatibility.

Where there is no chemical reaction between matrix and coupled fibre then it has been found that there is a definite maximum in physical properties for silanes that have optimum compatibility with the polymer as predicted from the solubility parameters of the polymer and silane[66].

1.8.3 Bonding by interpenetrating networks.

The formation of an interpenetrating network involves the silane on the glass surface dissolving in the matrix polymer (at processing temperatures). On cooling, the matrix loses its solubility and partially separates as an interpenetrating phase with the silane at the glass interface[67] (figure 1.8). This theory has largely superseded the chemical bonding theory[52].

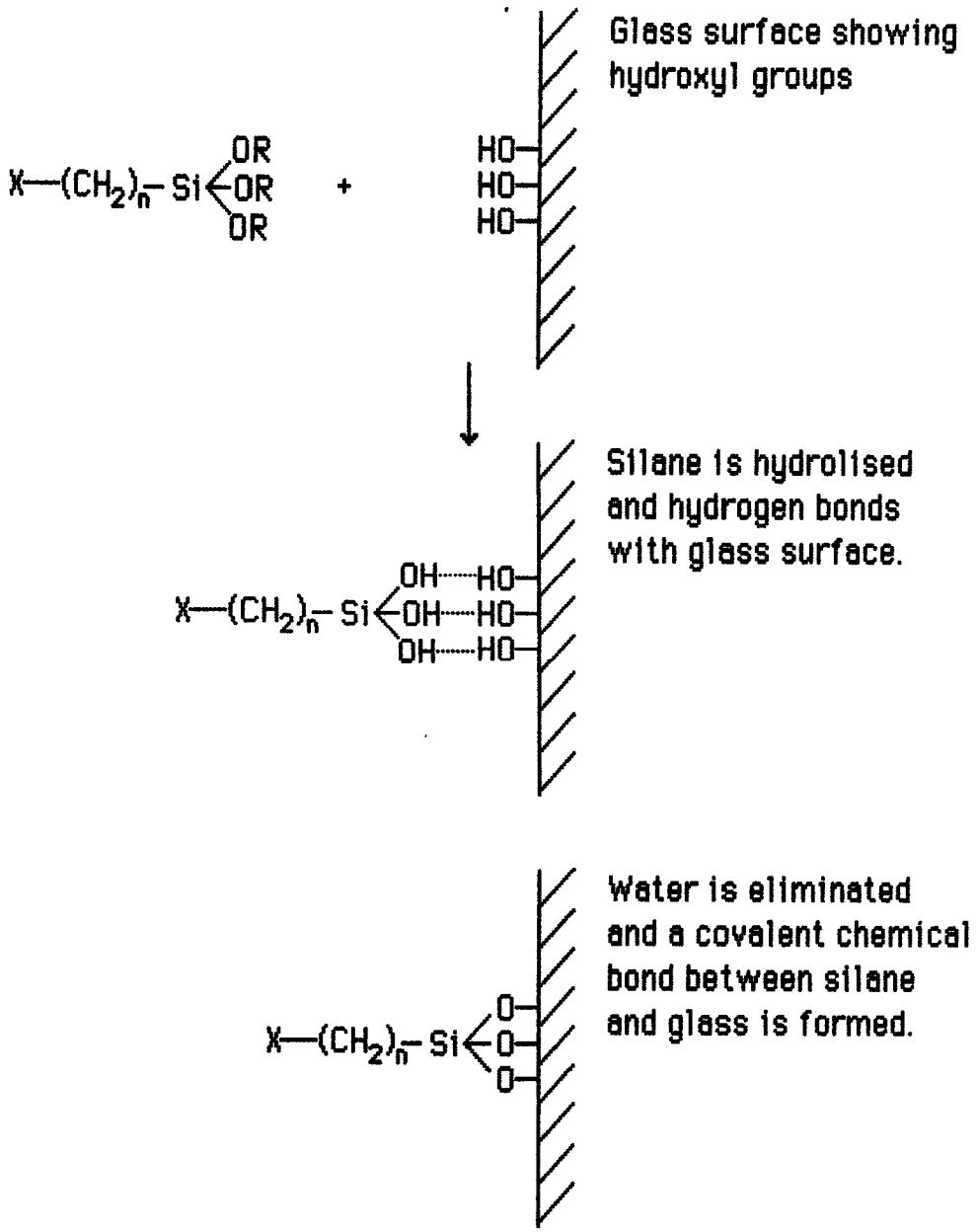


Figure 1.6 The mechanism of silane bonding to glass.

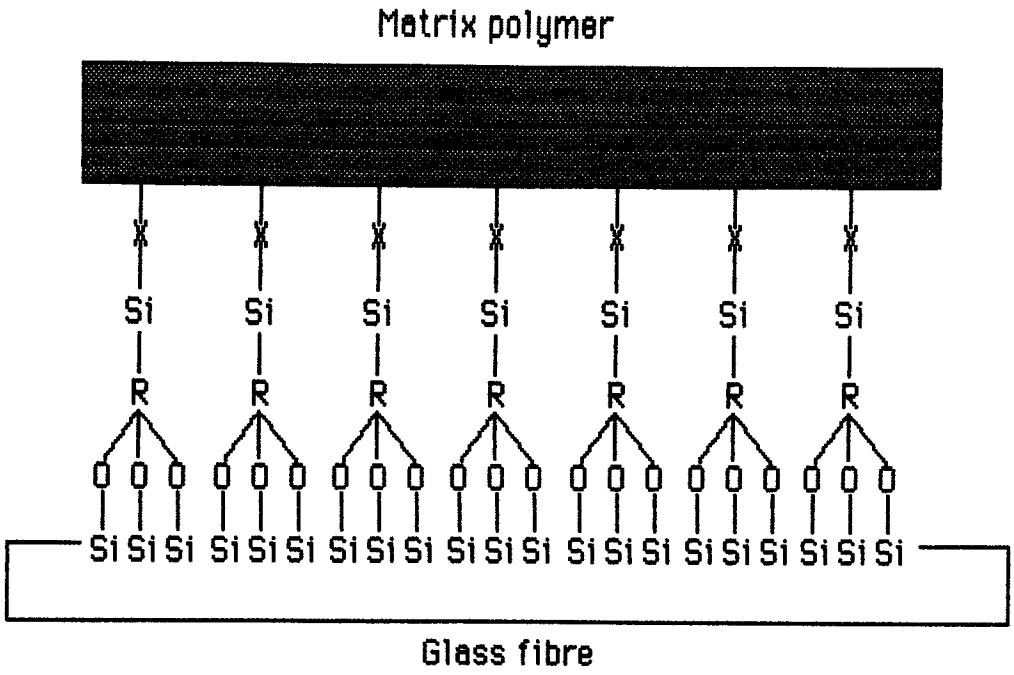


Figure 1.7 Idealised chemical bonding of glass fibre and matrix polymer by silane coupling agent.

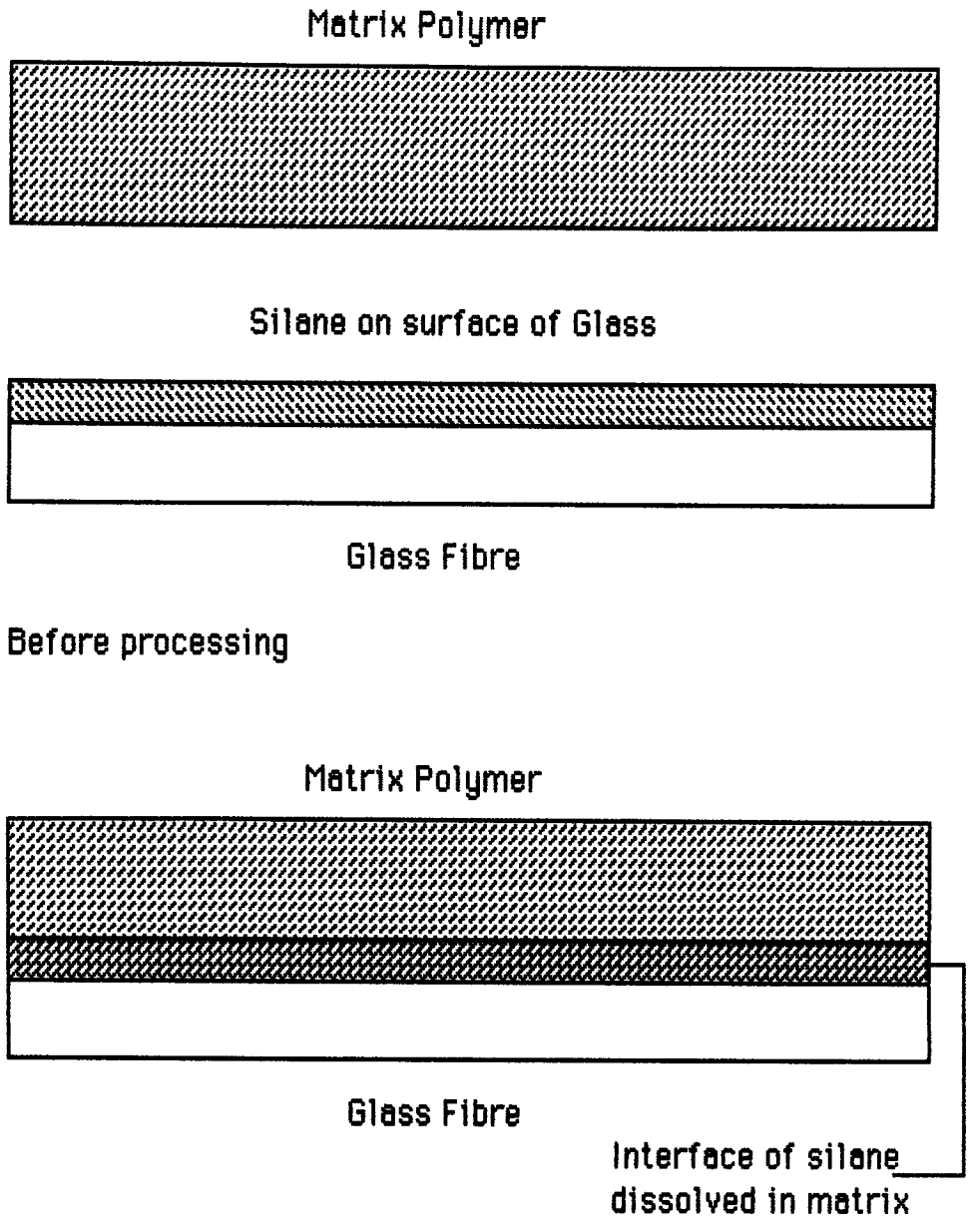


Figure 1.8 Bonding by interpenetrating networks.

1.9 Compounding of polymer composites.

The compounding stage of the composite manufacture involves the mixing and homogenisation of fibre and matrix to produce a compound which can be moulded[68]. Compounding is very important to the final properties of the product[69], during compounding energy is applied to the polymer by internal shear via screw rotation within the barrel[70]. The mixing action melts the polymer, mixes and homogenises the fibres[68,70]. Extensive fibre breakage occurs during compounding due to the large shearing forces involved[71]. The main processing requirements for optimum properties in the final composite are[68-72]:

1. Minimal thermal degradation of the matrix polymer.
2. Fibres must be totally enclosed by the matrix polymer.

3. There must be a uniform fibre dispersion.
4. Fibre breakage should be reduced to a minimum by (73):
   (a) Reducing screw speed to a minimum to avoid excessive fibre breakage at the screw periphery.
   (b) Setting a high barrel temperature at the feed zone and reducing the temperature profile towards the nozzle.

1.10 Injection moulding of polymer composites.

The fibre length is the most important factor in determining the final mechanical properties of a polymer composite, other important factors are fibre dispersion, orientation and void content in the final product(2,74-77). The injection moulding process may be divided into four specific operations, each of which will affect the final mechanical properties of the polymer composite and these processes are as follows(78-88) (figure 1.9):

1. Feeding the compounded polymer into the injection moulding machine. The feeding method may reduce fibre length, for example, forced feeding of dry blends.
2. Transporting and melting the compound while developing pressure, as with compounding the peripheral screw speed and pressure within the barrel will affect fibre length. It has been reported that nearly all fibre length attrition takes place during this phase (79).
3. Injecting the compound through runners and gates. During injection large shearing forces are developed in the runners and at the gates, these forces can reduce fibre length(80).
4. Flowing the moulding compound into the mould cavity, this effects the final fibre orientation(75,79,80).

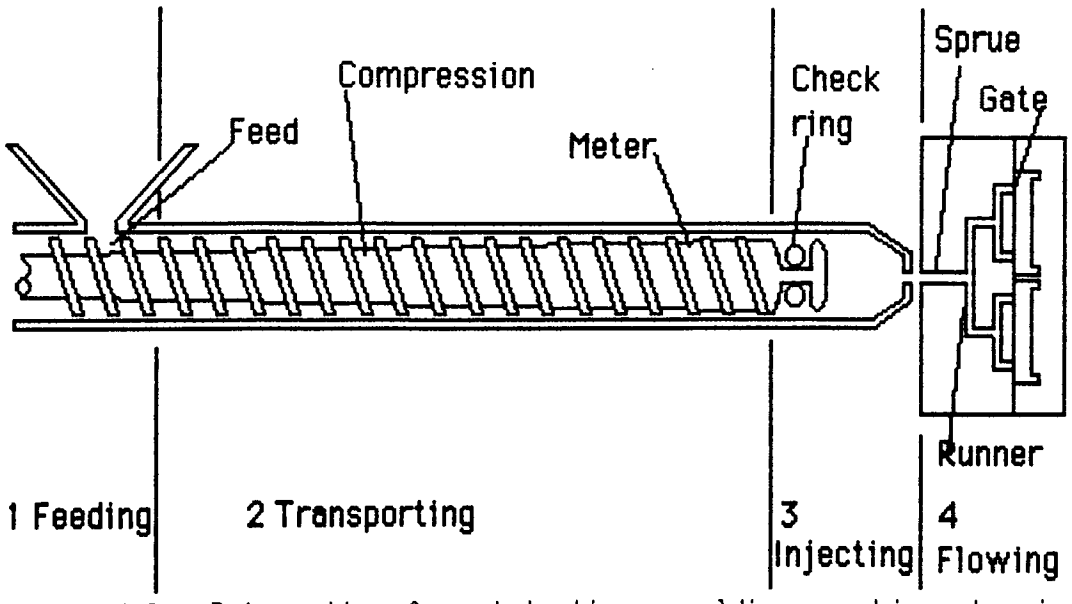


Figure 1.9 Schematic of an injection moulding machine showing zones of fibre length degradation.

1.11. Mechanochemistry.

Polymer reactions which are induced by stress are known as mechanochemical reactions, the major mechanochemical processes of commercial polymers include principally mixing and extrusion. Mechanochemical reactions can be induced in isolation by storage of elastic energy due to chain extension, however, in most cases the situation is not that simple and multiple reaction mechanisms operate, for example, in processing machinery at elevated temperatures reactions caused by heat, the presence of oxygen and mechanochemistry occur simultaneously.

The general mechanism for mechanochemistry is shown in figure 1.10, in its most simplistic form mechanochemistry takes place by the homolytic cleavage of the polymer chemical bonds, this homolytic cleavage gives rise to free radicals. The mechanisms for the propagation and termination of macro radicals formed during mechanochemical reactions are similar to radical reactions initiated by other means. The mechanism can thus be represented by the following schemes:

$R-R \rightarrow R^{\circ} + R^{\circ}$	(Rupture by shear)
$R^{\circ} + R^{\circ} \rightarrow R-R$	(Recombination)
$R^{\circ} + R^{\circ} \rightarrow R + R$	(Disproportionation to produce a saturated and unsaturated product)
$R^{\circ} + R-R-R \rightarrow R + R-R^{\circ}-R$	(Chain transfer.)
$R^{\circ} + A \rightarrow R-A$	(Acceptor reaction.)

The effects of mechanochemical reactions on a polymer is firstly to destroy any supermolecular structure by forces on intra and intermolecular bonds and then as the applied stress exceeds a critical value the chains rupture. Chain rupture is followed by a reduction in molecular weight, changes in the molecular weight distribution, cross linking and new functional group formation. The chemical bonds most likely to rupture are the thermodynamically weakest. During the mechanochemical modification of a polymer by the grafting of functional groups onto it, it is the final reaction that we wish to encourage since this produces a grafted polymer.

Most theories on the mechanism of mechanochemical reactions were developed in the 1950's with most of the mechanisms proposed being for amorphous chains in rubbers, melts and solutions. One of the first theories was proposed by Frenkle[89] with a related idea proposed by Kauzman and Eyring[90]. In these theories the sheared polymer molecule is extended in the direction of flow, bonds in the middle are most extended while those at the end retain their coiled shape. The forces of viscous drag strain the central bonds and at some critical shear rate the central bond fractures preferentially (figure 1.11). Generally, pure viscous forces are not a large

contributor to mechanochemical reactions as they cannot provide enough energy storage in the molecular bonds for breakage to occur.

In polymer melts and concentrated solutions it is the entanglement network which provides the elastic strains required. Since mechanochemical reactions lead to molecular fracture, one of the principal consequences of these reactions in polymers is a reduction in molecular weight and a change in the molecular weight distribution. Under certain conditions of shear on rubbers and polyolefins cross-linking and branching predominate and the molecular weight can increase. Generally, an exponential decrease is found for the molecular weight or a property related to the molecular weight. The decrease in molecular weight is severe at first, slowing until a limiting value is reached, the magnitude of this limiting value depends on shear and the more severe the shear the lower the limiting value.

Mechanochemical reactions can have positive and negative effects on the properties of a polymer, on the negitive side they produce a reduction in the molecular weight. It has been shown that the bond rupture which occurs can play a role in enviromental stress cracking, discoloration and embrittlement of the polymer. On the more positive side radicals which are formed on the surface of polyolefins have been shown to aid adhesive bonding.

Mechanochemical processes produce an alteration in both the chemical and physical structure of a polymer and as a result of these changes, changes in rheology and mechanical properties can result. The most important changes are destruction of supermolecular structures[91], alteration of the molecular weight and molecular weight distribution[92], cross-linking[93] and formation of new chemical functional groups[94]. The formation of new chemical functional groups depends on the chemical nature of the polymer and the environment in which the modification is performed. The chemical composition also determines the effects of these new functional groups on the polymer properties.

It is possible to significantly modify a polymer by carrying out mechanochemical reactions in the presence of active materials such as monomers or reinforcing agents. Such modification can be achieved by grafting polymers with active functional groups during processing, furthermore, these reactions may potentially be performed in standard processing machinery.

Polyethylene has been modified with MA in a disc extruder [95-99] and the following effects were noted, there was some crosslinking and a decrease in crystallinity. The extent of crosslinking was dependent on the amount of MA and the processing time. The reaction takes place between the macroradical and the MA double bond (figure 1.12). The crosslinked polymers were found to be less soluble the heat resistance, rigidity and strength properties were increased[95,96].

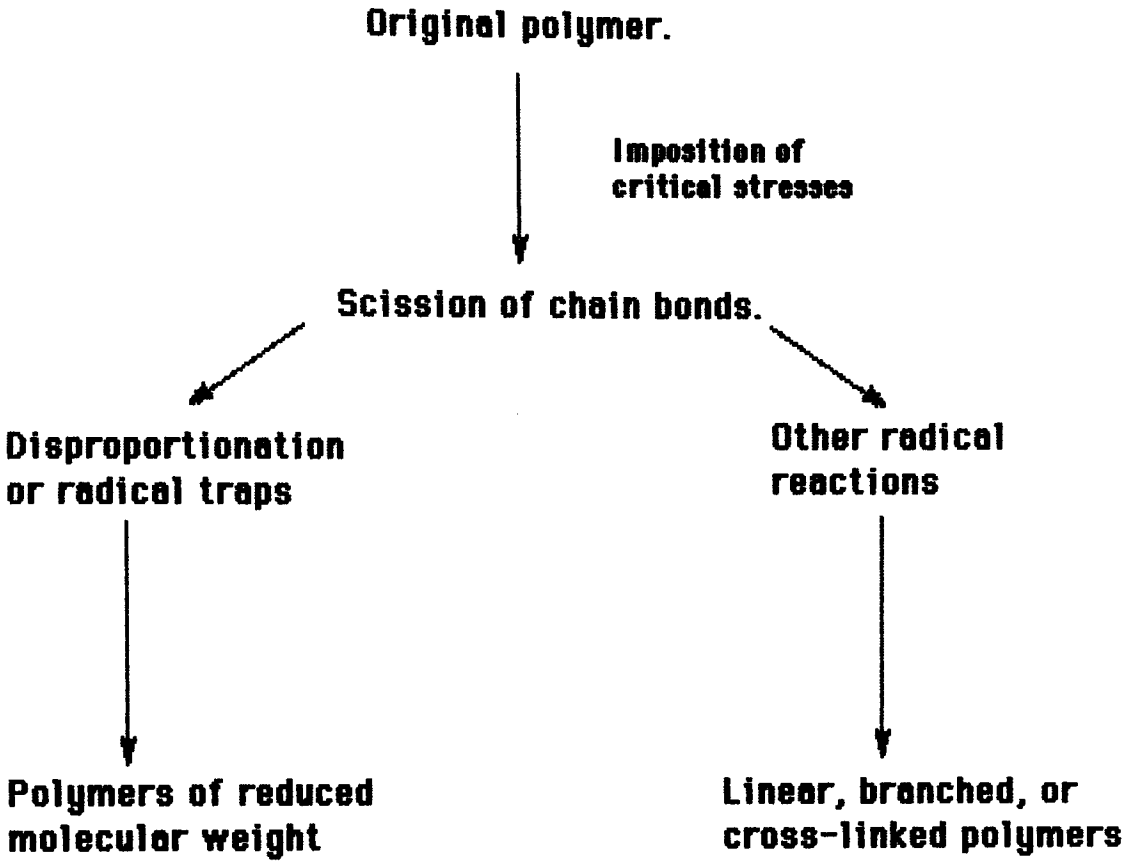
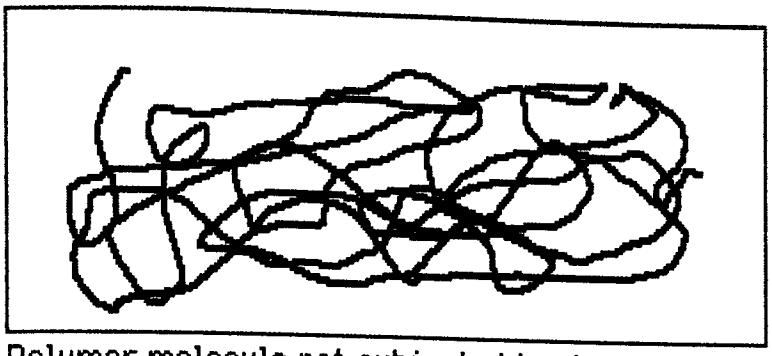
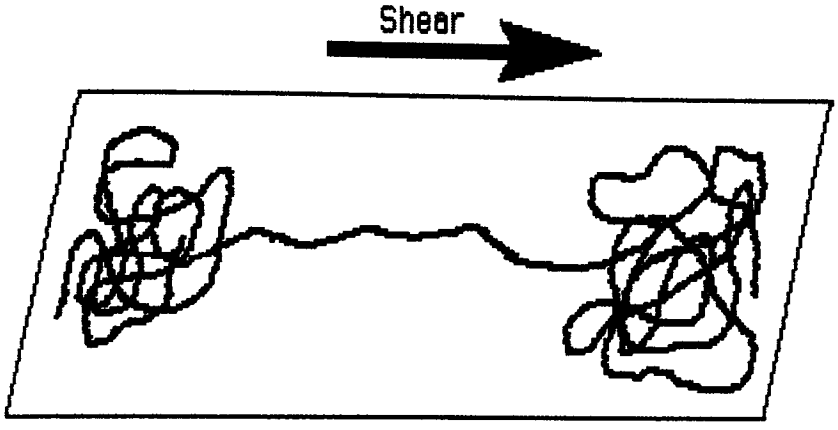


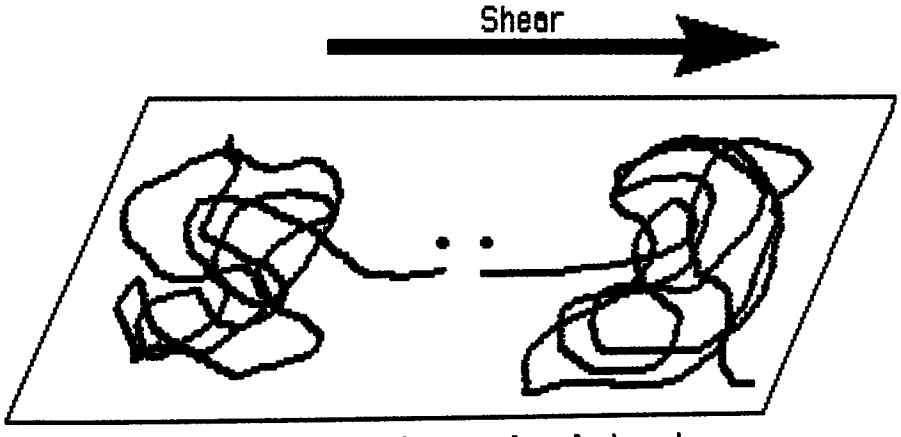
Figure 1.10. General mechanochemical reactions.



Polymer molecule not subjected to shear.



Shear applied to polymer molecule



Shear exceeds critical value, molecule breaks.

Figure 1.11 General mechanism of mechanochemical reactions.

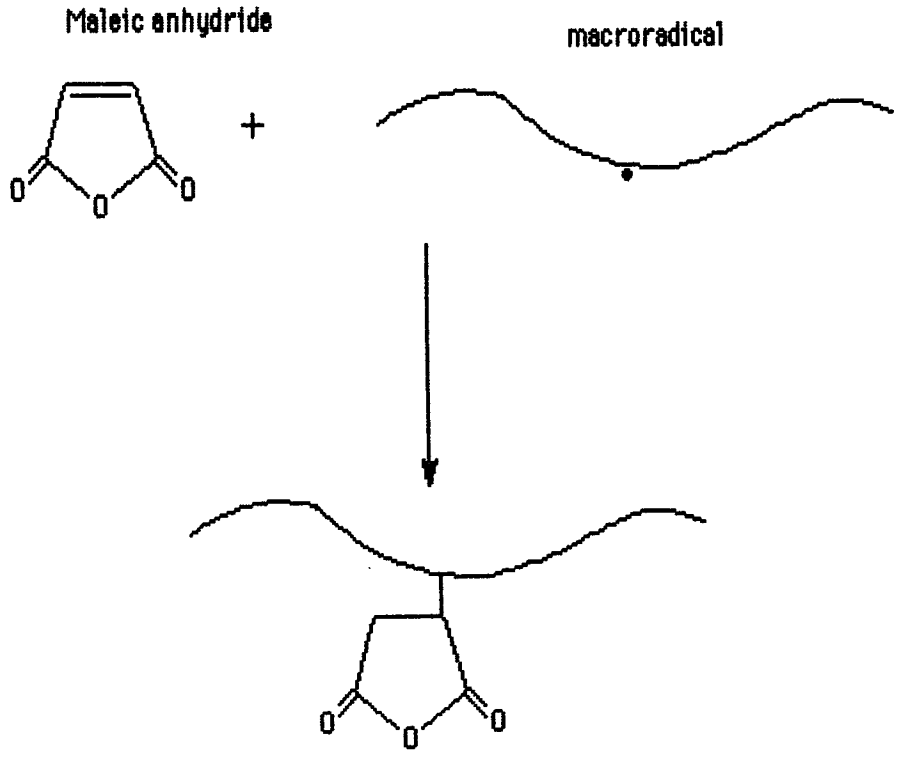


Figure 1.12 Reaction between a macroradical and maleic anhydride.

Chapter 2

Experimental.

2.1 Materials.

2.1.1 Polymers.

Three different grades of polypropylene (supplied by Imperial Chemical Industries Ltd) were used in this work. These are described in Table 2.1.

2.1.2. Glass fibres.

Two types of glass fibre were used in this work (supplied by Owens Corning Ltd) FGCS1640 (GF-CL) and R16E (GF-NH) grades. GF-CL is manufactured from borosilicate low alkali "E" type glass and is commercially used for incorporation into nylons and polyolefins. It has an average fibre length of 3mm and is coupled with 3-chloropropyltrimethoxysilane. GF-NH is also manufactured from "E" type glass, it has an average fibre length of 4.5mm and is coupled with 3-aminopropyltriethoxysilane. All the fibres were supplied coated with a layer of "size" to ensure good fibre dispersion. For the physical and chemical properties of these fibres see Table 2.2

2.1.3 Commercial chemicals.

Maleic anhydride (99.5% pure), Cyanuric chloride (97% pure), Allylamine (98% pure), Di-butylamine (99% pure) and 3-chloropropyltrimethoxy silane (97% pure) were used as supplied by Aldrich chemical Co. Ltd.

Sucinnic anhydride (99% pure), Di-cumyl peroxide (90% pure), 3-aminopropyltriethoxy silane (97% pure) and N-dodecane (99% pure) were used as supplied by BDH chemicals Ltd.

Table 2.4 shows the structures of the commercial chemicals

Table 2.1 ICI polypropylene grades used.

ICI Code Name	MFI* g/10min	Description
Propathene HF26	5.0	Unstabilised powder
Propathene HWM25	4.6	Highly stabilised injection moulding grade
Propathene HW60/GR30		30% coupled glass reinforced injection moulding grade

* 230°(±0.5°C), Die diameter 2.095mm, Load 2.16Kg.

Table 2.2 Physical and chemical properties of glass fibres [100, 101]

Fibre Property.	Fibre	
	FGCS1640 (GF-CL)	R16E (GF-NH)
Chemical Constitution (%).	B (3.4), Ca (1.9), O (61.2), Fe (1.4), Mg (0.6), Al (7.0), Si (24.3)	
Fibre diameter	10μm	
Fibre Length Weight average Number average	 3.0mm 3.0mm	 4.5mm 4.5mm
Aspect ratio	300	450
Split strand tex	95 tex	
Moisture content	0.2% (max)	
Size content	1.4% ($\pm$0.2%)	
Coupling agent	3-chloropropyl-trimethoxy silane.	3-aminopropyl-triethoxy silane.

Table 2.3A Commercial chemicals.

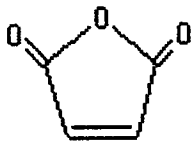
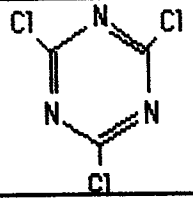
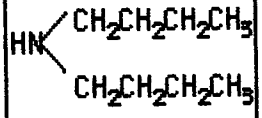
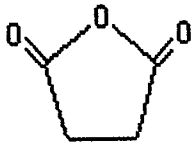
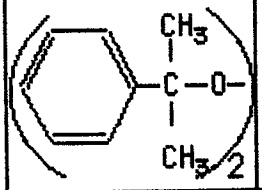
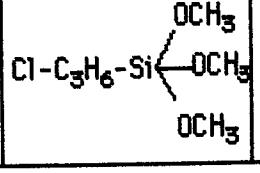
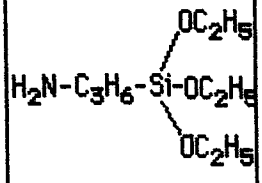
Code name	Chemical name	Structure	Mp (Bp) (°C)	FW
MA	Maleic anhydride		54-56	98
CCCT	Cyanuric chloride		145-148	184
ALM	Allylamine	$H_2NCH_2CH{=}CH_2$	(53)	57
DBA	Di-butylamine		(159)	129
SA	Succinic anhydride		119-120	100
DCP	Di-cumyl peroxide		Half life at 180°C 2 minutes	270
CLS	3-chloropropyl trimethoxy silane		(195)	198

Table 2.3B commercial chemicals.

Code name	Chemical name	Structure	Mp (Bp) (°C)	FW
AMS	3-aminopropy triethoxy silane		(217)	221
DD	N-dodecane	$C_{12}H_{26}$	(216)	170

MA e

Table 2.4A Synthesised modifiers based on maleimide.

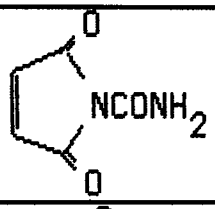
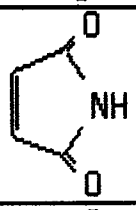
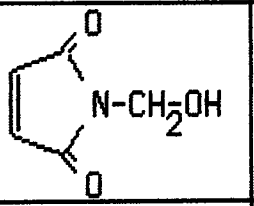
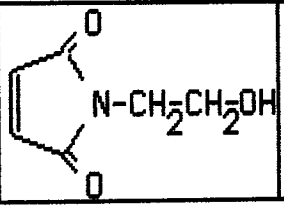
Code name	Chemical name	Structure	Mp (Lit value) (°C)	Ref	FW
NCA	N-Carbamyl-maleamic acid	$H_2NCONHCOCH$ $HOOCCH$	159 (160)	102	158
NCM	N-carbamyl-maleimide		156-158 (157)	102	140
MAL	Maleimide		91 (93)	102	97
NMM	N-methylol-maleimide		103-105 (105)	103	127
NEM	N-ethylol-maleimide		95 (96)	104	145

Table 2.4B Synthesised modifiers based on maleimide.

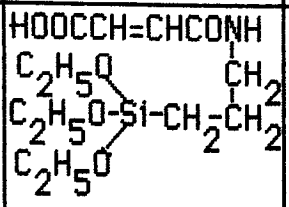
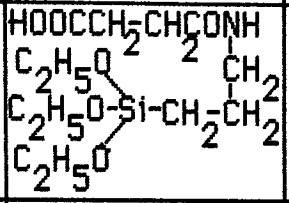
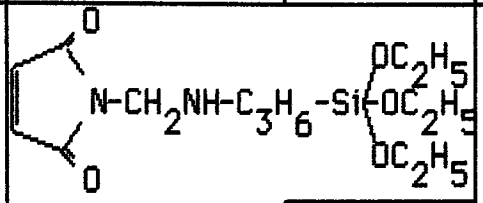
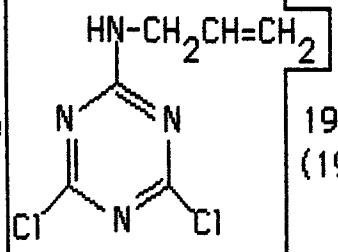
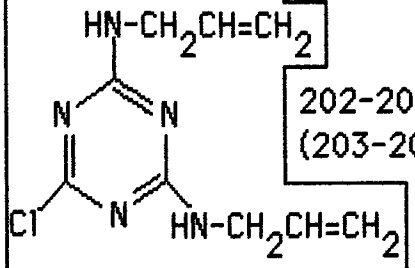
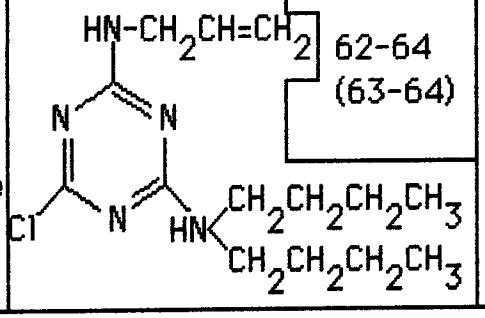
Code name	Chemical name	Structure	Mp (Bp) (°C)	Ref	FW
SMA	N-(-3-propyl-triethoxy-silane)-maleamic acid		Polymerised (red solid)		319
SSA	N-(-3-propyl-triethoxysilane)maleosuccinnic acid		Polymerised (red solid)		321
NMA	N-3-amino-propyltrieth-oxysilanemethanolmaleimide		Polymerised (red solid)		330

Table 2.4C Synthesised modifiers based on triazine.

Code name	Chemical name	Structure	Mp (Lit value) (°C)	Ref	FW
ACCT	2-allylamino-4,6-dichloro-1,3,5-triazine		196-198 (196-198)	105	204
AACT	2,4-diallyamino-6-chloro-1,3,5-triazine		202-204 (203-205)	106	225.5
ABCT	2-allylamino-4-chloro-6-dibutylamino-1,3,5-triazine		62-64 (63-64)	106	297.5

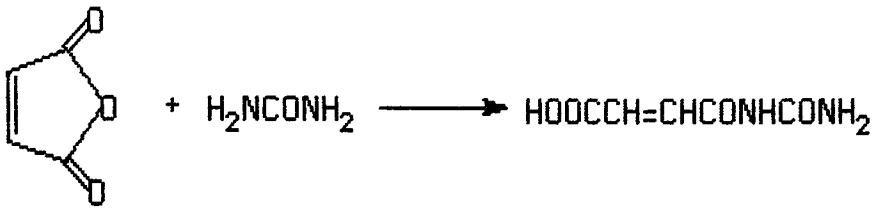
2.1.4 Synthesised modifiers.

A Summary of all modifiers synthesised in this work are shown in tables 2.4 A B C. Infrared spectra of these modifiers are shown (figure 2.1 to 2.10), together with spectral data (table 2.5) and elemental analysis (table 2.6).

2.1.4.1 Synthesis of maleimide (MAL)[102].

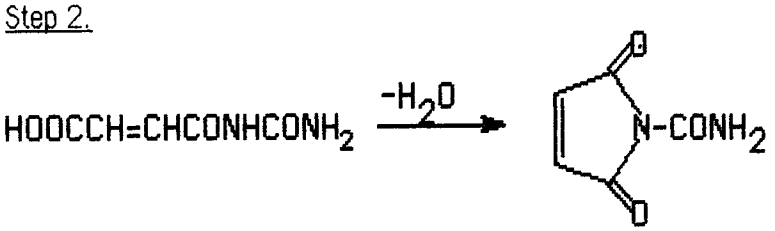
Maleimide was synthesised using the following three stage process.

Step 1.



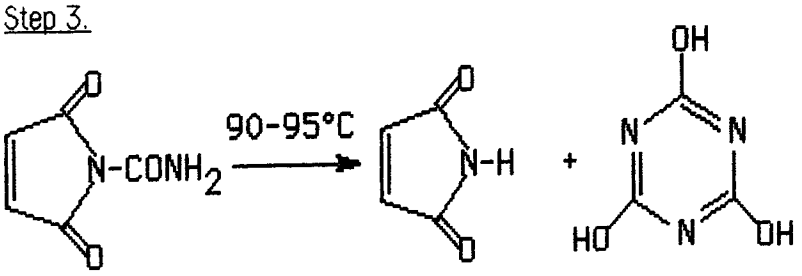
(MA) (NCA)

Step 2.



(NCA) (NCM)

Step 3.



(NCM) (MAL)

Step 1 N-carbamylmaleamic acid (NCA).

490g (5 moles) of maleic anhydride (MA) and 300g (5 moles) of urea were dissolved in 2000ml of glacial acetic acid at 55°C and maintained at this temperature for 12 hours. The solution was then allowed to stand at room temperature for 24 hours to give a white precipitate of N-carbamylmaleamic acid (NCA). This was filtered off, washed with glacial acetic acid and dried under vacuum at 50°C. To the remaining glacial acetic acid solution were added a further 196g (2 moles) of MA and 120g (2

moles) of urea. This solution was heated at 50°C for 5 hours, then allowed to stand at room temperature a further 12 hours to give a further precipitate of NCA, which was treated as before. The reuse of the glacial acetic acid solution was repeated a further 3 times after which it was finally discarded. The overall yield of product was 96%. The product NCA was used for step 2 without any purification.

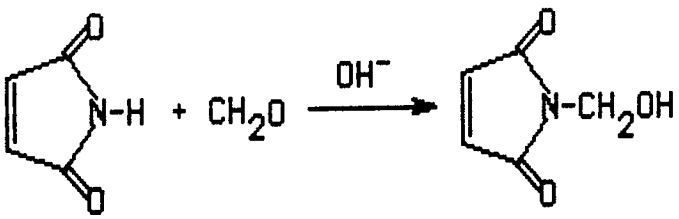
Step 2 N-carbamylmaleimide (NCM).

158g (1 mole) of N-carbamylmaleamic acid (NCA) was dissolved in 500ml acetic anhydride at 90°C. After 30 minutes the solution was filtered hot, then cooled to room temperature to give a white precipitate of N-carbamylmaleimide (NCM). The filtered product was washed with 100ml of cold acetone and dried under vacuum at room temperature; the product yield was 65% NCM and was used for step 3 without any further purification.

Step 3 Maleimide (MAL).

To 300ml of di-methyl formamide (DMF) at 90-95°C over an oil bath was added slowly with stirring 140g (1 mole) of N-carbamylmaleimide (NCM). During the exothermic reaction period which followed, a maximum temperature of 100°C was recorded, after which 90-95°C was maintained for 1 hour. After cooling to room temperature the white precipitate of cyanuric acid was filtered off and DMF removed under vacuum at 60°C. The product (MAL) was purified by recrystalisation from ethyl acetate (yield 25%).

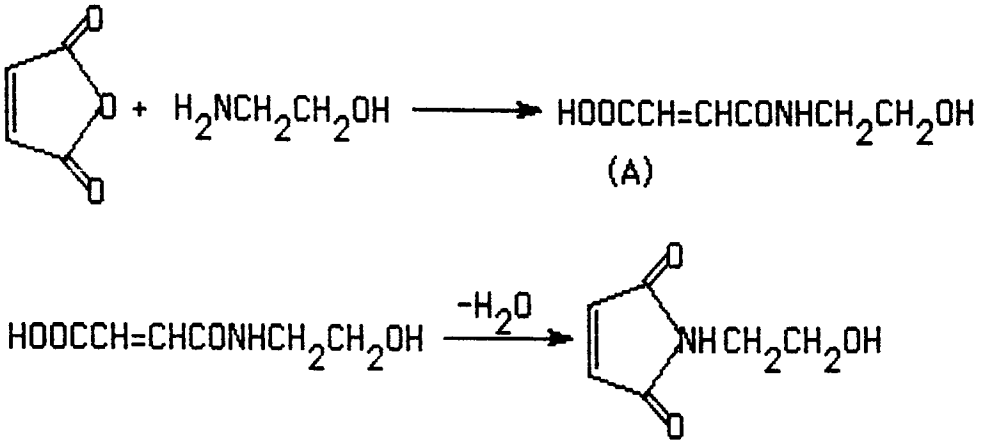
2.1.4.2 Synthesis of N-methylolmaleimide (NMM) (103).



(MAL) (NMM)

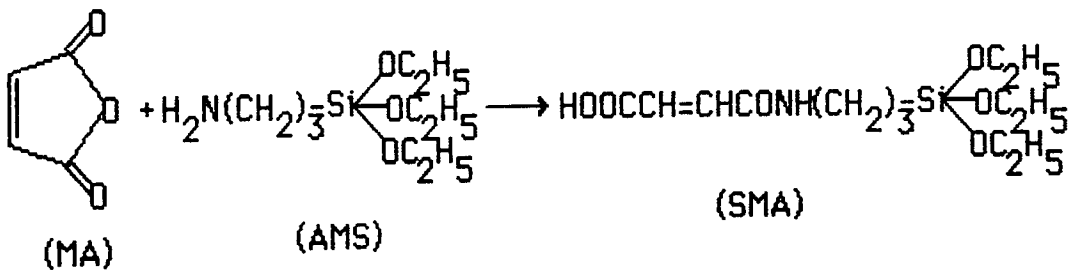
To a solution of 10g of 37% formalin solution (0.12 moles) and 0.5 ml 5% sodium hydroxide solution was added 9.7g (0.1 moles) of MAL. The solution was agitated for 10 minutes in an ultrasonic bath to ensure efficient dissolution of the MAL. The solution was allowed stand for 24 hours after which time a crop of colourless crystals of crude N-methanolmaleimide (NMM) were removed by filtration. The crude product (NMM) was purified by recrystallisation from ethyl acetate to give a white solid with a yield of 50%.

2.1.4.3 Synthesis of N-Ethanolmaleimide (104).



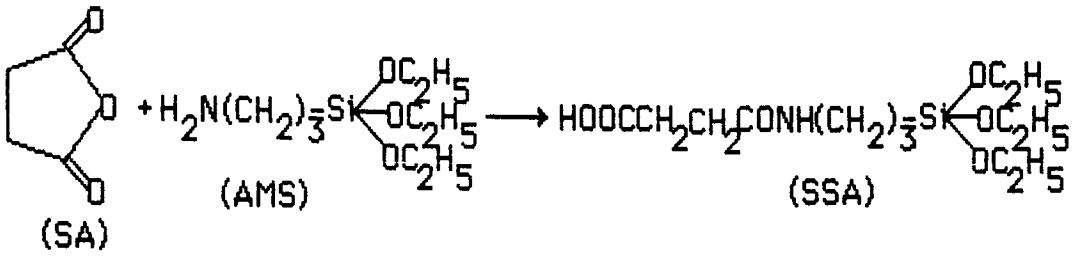
30.5g (0.5 moles) of 2-aminoethanol was slowly added with stirring to a solution of 49g (0.5 moles) of maleic anhydride (MA) in 500ml of dry di-methyl formamide (DMF). The solution was stirred for a further 2 hours to yield the intermediate (A) in DMF solution. The solution was heated to 60°C and acetic anhydride 250ml was added with stirring; the heating and stirring were continued for 30 minutes after the addition of the acetic anhydride. As much of the DMF as possible was removed under 5 mm Hg vacuum at 50°C to give a sticky brown solid which was filtered off and washed with a large excess of distilled water to give a white solid (yield 35%) of N-Ethanolmaleimide (NEM).

2.1.4.4 Synthesis of N-(-3-propyltriethoxysilane)maleamic acid (SMA). (11)



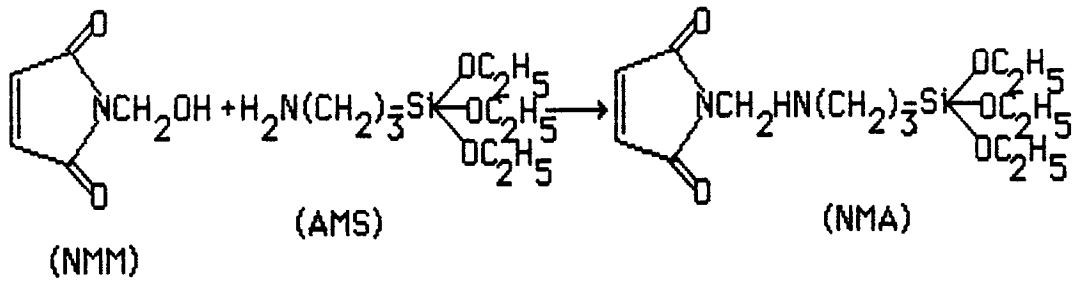
4.9g (0.05 moles) maleic anhydride (MA) were dissolved in 100ml chloroform at room temperature. To this solution was added 11.05g (0.05 moles) 3-aminopropyltriethoxy silane (AMS) and the solution was stirred for 1 hour at room temperature to yield a pale yellow solution. The chloroform was removed under 5mm Hg vacuum at room temperature to give a viscous yellow liquid (yield 80%), N-(-3-propyltriethoxysilane)maleamic acid (SMA).

2.1.4.5 Synthesis of N-(-3-propyltriethoxysilane)maleosuccinic acid (SSA) (12).



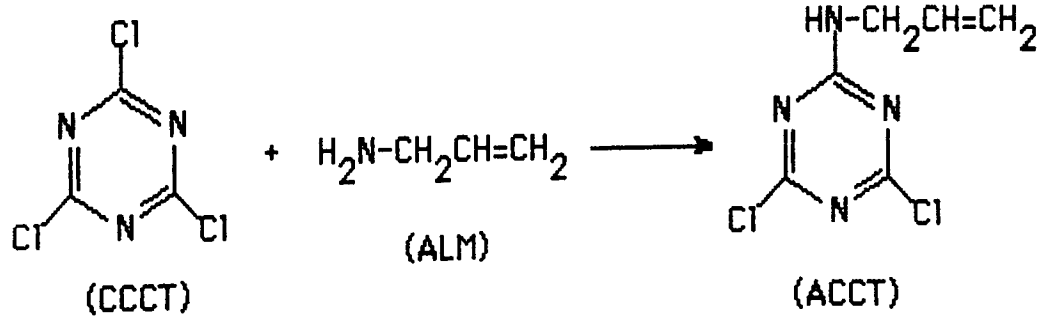
15g (0.05 moles) succinic anhydride (SA) was dissolved in 100ml chloroform at room temperature. To this solution was added 11.05g (0.05 moles) 3-aminopropyltriethoxy silane (AMS) and the solution was stirred for 2 hours at room temperature to yield a pale yellow solution. The chloroform was removed under 5mm Hg vacuum at room temperature to give a viscous yellow liquid (yield 80%) N-(-3-propyltriethoxysilane)maleosuccinic acid (SSA).

2.1.4.6 Synthesis of N-3-aminopropyltriethoxysilanemethylmaleimide (NMA).



2.54g (0.02 moles) N-methanolmaleimide (NMM) was dissolved in 80ml dioxane at room temperature. To this solution was added 4.42g (0.02 moles) 3-aminopropyltriethoxysilane (AMS). The solution was stirred for 24 hours at room temperature during which time it turned yellow. The dioxane was removed under 3mm Hg vacuum at room temperature to yield a yellow liquid (NMA); product 79%.

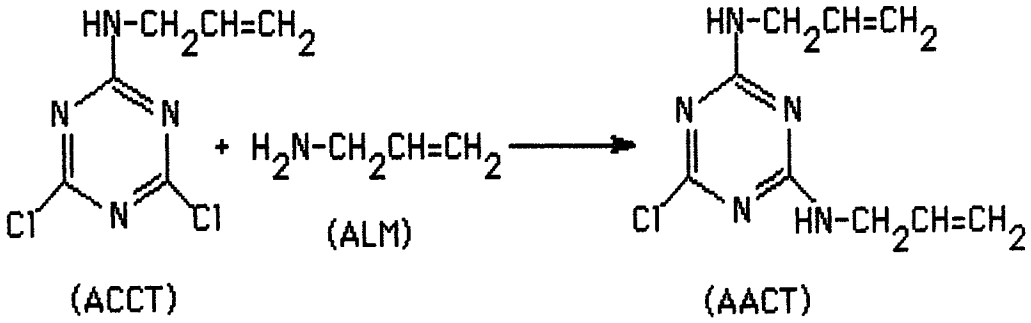
2.1.4.7 Synthesis of 2-allylamino-4,6-dichloro-1,3,5-triazine (105) (ACCT).



18.5g (0.1 moles) cyanuric chloride (CCCT) was dissolved in 200ml acetone, this

solution was poured over 1000ml of crushed stirred ice water, 8.4g (0.1 moles) sodium bicarbonate and 5.7g (0.1 moles) allylamine (ALM) were then added. The mixture was stirred until all the ice had melted. The white solid product (ACCT) was removed by filtration, washed with distilled water and dried under vacuum at room temperature. The product was obtained in a yield of 75% and used without further purification.

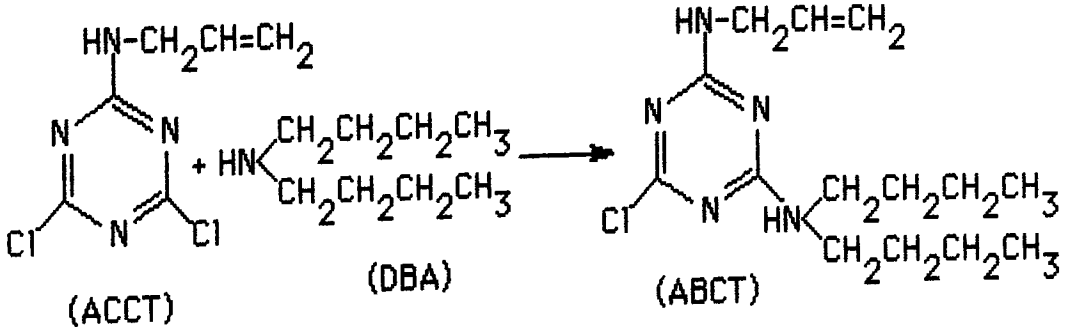
2.1.4.8 Synthesis of 2,4-di-allylamino-6-chloro-1,3,5-triazine[106] (AACT).



(ACCT) (AACT)

2-Allylamino-4,6-dichloro-1,3,5-triazine (ACCT) was prepared as in section (2.1.4.9) except that the solid product was not removed from the aqueous solution. The solution was warmed to 40°C in a water bath and a further 5.7g (0.1 moles) allylamine (ALM) and 8.4g (0.1 moles) sodium bicarbonate were added. The solution was stirred at 40°C for 60 minutes after which it was allowed to cool to room temperature. The white precipitate of 2,4-di-allylamino-6-chloro-1,3,5-triazine (AACT) was removed by filtration, washed with distilled water and dried in a vacuum oven at room temperature; the product of AACT was 68%.

2.1.4.9 Synthesis of 2-Allylamino-4-chloro-6-dibutylamino-1,3,5- triazine[106] (ABCT).



(ACCT) (ABCT)

2-Allylamino-4,6-dichloro-1,3,5-triazine (ACCT) was prepared as in section (2.1.4.9) except that the solid product was not removed from the aqueous solution. The solution was warmed to 40°C, 13g (0.1 moles) di-butylamine (DBA) and 8.4g (0.1

moles) sodium bicarbonate were added and the solution stirred at 40°C for 60 minutes. The solution was allowed to cool to room temperature, the white product 2-allylamino-4-chloro-6-dibutylamino-1,3,5-triazine (ABCT) was removed by filtration, washed with distilled water and dried in a vacuum oven at room temperature. The product ABCT was obtained in a yield of 65% and used without further purification.

Table 2.5. Infrared characteristics of synthesised modifiers.

Code name.	Wavenumber (Cm^{-1})	Description
MAL	3257 1732	-CONH, solid state, N-H stretching C=O, anhydride
NMM	3462 1718	Hydrogen bonded -OH C=O, anhydride
NEM	3492 1717	Hydrogen bonded -OH C=O, anhydride
SMA	1717	C=O, α,β unsaturated carboxylic acid
SSA	1725	C=O, carboxylic acid
ACCT	1642 1296	C=C stretching Triazine
AACT	1642 1309	C=C stretching Triazine
ABCT	1600 1309	C=C stretching Triazine

Table 2.6 Elemental analysis results.

Code Name	Formula	% carbon		%Hydrogen		%Nitrogen	
		Calc	Fd	Calc	Fd	Calc	Fd
MAL	$C_4H_3NO_2$	49.6	49.5	2.9	3.1	14.5	14.7
NMM	$C_5H_5NO_3$	47.2	47.1	4.0	4.2	11.0	11.5
NEM	$C_6H_7NO_3$	51.1	50.8	5.0	4.7	10.0	10.9
ACCT	$C_6H_6Cl_2N_4$	35.3	35.0	3.0	3.6	27.4	28.1
AACT	$C_9H_{12}ClN_5$	47.9	47.1	5.3	5.7	31.0	31.8
ABCT	$C_9H_{24}ClN_5$	56.4	56.3	8.1	7,8	23.5	23.4

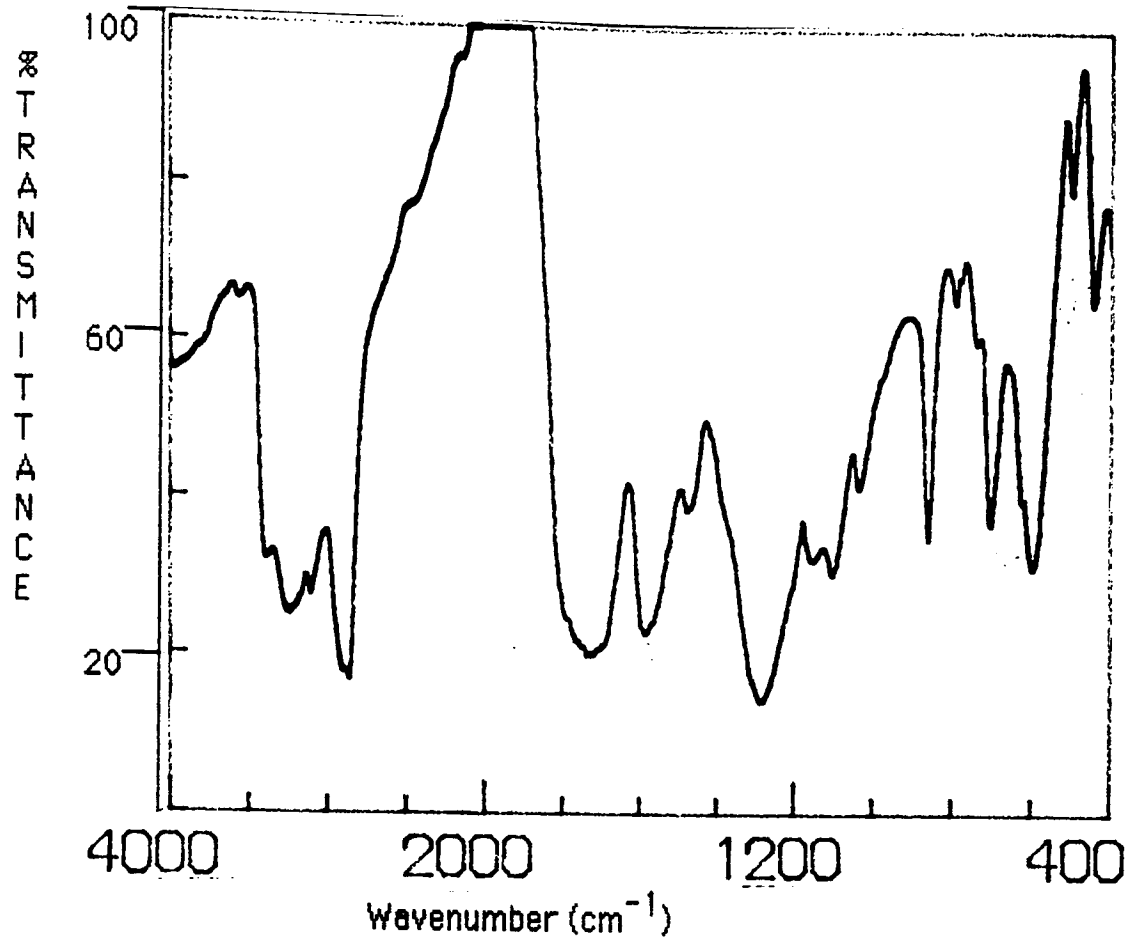


Figure 2.1 The infrared spectrum of MAL, (section 2.1.4.1), nujol mull (ref air).

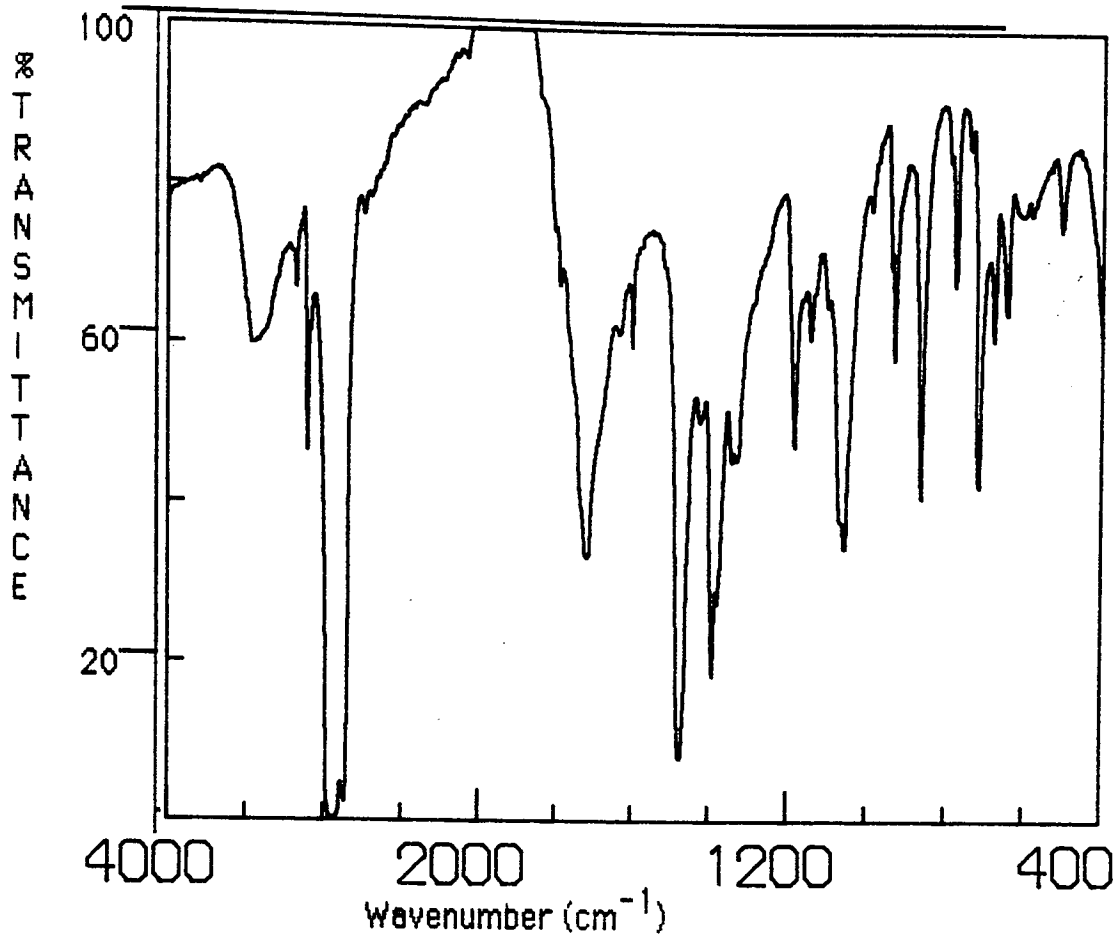


Figure 2.2 The infrared spectrum of NMM, (section 2.1.4.2), nujol mull (ref air).

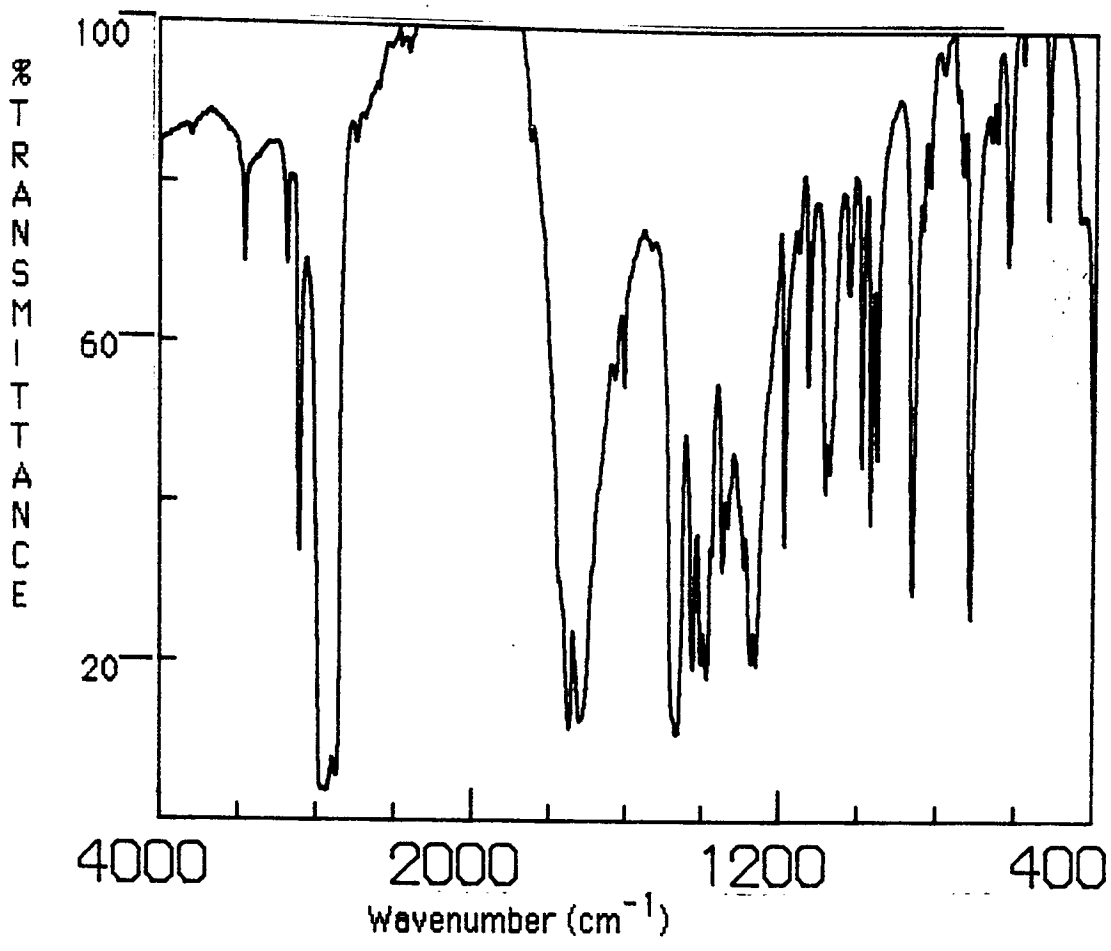


Figure 2.3 The infrared spectrum of NEM, (section 2.1.4.3), nujol mull (ref air).

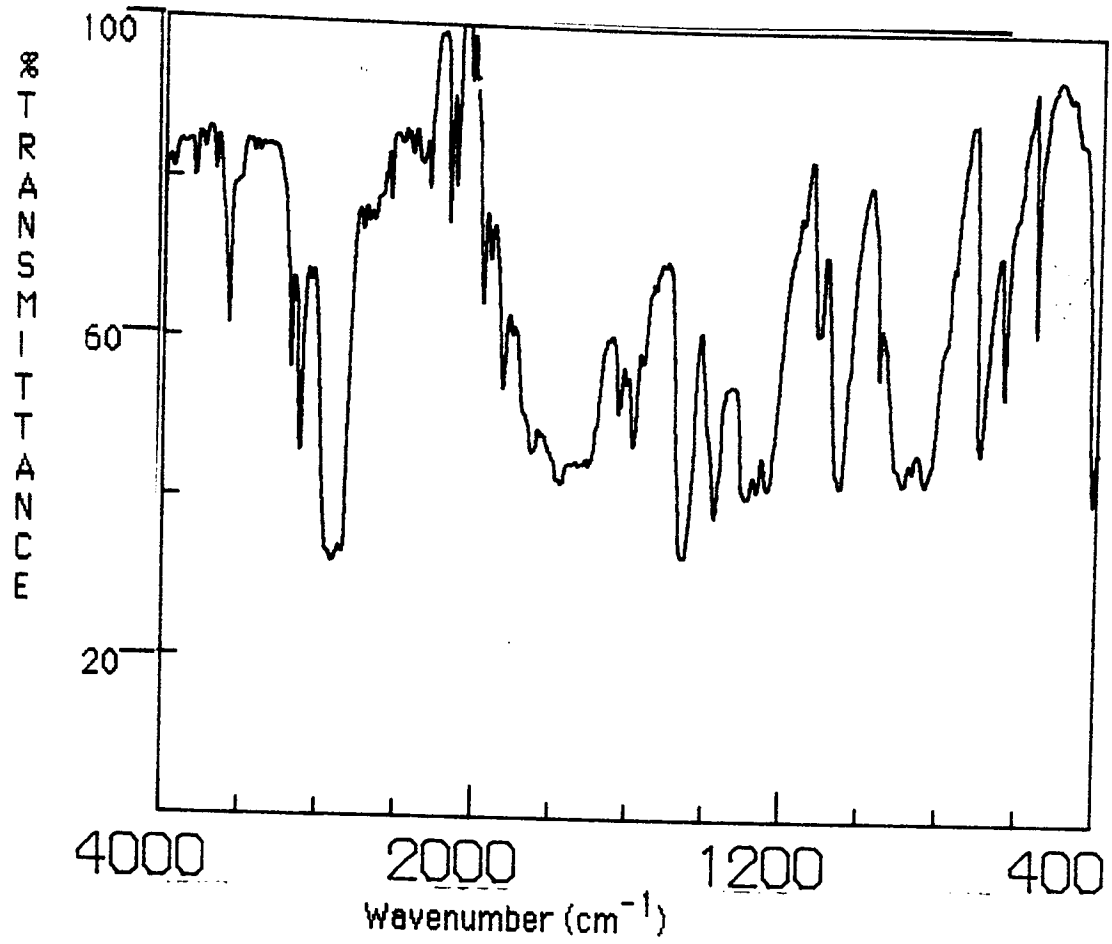


Figure 2.4 The infrared spectrum of ABMA, (section 2.1.4.4), nujol mull (ref air).

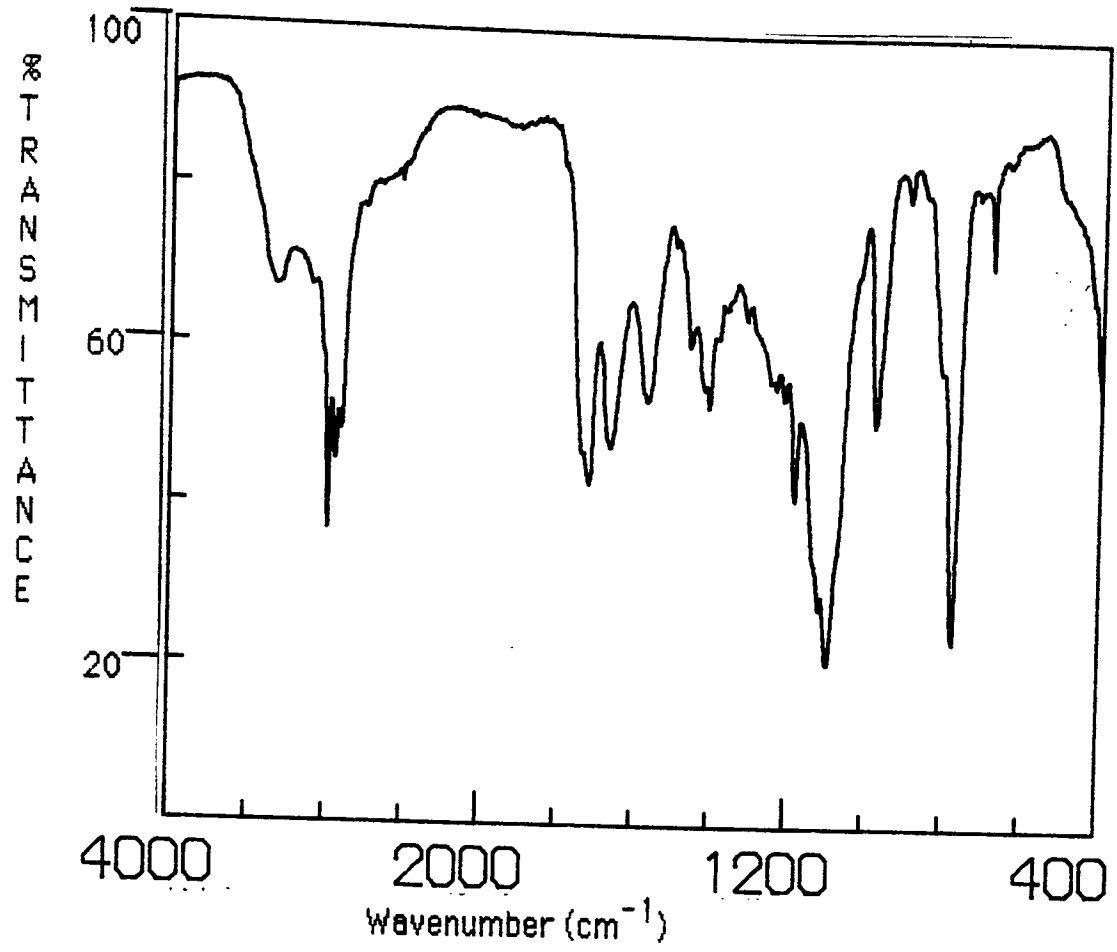


Figure 2.5 The infrared spectrum of SMA, (section 2.1.4.5), nujol mull (ref air).

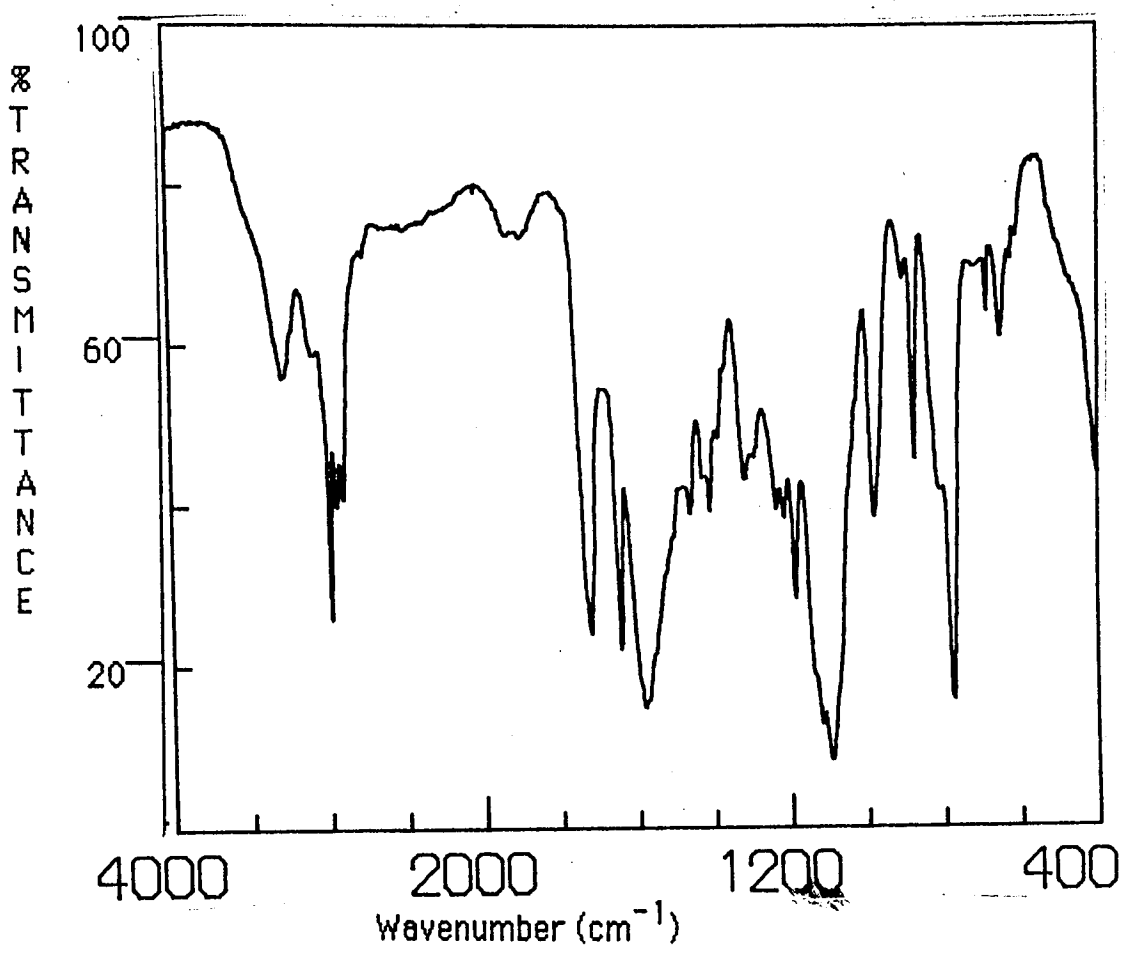


Figure 2.6 The infrared spectrum of SSA, (section 2.1.4.6), nujol mull (ref air).

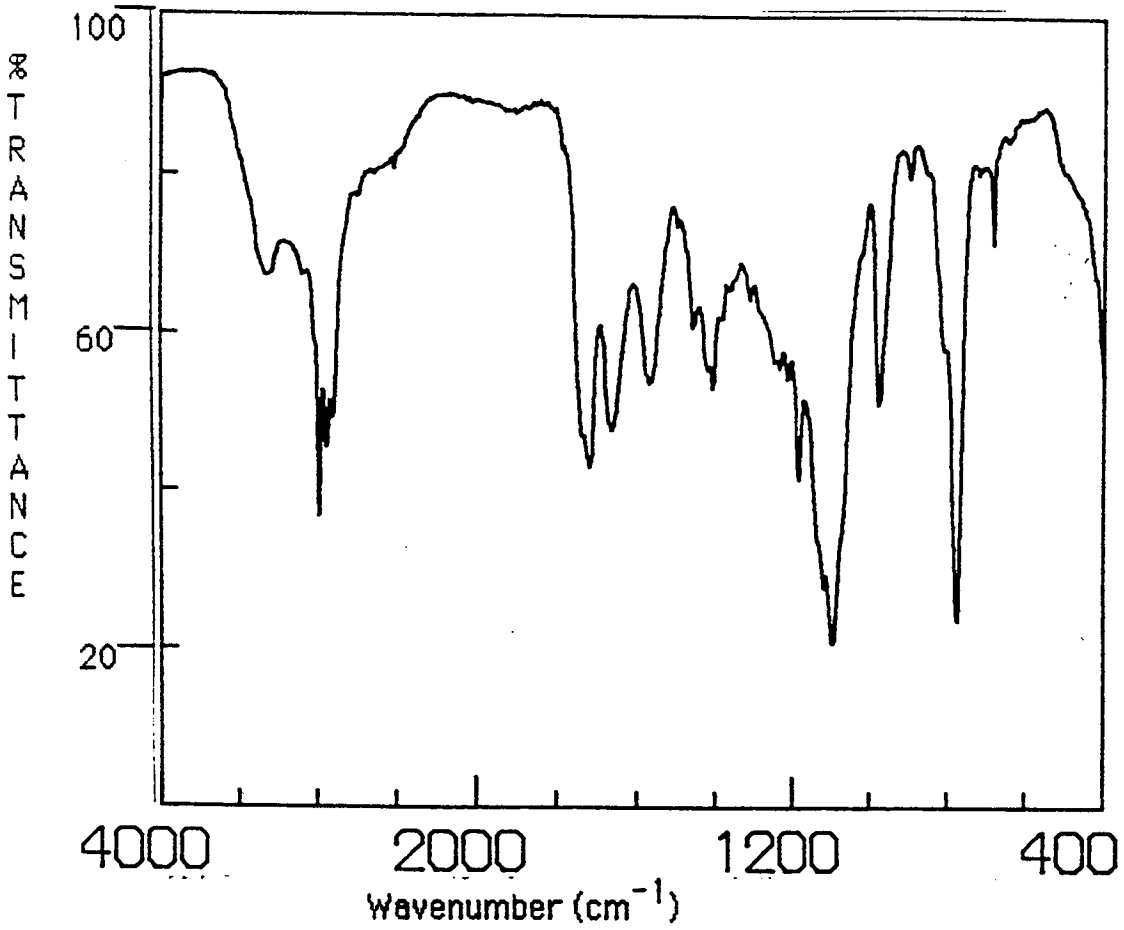


Figure 2.7 The infrared spectrum of NMA, (section 2.1.4.7); nujol mull (ref air).

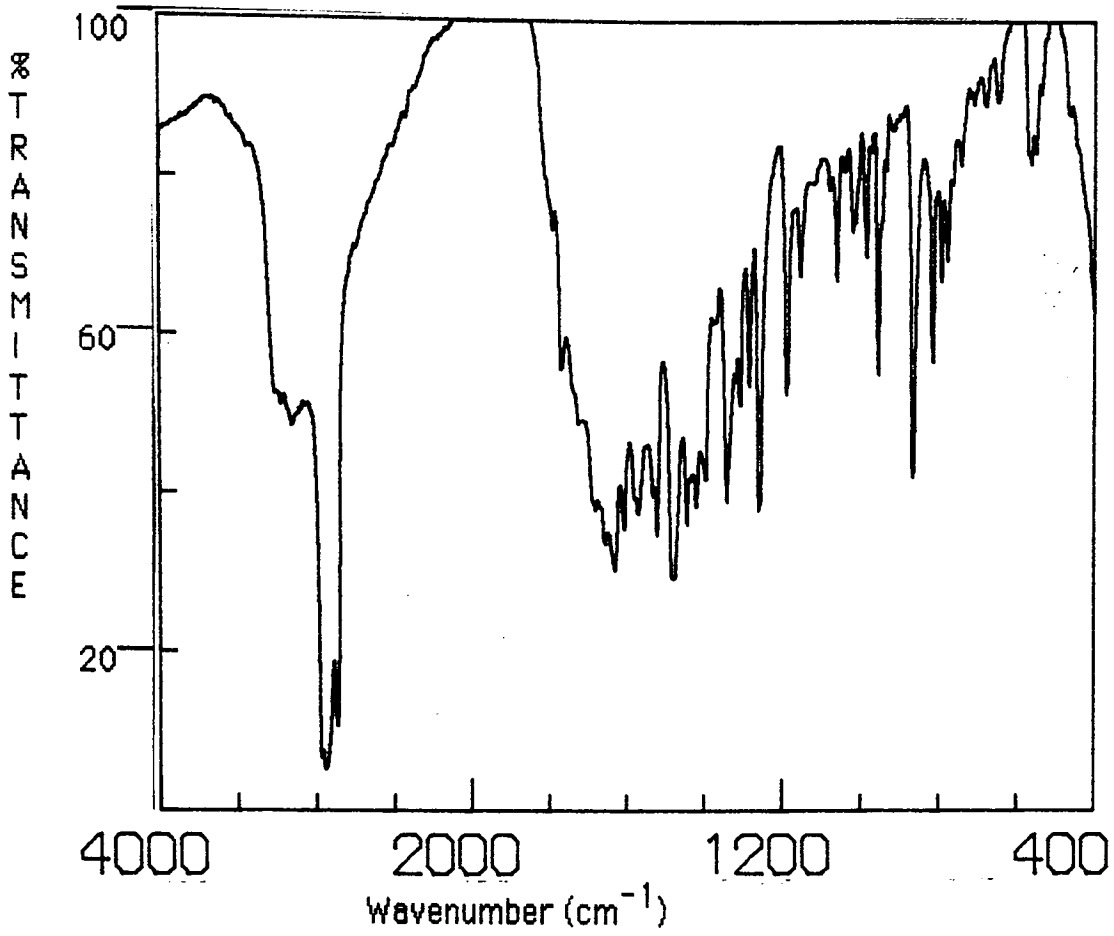


Figure 2.8 The infrared spectrum of ACCT, (section 2.1.4.8), nujol mull (ref air).

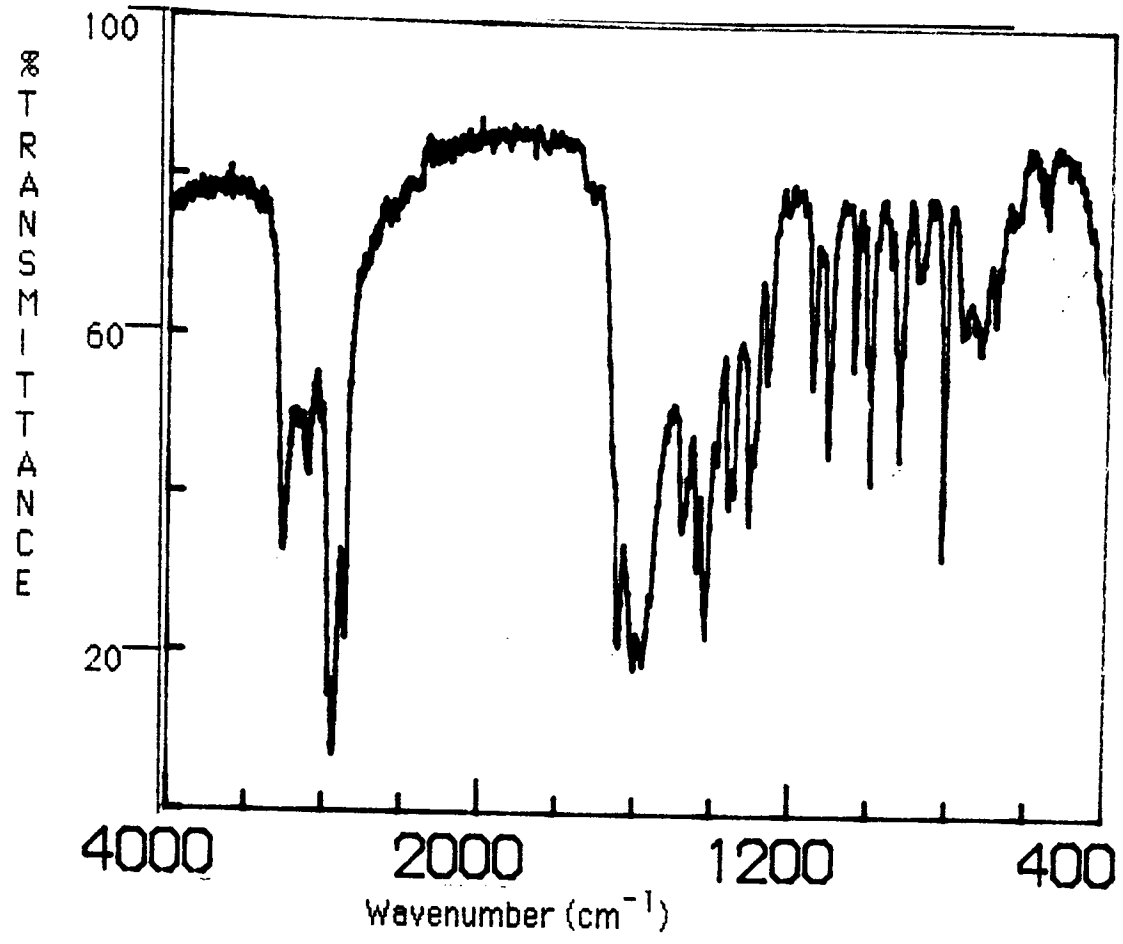


Figure 2.9 The infrared spectrum of AACT, (section 2.1.4.9), nujol mull (ref air).

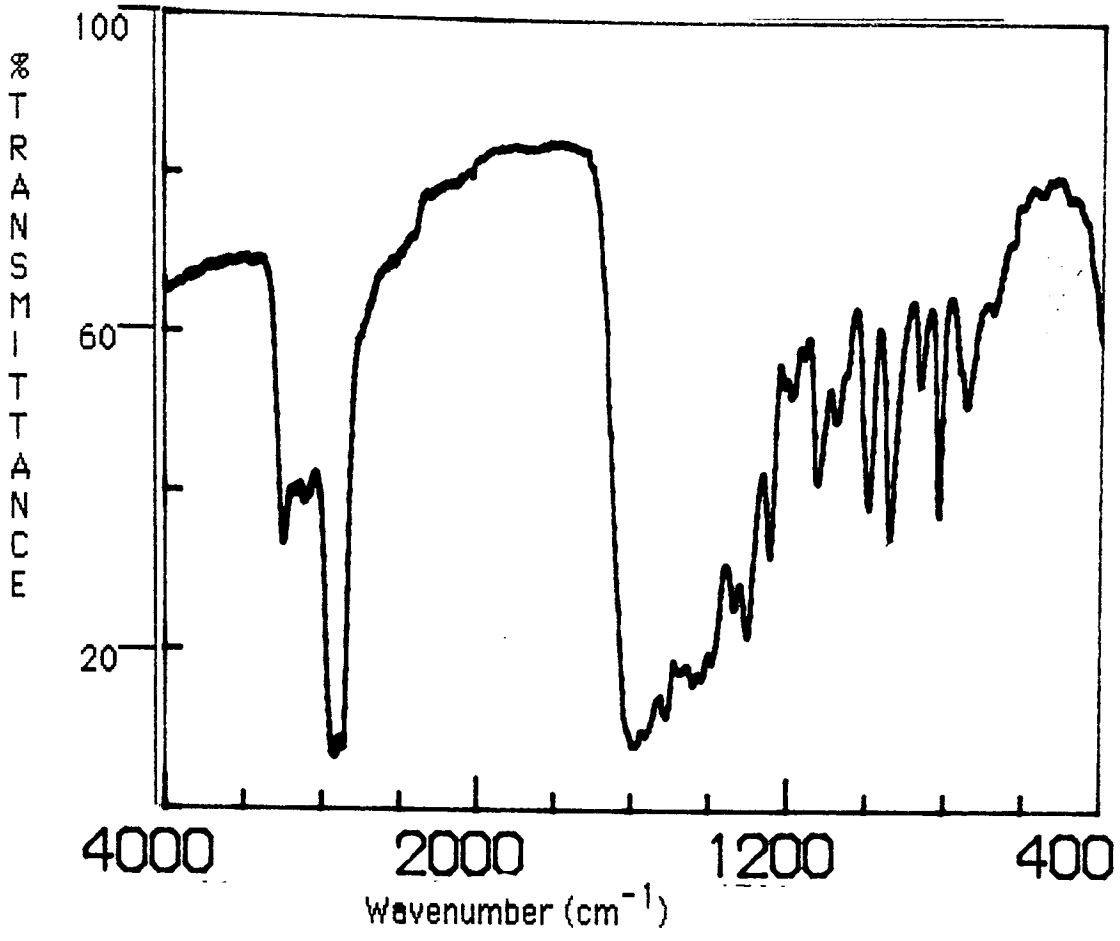


Figure 2.10 The infrared spectrum of ABCT, (section 2.1.4.10), nujol mull (ref air).

2.2 Composite preparation.

2.2.1 Continuous processing of modifiers and fibres for composite preparation, in a Buss Ko-Kneader.

Modifiers or fibres were mixed and homogenised with the base polymer by means of a laboratory scale Buss Ko-Kneader (model PR46). The Buss Ko-Kneader is a modified screw extruder, with the rotation of the screw being supplemented by a reciprocation of the screw to ensure high shearing and good mixing[107]. The screw speed is variable in the range 32 to 48 R.P.M. The temperature is controlled by means of an oil heater up to a maximum of 230°C. Back pressure from the die excludes air from the polymer melt. Polymer is fed in the screw by a pneumatic ram set vertically over the neck of the hopper. The up-stroke of the ram allows polymer to fall under gravity into the neck, the down-stroke forces the polymer through the neck into the screw. The up and down strokes of the ram are controlled by timers with a range 0 to 30 seconds, variation of the time allows the feed rate of the polymer to be controlled. The conditions used for the homogenisation of fibres and modifiers are shown in table 2.7.

Table 2.7 Buss Ko-Kneader compounding conditions.

Compounding material	Screw speed (RPM)	Barrel temp (°C)	Ram feed times (Sec)	
			Up	Down
Modifiers	48	175	2	4
Glass fibres	32	230	2	4
Rockwool	32	230	Material hand fed	

2.2.2 Grinding of homogenised polymers.

Polymer prepared on the Buss Ko-Kneader was granulated using a Maskin AB Rapid, granulator type GK75 EB. Polymer which had first been water cooled, if no glass fibre had been added or direct from the nozzle if glass fibre had been added was carried to the throat of the granulator by means of a conveyer belt. The polymer was granulated by blades mounted on a horizontal cylinder until it was small enough to pass through the 6mm diameter holes in the mesh underneath the blades. The polymer granules were then conveyed to a holding hopper by an air current.

2.2.3 Injection moulding.

The injection moulding of the test pieces for impact, tensile, flexural and creep testing was carried out in an Edgwick 1214-HY Type S (MkII) machine, see Table 2.8.

Table 2.8 Edgwick 1214-HY Type S (MK II) injection moulding machine parameters.

Machine parameter	Value
Maximum shot volume	95 cm^3
Injection rate	82 cm^3 sec^{-1}
Injection stroke	82.5 cm
Screw diameter	4.1 cm
Injection force	15311 Kg
Injection pressure range	0 to 1153 Kg cm^2
Die locking force	45000 Kg
Minimum batch size	300 g
Injection temperature	200-220°C
Mould temperature	25°C

2.3 Composite testing.

2.3.1 Tensile property tests.

Tensile testing was performed on a Testometric 500M tensometer[108] controlled by the tensile programme (appendix 1) running on an Apple IIe computer, according to ASTM D638M[109]. Five injection moulded dumb-bell test pieces from a mould of dimensions 12.5mm by 3.125mm were used for each determination. Prior to testing all the samples were stored at -10°C and removed 24 hours prior to testing to allow

them to condition to room temperature. A cross-head speed of 20mm min^{-1} was used so that rigid composites and unmodified polypropylene could be compared directly in one test. The following properties were recorded (see Figure 2.11).

Yield strength (YS) $\frac{\text{Load at yield X 100}}{\text{Cross sectional area (mm2)}}$ (Mpa)

Tensile modulus (TM) $\frac{\text{Stress (KN mm-2)}}{\text{Strain}}$ (Gpa)

Elongation at yield (EY) $\frac{\text{Extension at yield (mm)}}{\text{Original length (mm)}} \times 100$ (%)

Elongation at break (EB) $\frac{\text{Extension at break (mm)}}{\text{Original length (mm)}} \times 100$ (%)

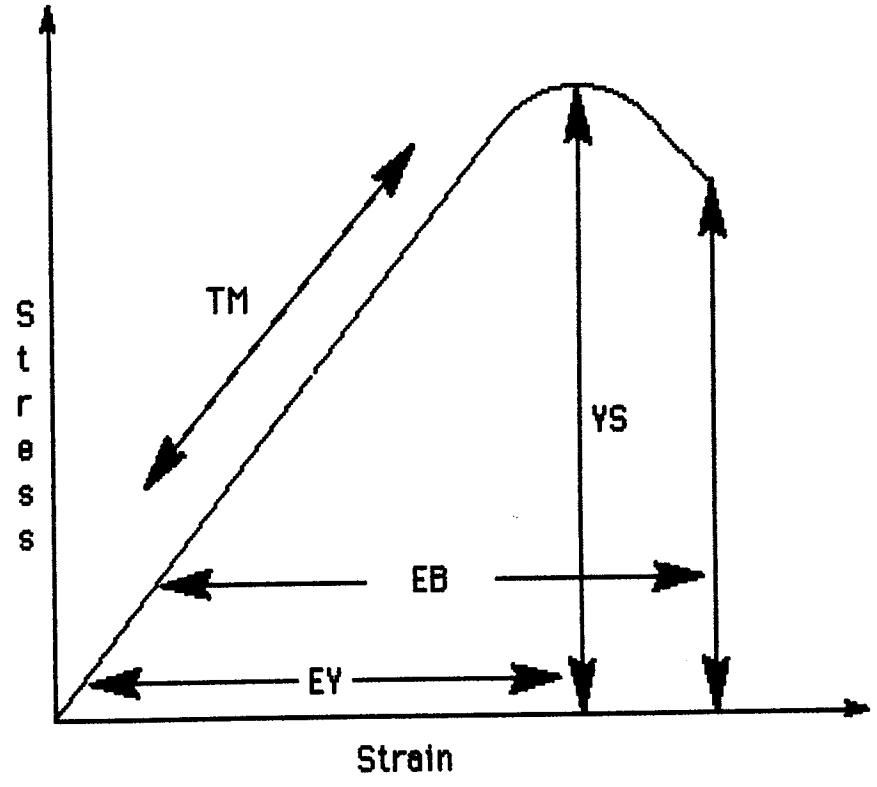


Figure 2.11 Typical polymer stress strain curve showing yield strength (YS), Tensile modulus (TM), Elongation at yield (EY) and Elongation at break (EB).

All the necessary calculations were carried out by the computer (see appendix 1).

2.3.2 Flexural property tests.

Three point flexural testing was carried out on a Testometric 500M tensometer[108] controlled by the flexural programme running on an Apple IIe computer, (appendix 2) according to ASTM D790M method 1[110]. Four injection moulded bars from a mould of dimensions, length 50mm, width 12.5mm and thickness 3.125mm were used for each test. Prior to testing all the samples were stored at -10°C and removed 24 hours prior to testing to condition to room temperature. A crosshead speed of 2mm min^{-1} was used so that rigid composites and unmodified polypropylene could be compared directly. The following properties were recorded.

Flexural strength (FS) $3PL/2bd^2$

Flexural modulus (FM) $(P/Q)/(L^3/4bd^2)$

Where L = Span (50mm).
b = Width (mm).
d = Thickness (mm).
p = Load (KN).
Q = Deflection (mm).

All necessary calculations were carried out by the computer (see appendix 2).

2.3.3 Impact property tests.

A Hounsfield plastic impact machine was used to measure the impact of un-notched samples. Five injection moulded bars of mould dimensions 3.125 mm by 12.5 mm were used for each determination. The sample was supported at both ends and subjected to impact from a falling pendulum onto a stress concentrator then onto the sample. The impact strength test was used only to rank samples on a comparative basis since such tests cannot be used to satisfactorily to predict the in service performance of a composite, due to the influence of temperature, geometry, orientation and impact velocity[111]. Tests were performed on samples at temperatures of -10 and 20°C. The following properties were recorded

Impact strength (IS) $\frac{\text{Energy of break (J).}}{\text{Width X Thickness } (mm^2)}$ (J mm-2)

All calculations were carried out by a computer (Appendix 3).

2.3.4 Water resistance tests of composites.

The attack of water on the glass polymer interface is a serious problem for composites which can result in a reduction in physical properties, the appearance of fibres and a roughening of the surface (112). There is no real correlation between these accelerated tests and the performance of a composite in outdoor conditions(112). The test used was a two hour water boil test which is considered to be equivalent to 30 days immersion in room temperature water(113). Three tensile test pieces were placed in boiling water for two hours, dried on paper, then left for 24 hours before tensile testing (See section 2.3.1). The performance of the composite before and after water immersion was compared.

2.3.5 Solvent resistance testing of composites.

The effect of a harsh chemical environment on the tensile properties of the prepared composites were determined by refluxing 4 tensile test pieces in Hexane and removing the samples at periods of 1, 24, 48 and 120 hours. The tensile properties were determined as in section 2.3.1. Hexane was chosen as the solvent to simulate petrol.

2.3.6 Fibre length determination.

Fibre lengths were recorded by photographing the fibres on a glass slide through a Vickers Photoplan optical microscope. To obtain statistically representative ranges of fibre lengths 500 individual fibre lengths were recorded. A photograph of a calibrated grating was taken so the lengths of the fibres on the photograph could be translated into their actual lengths. To calculate the initial fibre length before processing the raw fibres were simply spread over a glass slide. For processed samples the embedded fibres were removed from the polymer matrix by hot soxhlet extraction of the sample with xylene. The results were used to produce histograms of % total content at each fibre length versus fibre length. From this the weight average and number average lengths were calculated using the following formula:

$$\text{Number average length} = \Sigma NL / N$$

$$\text{Weight average length} = \Sigma NL^2 / \Sigma NL$$

Where

N = Number of fibres

L = Length of fibre (mm)

See Figures 2.12 and 2.13 for fibre length distributions of GF-CL and GF-NH respectively.

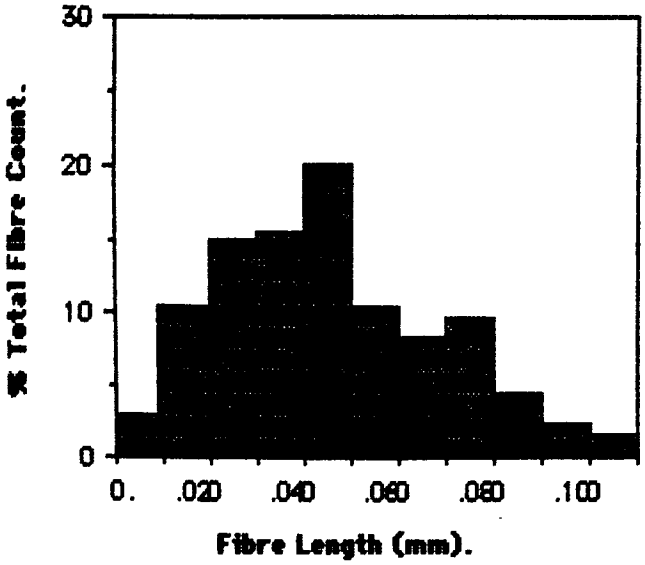


Figure 2.12 Histogram of fibre length distribution for injection moulded GF-CL homogenised in Buss Ko-Kneader 240°C, 48rpm.

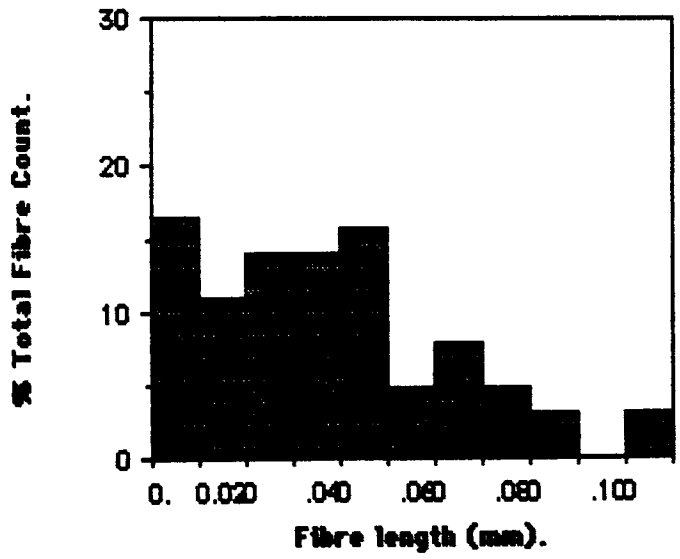


Figure 2.13 Histogram of fibre length distribution for injection moulded GF-NH homogenised in Buss Ko-Kneader 240°C, 48rpm.

2.4 Batch processing in an internal mixer (Hampden RAPRA torque rheometer).

Melt processing was carried out in a Hampden RAPRA Torque rheometer(114) which is a laboratory scale internal mixer with a capacity of 36g in the case of polypropylene. The temperature of the mixing chamber is controlled by means of an oil jacket. The mixing chamber can be closed by means of a pneumatic ram to limit the access of atmospheric oxygen to the polymer, (closed mixing, CM) or it can be left open (open mixing, OM). The torque applied to the variable speed rotor blades can be recorded. The torque is related to the viscosity of the polymer, but because of the complex flow pattern in the rheometer it cannot be used to directly measure the viscosity. Measurement of the torque does however supply information concerning fusion, cross-linking, polymerisation and degradation of the polymer. Immediately on removal from the mixing chamber the polymer melt was immersed in cold water to quench any further reactions.

2.4.1 Polymer film preparation.

Polymer films approximately 0.2mm thick were prepared by placing 8g of polymer between two sheets of cellophane then sandwiched between two steel plates. The whole assembly was then placed in a preheated press at 180°C. Both platens were brought into contact with the plates and the assembly left to preheat for 1 minute. Full pressure (1 ton $in^{2)}$ was applied and the press was subsequently cooled, on reaching 60°C, (after approximately 10 minutes), the pressure was released, the press opened and the film removed.

2.4.2 Melt stability testing.

2.4.2.1 Gel permeation chromatography.

Thermal degradation of polypropylene involves chain scission associated with a decrease in molecular weight. Gel permeation chromatography (GPC) is a method by which the weight average (Mw) and number average (Mn) molecular weight of a polymer may be directly measured. Hence these measurements may be used to estimate the stability of a polymer melt. GPC measurements were carried out by RAPRA polymer supply and characterisation centre. The operating variables used were.

I	Columns	1×10^6A
		1×10^4A
		5×10^2A
II	Flow rate	1 ml min^{-1}
III	Solvent	1,2-dichlorobenzene stabilised with 2,6-di-tert-butyl-p-cresol.

IV Temperature 140'C

V Calibration Mark Houwink constants used for conversion via universal calibration.

(a) Polystyrene $K=1.38 \times 10^4$ dl g^{-1} a=0.7

Polypropylene $K=1.03 \times 10^4$ dl g^{-1} a=0.78

(b) Not corrected for peak broadening effects.

(c) Not corrected for variation of refractive index with molecular weight.

2.4.2.2 Melt flow index measurements.

The melt flow index (MFI) is defined as the weight of sample extruded through a standard die under standard conditions of load and temperature. The British standard 2782 (115) was used. A temperature of 230°C (±0.5°C) and a 2.16Kg weight were used with a die diameter of 2.095mm. The barrel was loaded with 4g of polymer in 1 minute excluding all trapped air, the material was then left for 4 minutes to come to equilibrium after which the 2.16Kg weight was applied and after a further minute extruded samples were cut every 30 seconds. The MFI was then calculated as follows:

MFI = Average weight extruded in 30 seconds X (600/30) g/10min

MFI is only suitable for comparative purposes and is normally used as a quality control test.

2.4.4 Chemical binding studies of polypropylene additives.

2.4.4.1 Continuous hot soxhlet extraction of polypropylene films

Polypropylene films were continuously extracted for a total of 72 hours with for 24 hours each dichloromethane, acetone and hexane. The dichloromethane and acetone were used to extract the modifiers, all the modifiers being soluble in one or both of these. The hexane was used as a wash to remove all traces of the other extraction media. All extractions were carried out in a soxhlet under a nitrogen atmosphere. The films were dried under vacuum for 12 hours at room temperature.

2.4.4.2 Continuous hot soxhlet extraction of polypropylene granules.

The extraction of granules was carried out in the same way as for films except that the extraction time was raised to 72 hours per solvent and the drying time to 24 hours.

2.4.4.3 Percentage binding calculations for polypropylene additives.

The percentage of modifier bound to polypropylene during melt processing was measured using infrared and ultraviolet spectroscopy.

2.4.4.4 Percentage binding from infrared spectroscopy.

The infrared spectra of extracted (section 2.4.5.1) and unextracted films were measured using a Perkin-Elmer 599A spectrometer controlled by Heyden Datasystems Spectrafile programme[116] version 1.1, running on an Apple IIe computer, see Figure 2.14.

$$\% \text{ binding} = \frac{A_2 - A_1}{A_3 - A_1}$$

Where

A_1 = Absorbance of polypropylene film with no modifier

A_2 = Absorbance of polypropylene film with modifier after extraction.

A_3 = Absorbance of film with additive before extraction.

For each additive a specific wavenumber corresponding to a strong absorbance was chosen.

2.4.4.5 Percentage binding from ultra violet spectroscopy.

The ultraviolet spectra of extracted and unextracted films were measured using a Beckmann DU7 spectrometer, controlled by the Beckmann mass storage accessory software[117], running on an Apple IIe computer. The percentage binding was calculated directly using the U.V data manipulation software Appendix 4. Figure 2.15.

$$\% \text{ Binding} = \frac{A2}{A3} \times 100$$

Where

A2 = Absorbance of polypropylene film with additive after extraction.

A3 = Absorbance of polypropylene film with additive before extraction.

It should be noted that the percentage binding results only account for the material present after melt processing and does not account for volatilised material.

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2.4.6 Quantitative determination of bound additive concentration in polypropylene films.

The molar concentrations of bound additives, after hot soxhlet extraction (see section 2.4.5.1) was determined from ultraviolet and infrared spectra of the extracted films.

2.4.6.1 Quantitative determination of bound additives from ultraviolet spectra.

The ultraviolet spectra of extracted films were measured using the procedure in section 2.4.5.5. At a particular λ max for each modifier the absorbance (A) was read from the spectra. Then from the path length (thickness of film) (L) and the molar extinction coefficient (E) calculated from characterisation of prepared compounds the molar concentration of the additive was calculated using the Beer-Lambert law (118).

$$C = \frac{A}{\epsilon L} = \text{concentration in (mol dm}^{-3}\text{).}$$

All calculations were carried out by the ultraviolet data manipulation programme (Appendix 4).

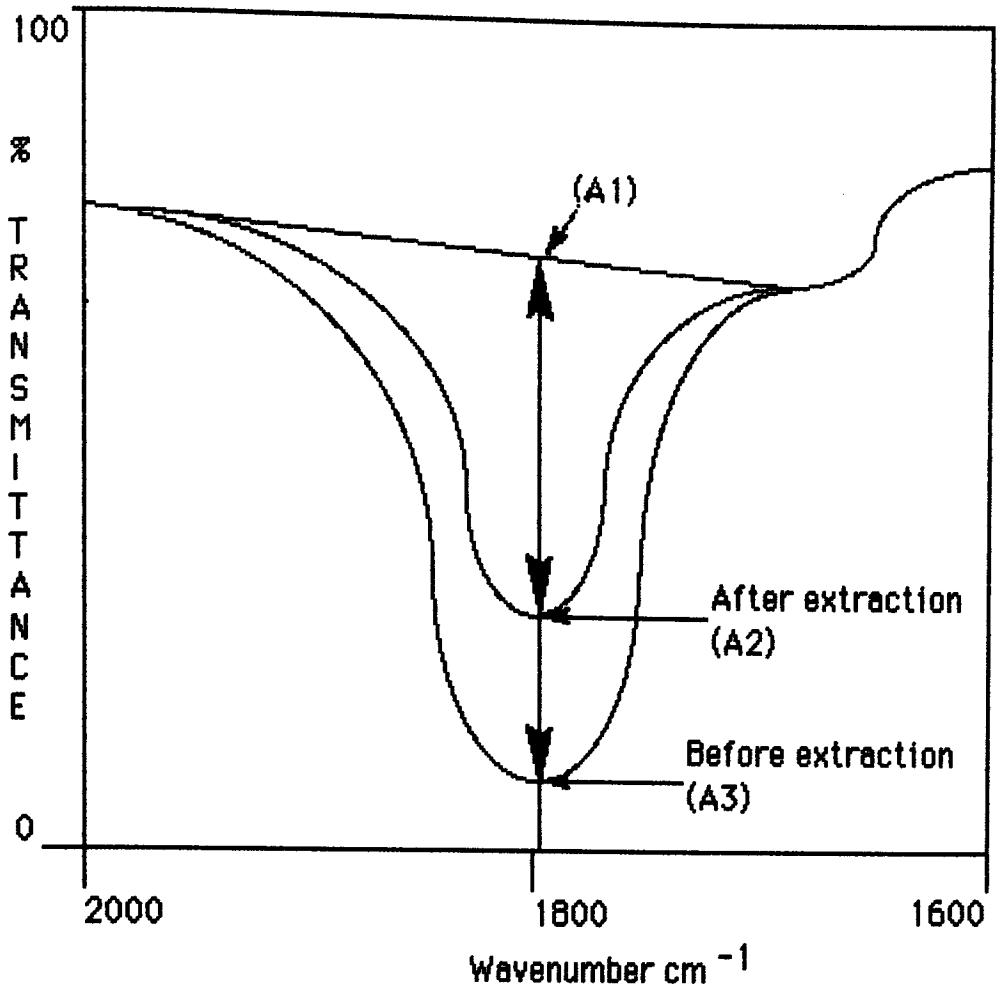


Figure 2.14. Typical infrared spectrum of a compound with an absorbance at 1795 cm^{-1}, before and after extraction.

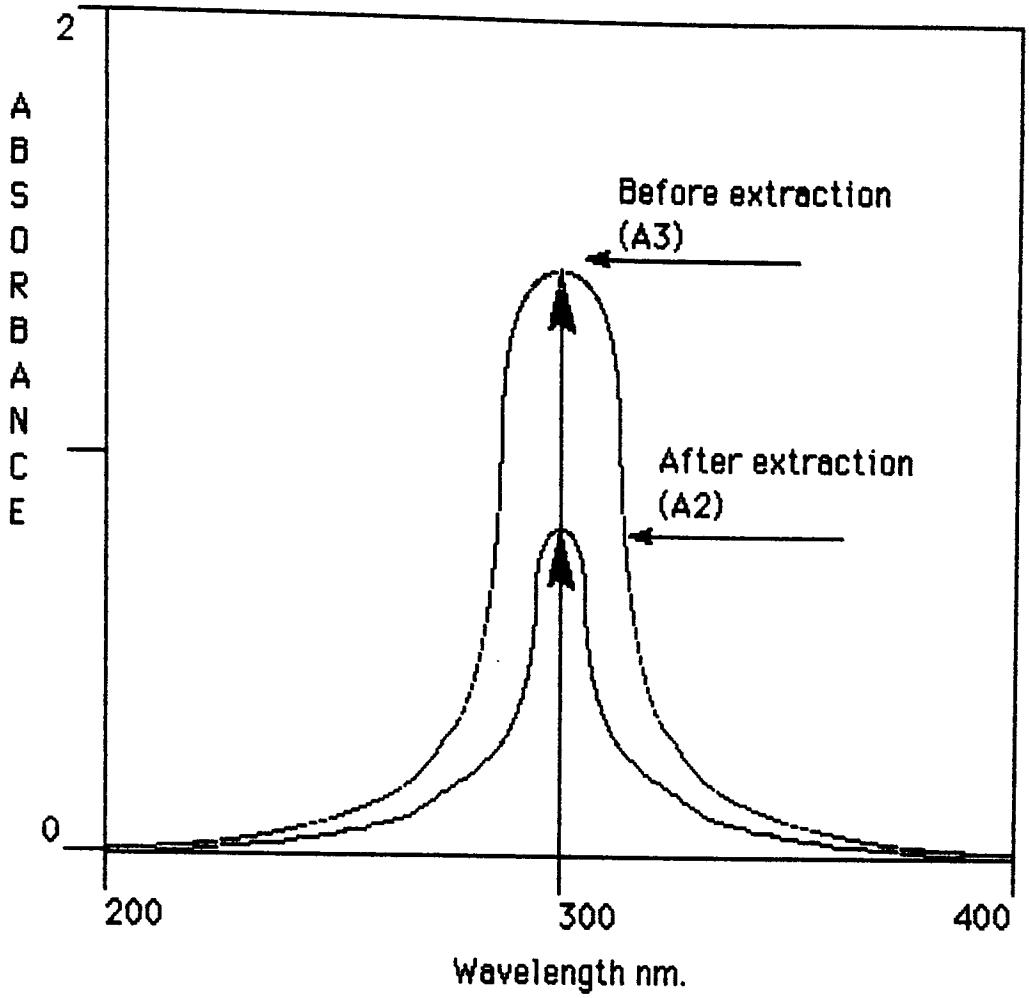


Figure 2.15. Example ultraviolet spectrum of a compound with an absorption at 300nm before and after extraction.

2.4.6.2 Quantitative determination of bound additive from infrared spectra.

The infrared spectra of extracted polypropylene films (see section 2.4.5.1) were measured using the procedure in section 2.4.5.4. At a particular wavenumber for each modifier, corresponding to a strong absorbance, the absorbance was calculated according to the procedure in section 2.4.5.4. The absorbance was then correlated against a calibration graph obtained by plotting absorbance of modifier in a suitable solvent) against modifier concentration (moles dm^{-3}) hence the modifier concentration could be determined. The figure obtained was multiplied by:

$$\frac{\text{Path length used in calibration curve}}{\text{Path length (width) of polypropylene film}}$$

to give the molar concentration (dm^{-3}) in polypropylene. Figures 2.16-2.22 for calibration graphs, the wavelength used to determine the binding is shown in the appropriate figure The equations above each graph show the slope, intercept and Spearmann rank correlation coefficient (r) for each graph.

2.5 Solution modelling of mechanochemical modification reactions.

In order to look in more detail at the chemical reactions involved during the mechanochemical modification of polypropylene a solution model was devised in order to allow easier analysis of the resulting products. The accurately weighed reactants were placed in a 25ml round bottomed flask along with 5g of N-dodecane to act like PP as a dispersive medium, a 1cm long PTFE coated magnetic follower was also added to allow for mixing of the reactants. The flask was purged with oxygen free nitrogen for 1 minute, stopped then placed in a preheated silicone oil bath for 5 minutes at 175°C. The flask was then removed, cooled rapidly in cold water and the liquid and solid products separated into sample bottles which were stored at -10°C until analysis.

2.5.2 Ultraviolet analysis of solution models.

The ultraviolet spectra of both the solid and liquid products of the solution models were measured on a Beckmann DU7 spectrometer connected to an Apple 11e computer running the Beckmann mass storage accessory software (117). The dodecane solutions were measured against a dodecane background in a 1cm quartz cell. Solid products were dissolved in 95% ethanol and measured against a 95% ethanol background in a 1cm quartz cell.

2.5.2 The infrared analysis of the solution models.

The infrared spectra of the solid and liquid products of the solution models were measured using a Perkin Elmer 1710 Fourier transform infrared (FTIR) spectrometer. Liquids were measured in a liquid cell with a path length of 0.544mm. Gels were measured as thin films between KBr plates. Solids were made into a mull with Nujol and measured as a thin film between KBr plates. All spectra were recorded as 20 scans at a resolution of $4cm^{-1}$ between $4000cm^{-1}$ and $220\ cm^{-1}$.

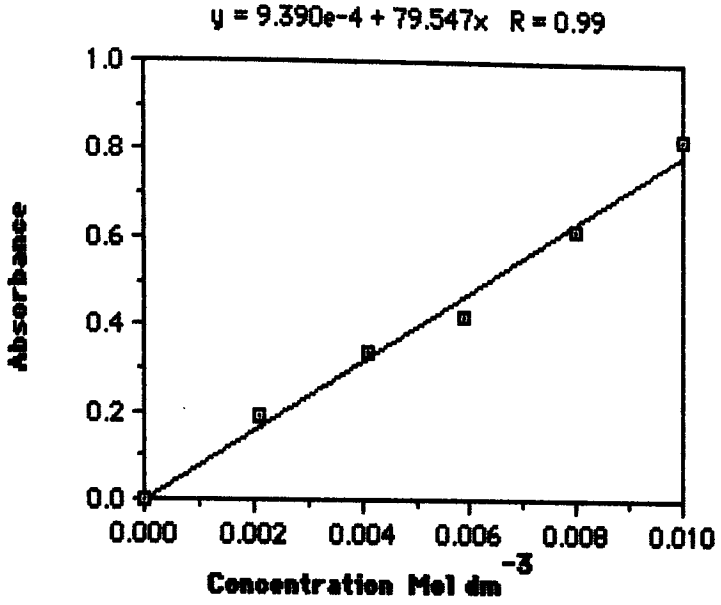


Figure 2.16. Calibration curve of infrared absorbance ($1792cm^{-1}$) for maleic anhydride (MA), path length 0.533mm in chloroform (ref.air).

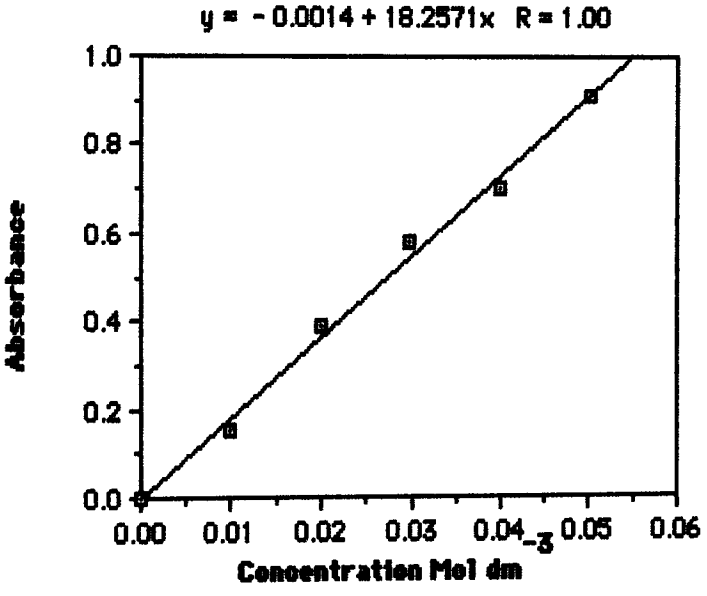


Figure 2.17. Calibration curve of infrared absorbance ($1720cm^{-1}$) for maleimide (MAL), path length 0.533mm in chloroform (ref.air).

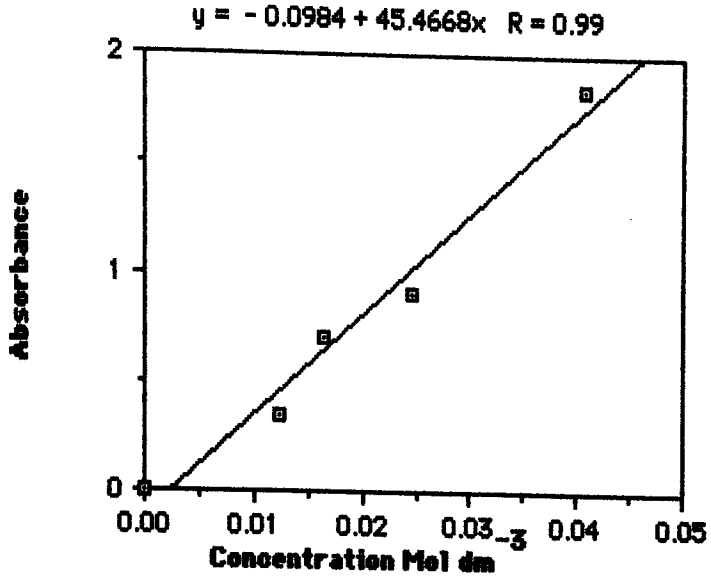


Figure 2.18. Calibration curve of infrared absorbance ($1718cm^{-1}$) for N-methanolmaleimide (NMM), path length 0.20mm in chloroform (ref.air).

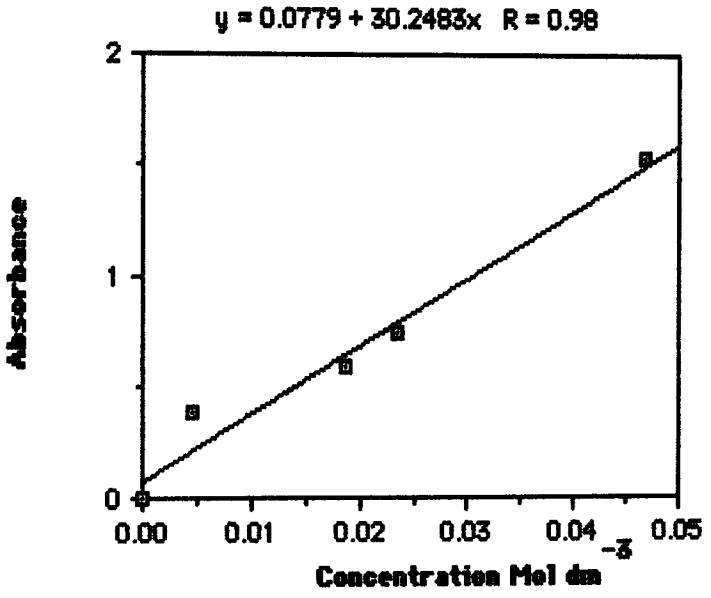


Figure 2.19. Calibration curve of infrared absorbance ($1717cm^{-1}$) for N-ethanolmaleimide (NEM), path length 0.20mm in chloroform (ref.air).

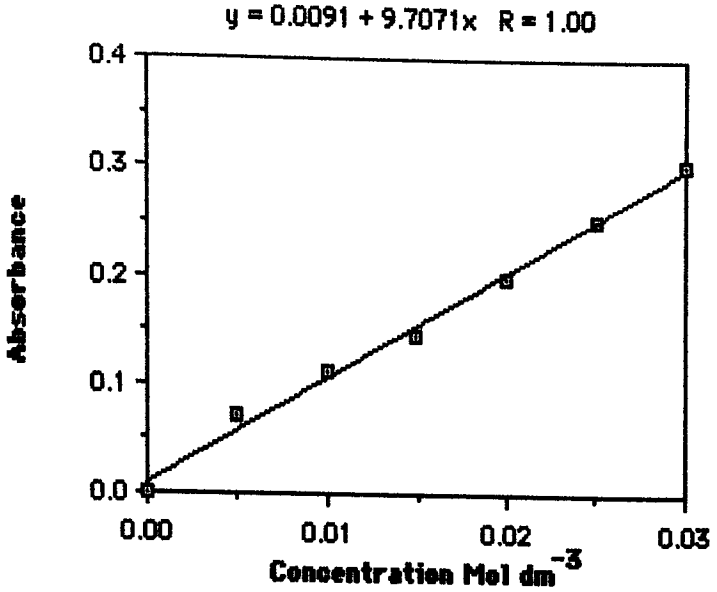


Figure 2.20 Calibration curve of infrared absorbance ($1565cm^{-1}$) for 2-allylamino-4,6-dichloro-1,3,5-triazine (ACCT), path length 0.20mm in chlorobenzene (ref.air).

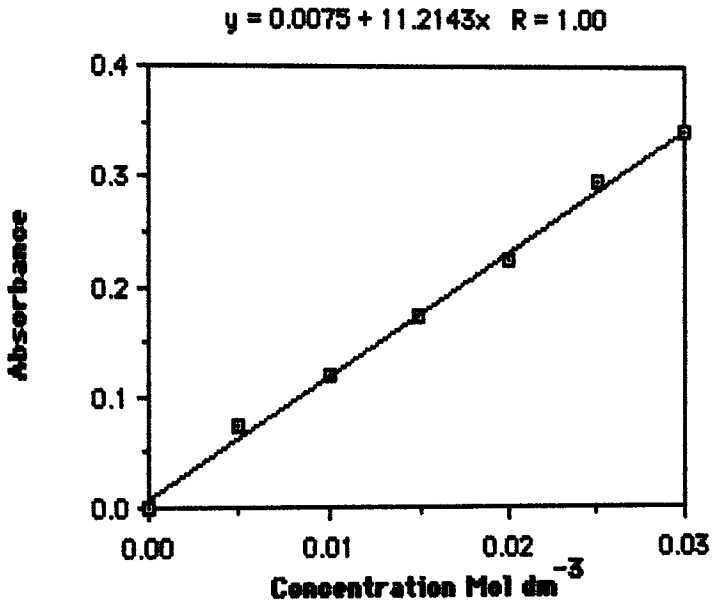


Figure 2.21 Calibration curve of infrared absorbance ($1565cm^{-1}$) for 2-chloro,4,6-diallylamino-1,3,5-triazine (AACT), path length 0.20mm in chlorobenzene (ref.air).

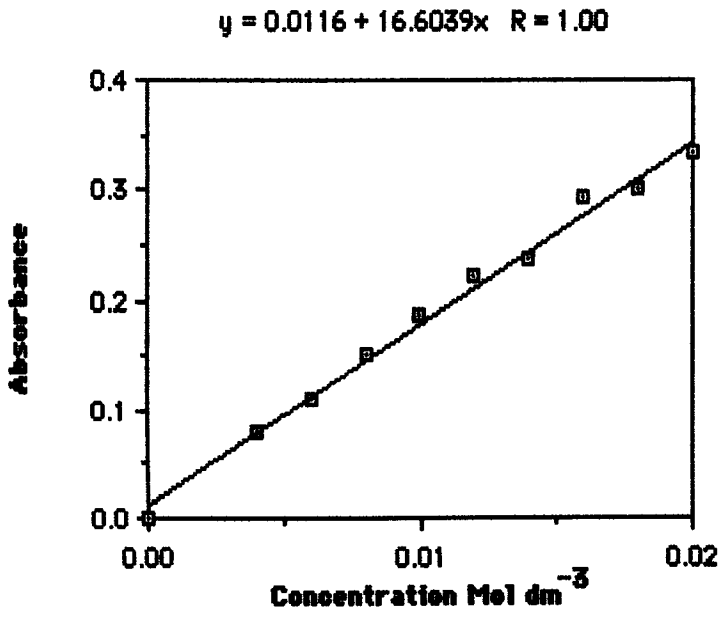


Figure 2.22 Calibration curve of infrared absorbance ($1565cm^{-1}$) for 2-allylamino-4-chloro-6-dibutylamino-1,3,5-triazine (ABCT), path length 0.20mm in chlorobenzene (ref.air).

Chapter 3.
The mechanochemical modification of polypropylene with di-cumyl peroxide, maleic anhydride and N-subsituted maleimides.

3.1 Outline and Plan.

The main objective of the study described in this chapter is to enhance the mechanical properties of glass fibre polypropylene (PP) composites by reactive processing of the PP with the modifiers (table 3.1). Generally, the modifiers chosen possess two reactive organic functional groups. One of the groups is a double bond. The double bond has been chosen since it can potentially bind to the PP by a free radical mechanism. The other organic functional group, which makes up the modifier, has been chosen for its potential reactivity towards the silane coupling agents, 3-chloropropyltrimethoxy silane (CLS) and 3-aminopropyltriethoxy silane (AMS) (table 3.1). These are present on the surface of the glass fibres GF-CL and GF-NH respectively. By forming a chemical bond with both glass fibre and PP, it is believed that the interfacial shear strength (τ) (see section 1.3) will be increased. Thus, the mechanical properties of the composite will be improved.

In this chapter, the chemical reactions which take place during the melt processing of PP HF26 (unstabilised PP) with modifiers (see scheme 3.1, table 3.1) are examined. To facilitate their examination these reactions have also been modelled in dodecane solution (see scheme 3.2). Finally, the mechanical properties of PP, GF-CL and GF-NH, composites reactively processed with the modifiers (see scheme 3.3) are examined.

Di-cumyl peroxide (DCP) was employed during the reactive processing to act as a free radical initiator. This was to encourage the reaction between the PP and the modifiers which contain a polymer reaction function (unsaturation).

Maleic anhydride (MA) was examined as a modifier since it has been extensively studied by other workers. The results obtained with MA may act as a milestone by which the other modifiers may be evaluated.

Succinic anhydride (SA) has been chosen for its similarity to MA whilst not possessing the unsaturation of the MA and thus reactivity towards the PP. It is hoped that studies of SA may help to elucidate the reactions of the MA with the silane coupling agents.

Cis maleic acid (MAC) has been studied to help to further elucidate the reactions of the MA. MAC possesses unsaturation but its potential reactivity towards the coupling agent is different.

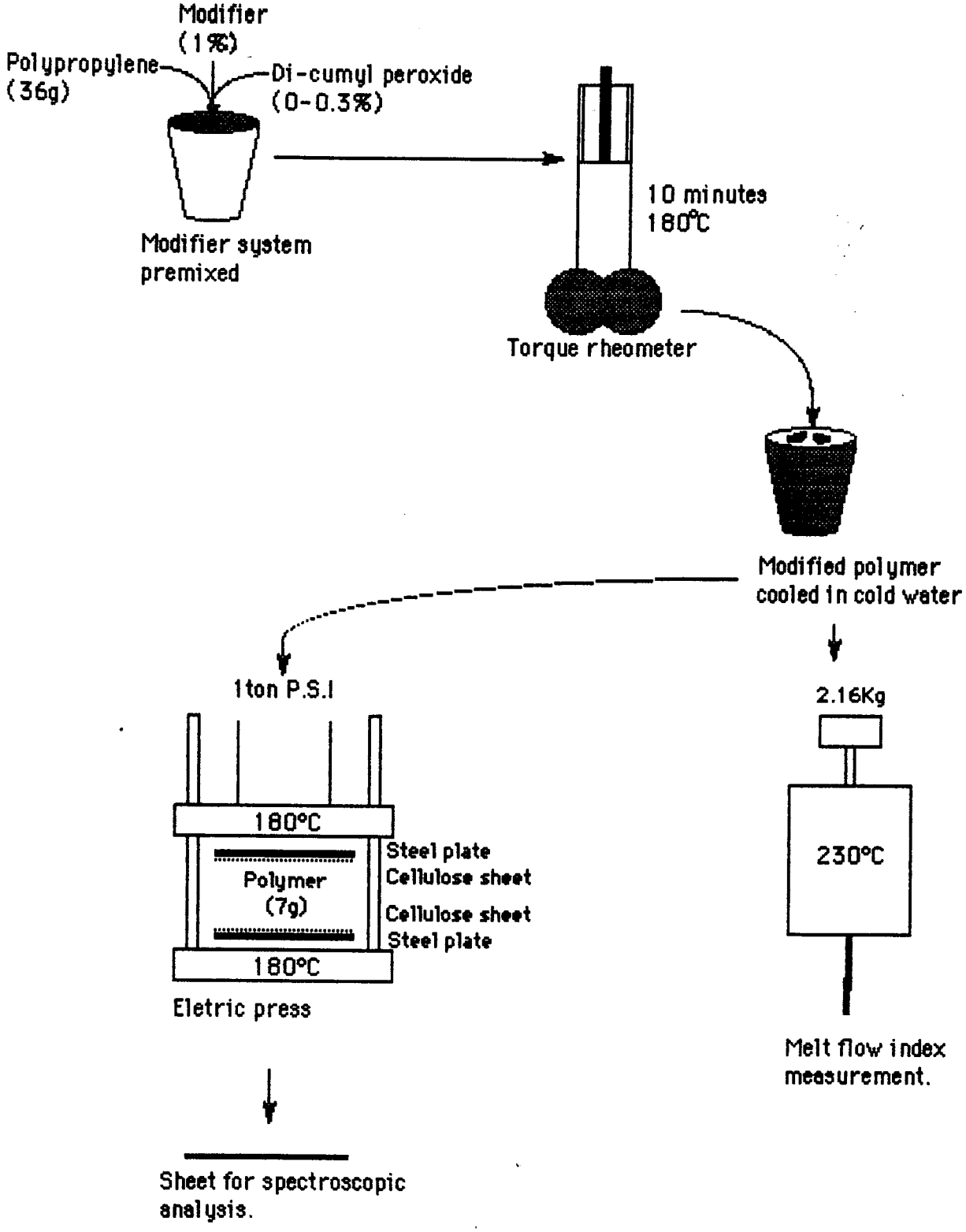
N-methylolmaleimide (NMM) has been included for study since it is unsaturated (potentially reactive to the PP) and has been reported [103] to react via a condensation reaction with amines. It is, therefore, potentially reactive towards the GF-NH.

The N-ethanolmaleimide has been evaluated as since it is a homologue of NMM it may possess similar reactivity.

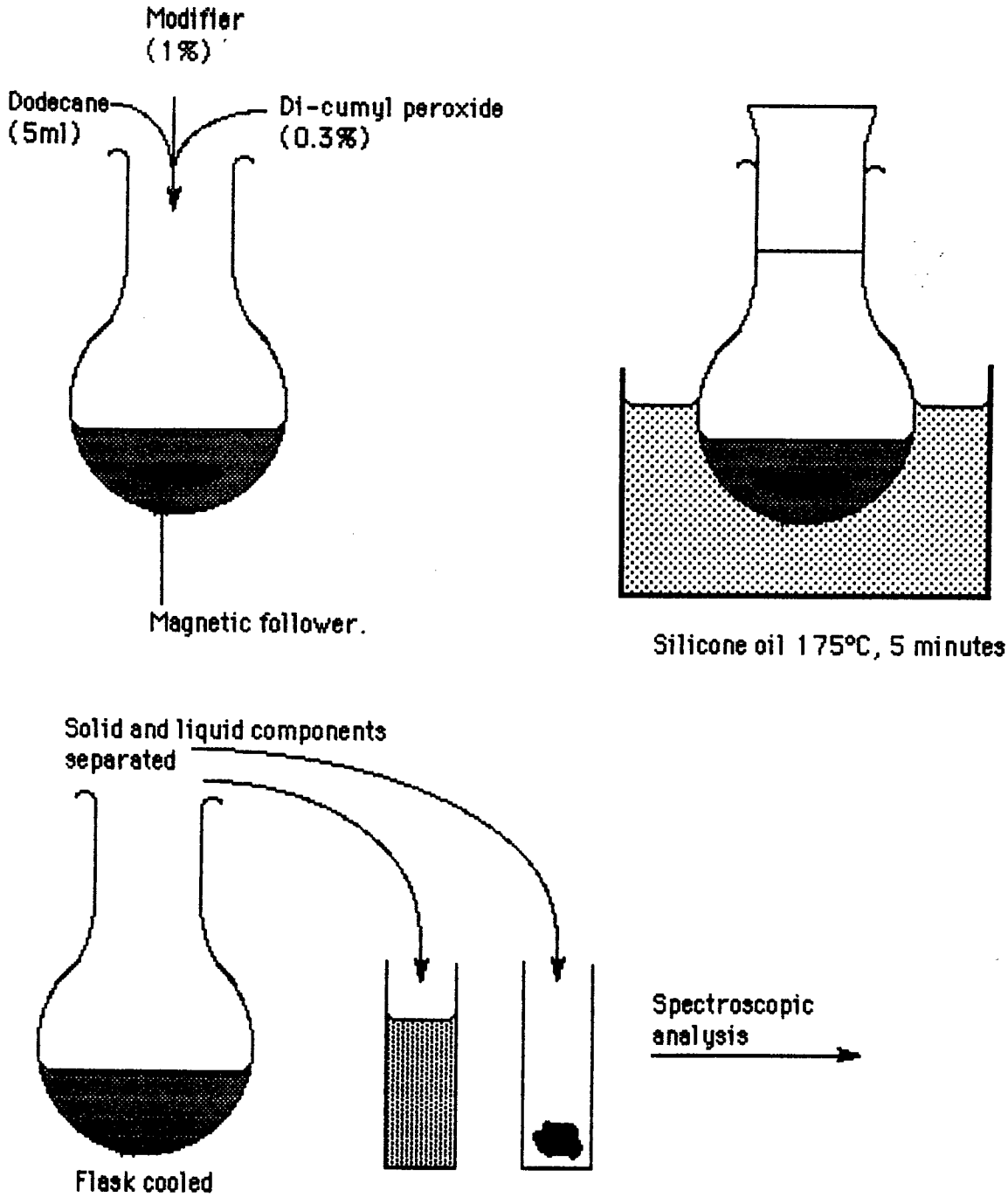
Two commercially available polymers were used in this study. The first is ICI's HW60/GR30 (30% glass fibre reinforced PP). The second is ICI's HWM125 (unreinforced stabilised PP). The purpose of including these two polymers is to allow a comparison between the experimental systems discussed in this chapter and some commercially available polymers.

The effects of adverse environments on all composites discussed in this chapter have been examined. This includes, boiling water and hexane (their effect on tensile properties) and low temperatures (-10°C) (effect on impact properties). Water was chosen since the bond between the coupling agent and glass fibre can be hydrolysed, thus weakening the bond and reducing the mechanical properties. Hexane was chosen as a substitute for petrol since one application of such composites could be in automobiles. The low temperature impact properties were examined since low temperature impact strength is a particular weakness of glass fibre reinforced composites.

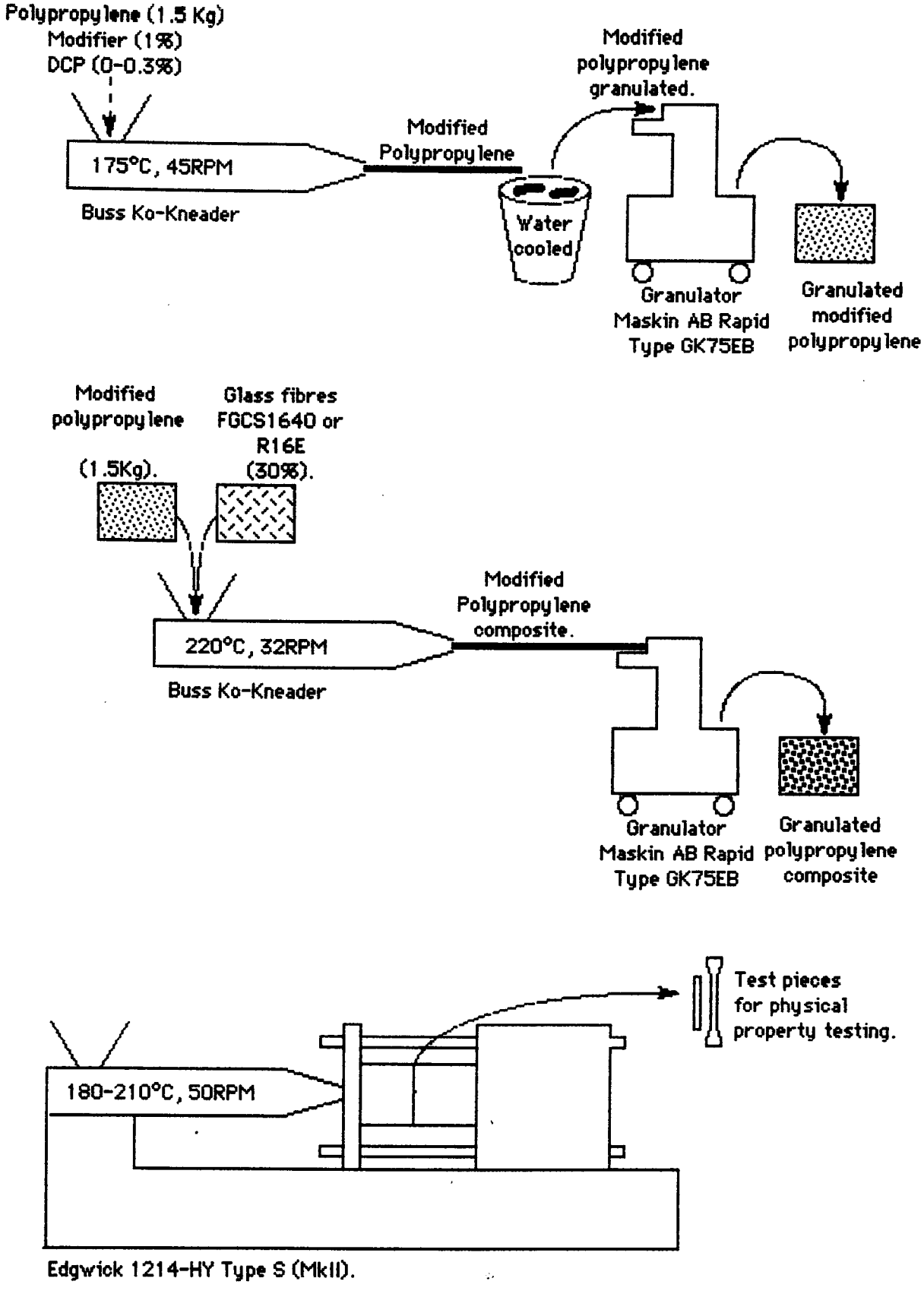
The chemical and mechanical results obtained for each modifier are discussed together. The conclusions for all the results presented in this chapter are made at the end. The results begin with systems modified with DCP only followed by the MA system and, finally, the other modifiers are presented.



Scheme 3.1. The mechanochemical modification of PP to produce samples for MFI and spectroscopic studies.

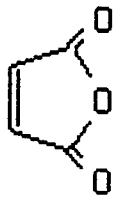
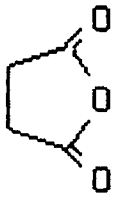
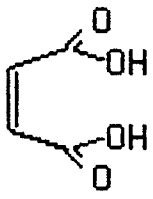
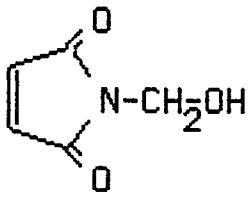
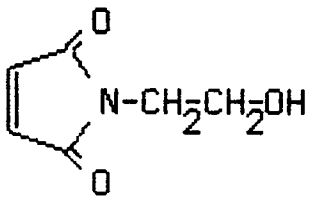


Scheme 3.2. The solution modelling of mechanochemical reactions.



Scheme 3.3. Mechanochemical modification of PP with the modifiers table 3.1 and glass fibres GF-CL or GF-NH to produce samples for mechanical property testing.

Table 3.1 Modifiers discussed in this chapter.

Structure	Name
	Maleic Anhydride (MA)
	Sucinnic anhydride. (SA)
	Maleic Acid (MAC)
	N-methanolmaleimide (NMM)
	N-ethanolmaleimide (NEM)

3.2 Mechanical modification of PP (HF26) with DCP and the mechanical performance of corresponding glass fibre containing composites.

Figure 3.1 shows the infrared spectrum in the regions 1400cm^{-1} to 2000cm^{-1} of PP modified according to scheme 3.1 containing 0, 0.1 and 0.3% DCP respectively. As the concentration of DCP increases a peak at 1710cm^{-1} increases. This peak is normally attributed to a carbonyl group formed during the free radical oxidation of PP. When the experiment is repeated in the presence of 1% CLS (figure 3.2) or AMS (figure 3.3) to represent the presence of the glass fibres containing the chloro (GF-CL) or amino (GF-NH) coupling agents, the same trend is observed. In either figure 3.2 or 3.3 there is no evidence for the presence of CLS or AMS, the spectra of which are shown in figures 4.3 and 3.5. The melt flow index (MFI) is an indicator of the molecular weight of a polymer. As the DCP concentration increases so the MFI increases, indicating a decrease in molecular weight for those samples (figure 3.6).

Figures 3.7 to 3.9 show the effect of DCP concentration on the mechanical properties of PP (HF26) in the absence and presence of glass fibre containing chloro (GF-CL) and amino (GF-NH) silane coupling agents (see scheme 3.3). It is clear that in general the glass containing samples show lower elongation (EL), impact strength (IS) and flexural modulus (FM), but higher tensile strength (TS) and flexural yield strength (FS) than the PP samples. Varying the DCP concentration (up to 0.3%) does not have a significant effect on the glass filled samples. However, DCP concentration effects on the unfilled system are much more significant. Figures 3.7 to 3.9 show that all properties examined except TS reduce with increasing DCP concentration. The mechanical properties of the GF-NH filled polymer system are, in general, higher than the GF-CL system (see table 3.2 and figures 3.7 to 3.9).

The effects of aggressive environments such as immersion in boiling water for two hours or in boiling hexane for 120 hours is shown in figure 3.10 and table 3.3. Immersion in water had no effect on unfilled polymer, a much higher loss was observed for the GF-NH filled systems when compared with its GF-CL analogue.

The overall loss in hexane is much higher for all systems when compared to water. A much higher loss was observed for the GF-CL filled system when compared with its GF-NH analogue. The IS of all the systems at -10^{o}C are shown in figure 3.10 and table 3.3. In general, the unfilled system shows the greatest losses, a much higher loss was observed for the GF-NH filled system when compared with the GF-CL analogue.

A comparison of the mechanical properties of the polymer systems with the commercial

systems are shown in table 3.2. There is no significant difference between the TS, EL, FS and FM of the unfilled PP system without DCP and the unfilled stabilised HWM25. The mechanical properties of the GF-CL and GF-NH filled systems are in general less than those of the the glass fibre filled commercial system (HW60/GR30). However, the TS, EL and IS of the GF-NH filled system containing no DCP do not differ significantly from those of the commercial system.

The mechanical properties of the commercial systems in aggressive environments are shown in table 3.3. In general, the unfilled commercial system did not differ significantly from the unfilled PP (HF26) without DCP whilst the GF-CL and TS in water of the GF-NH filled system showed a greater loss than the filled commercial system. The TS after hexane exposure and the IS at -10^{0}C of the GF-NH filled system did not differ significantly from those of the commercial system.

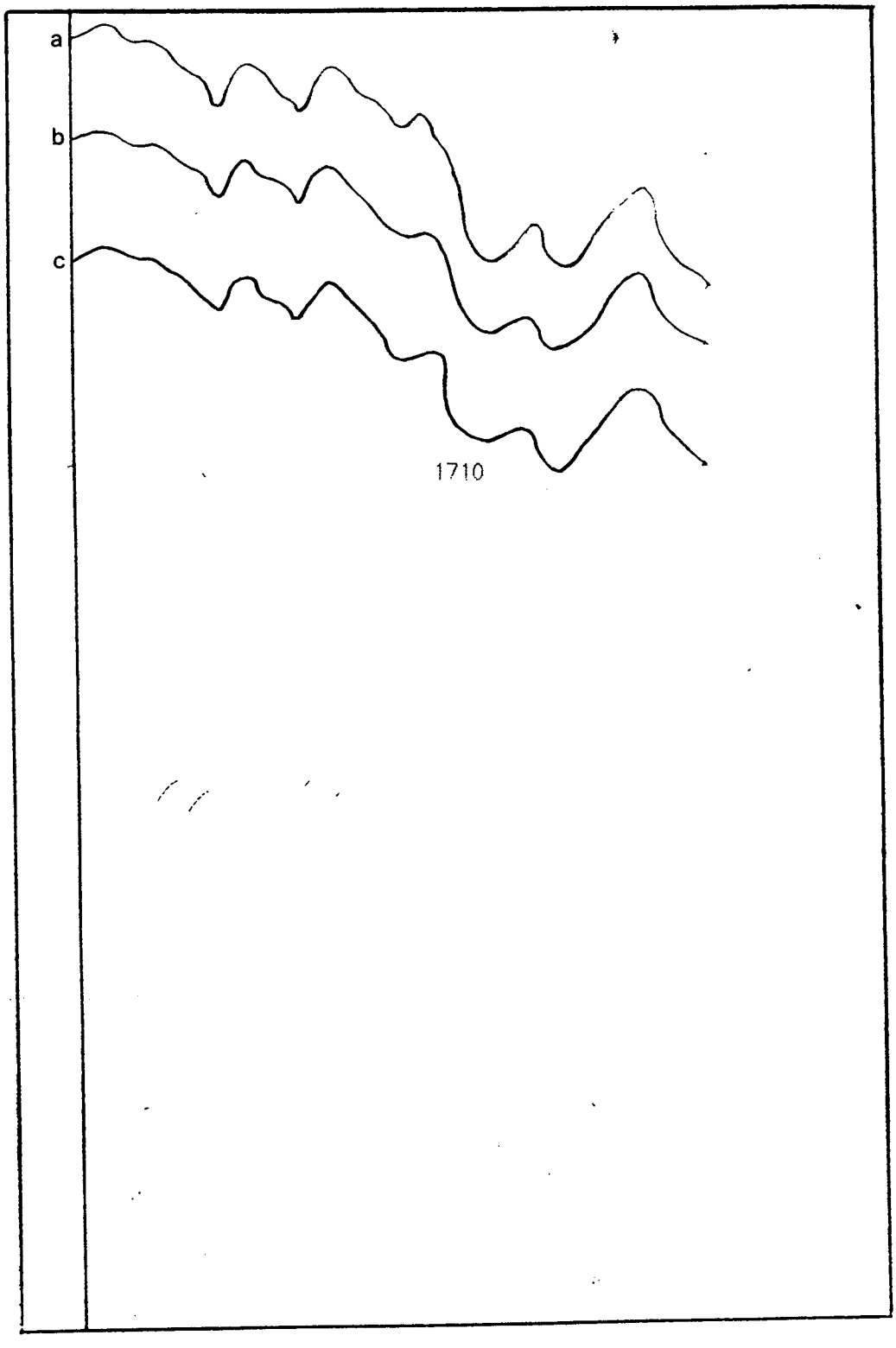


Figure 3.1 The infrared spectra of PP modified with DCP according to scheme 3.1.

a= PP, **b**= PP + 0.1% DCP, **c**= PP + 0.3% DCP.

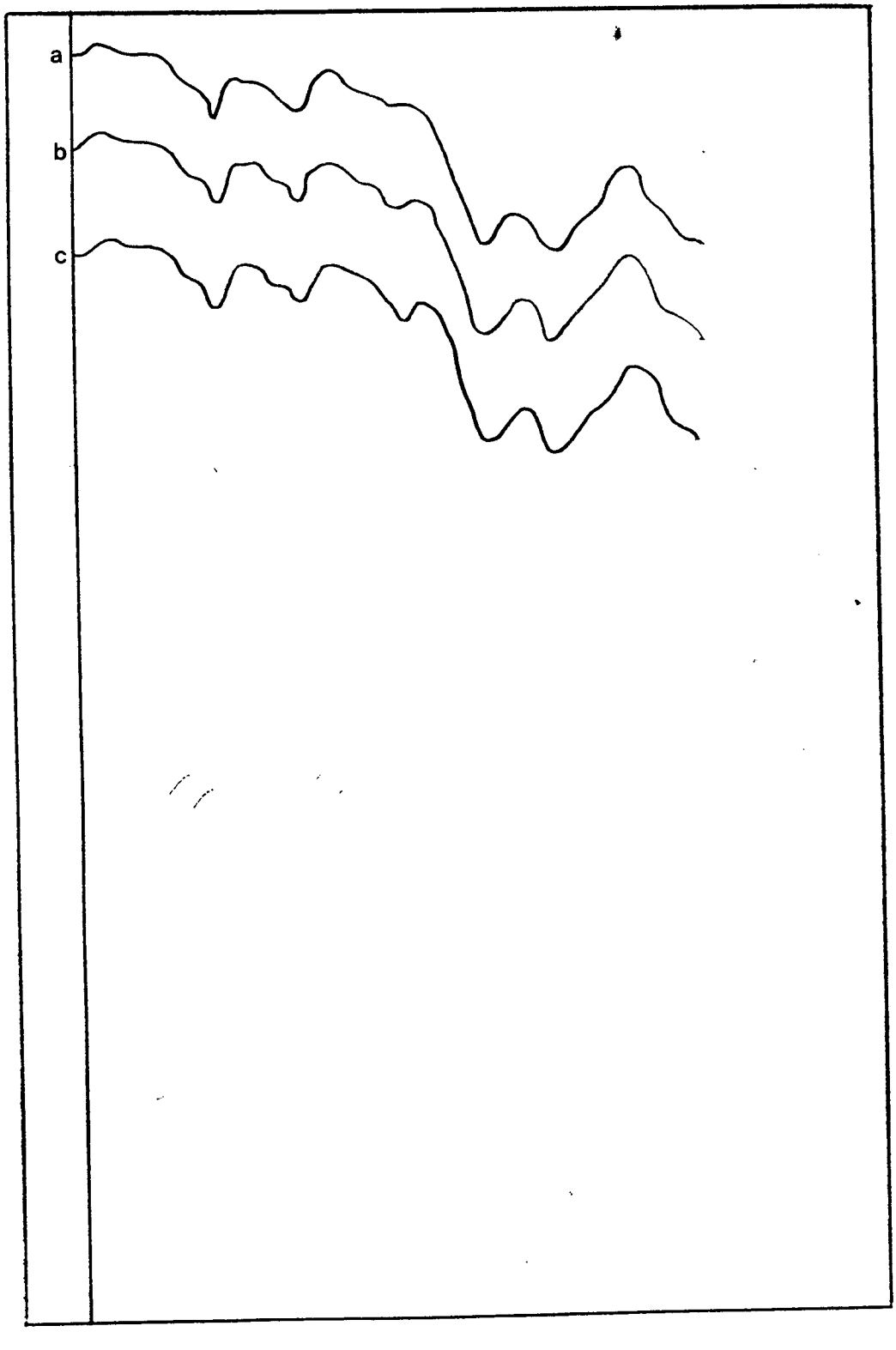


Figure 3.2 The infrared spectra of PP modified with DCP and CLS according to scheme 3.1.

a= PP + 1% CLS, **b**= PP + 0.1% DCP + 1% CLS, **c**= PP + 0.3% DCP + 1% CLS.

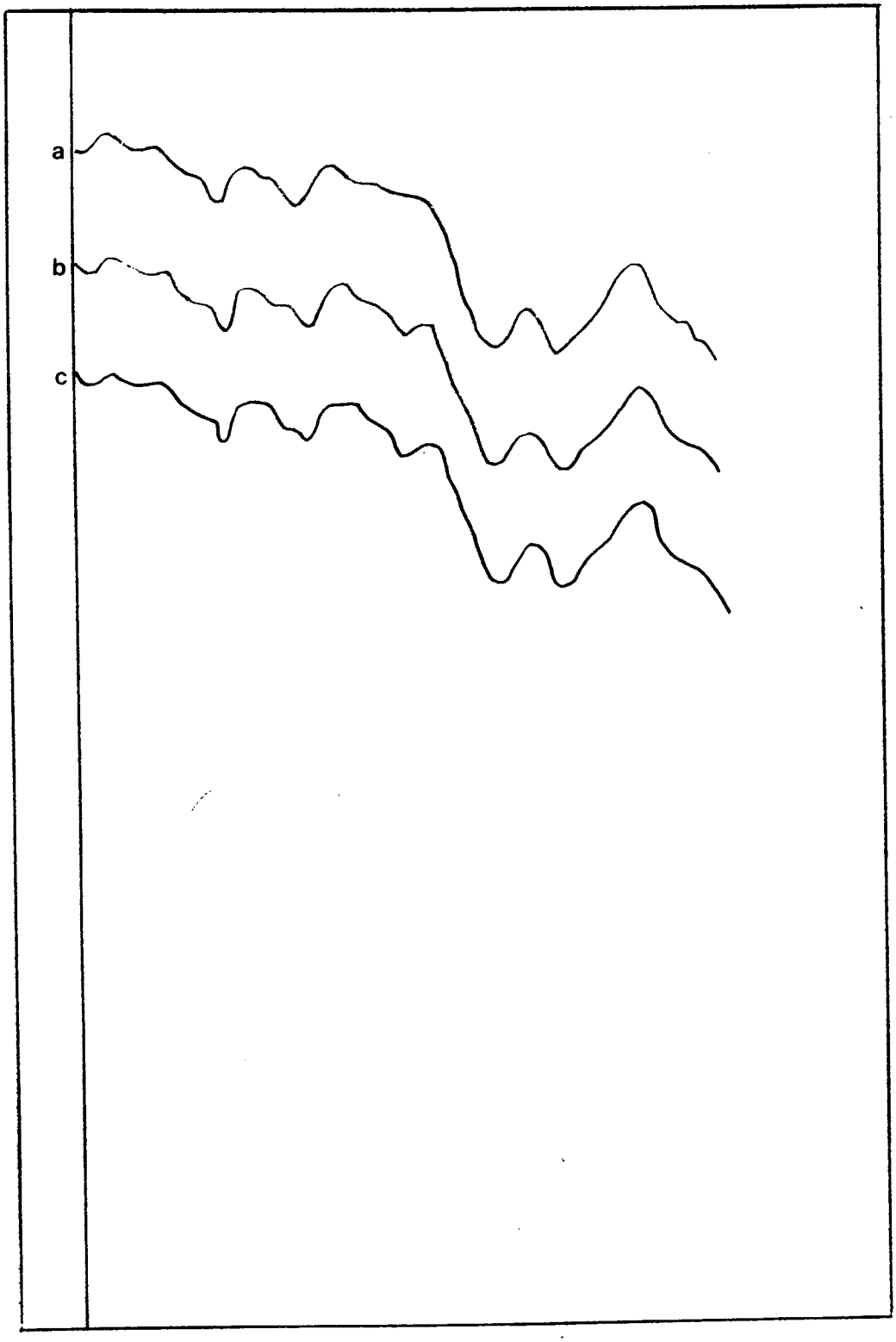


Figure 3.3 The infrared spectra of PP modified with DCP and CLS according to scheme 3.1.

a= PP + 1% AMS, **b**= PP + 0.1% DCP + 1% AMS, **c**= PP + 0.3% DCP + 1% AMS.

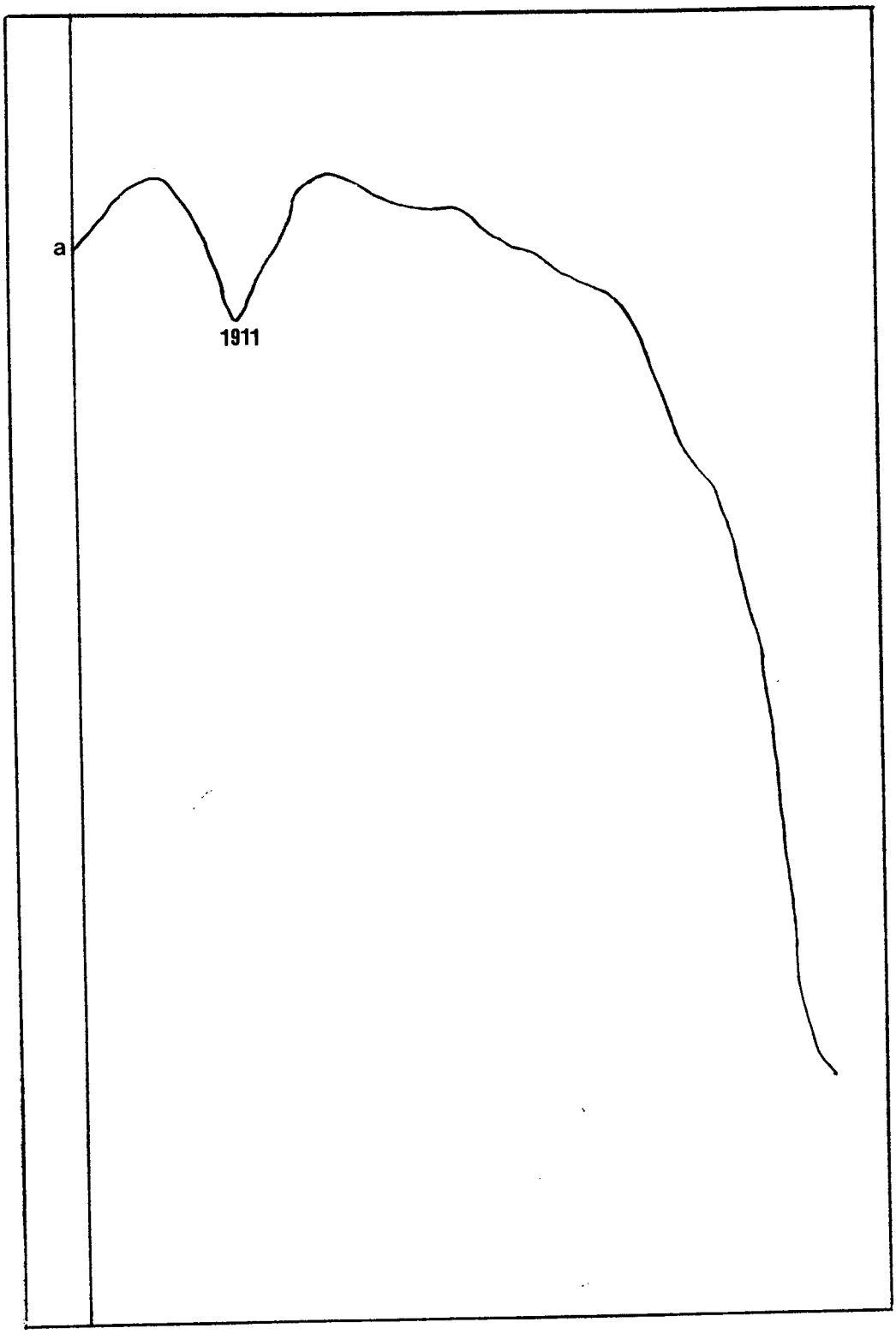


Figure 3.4 the infrared spectra of CLS.

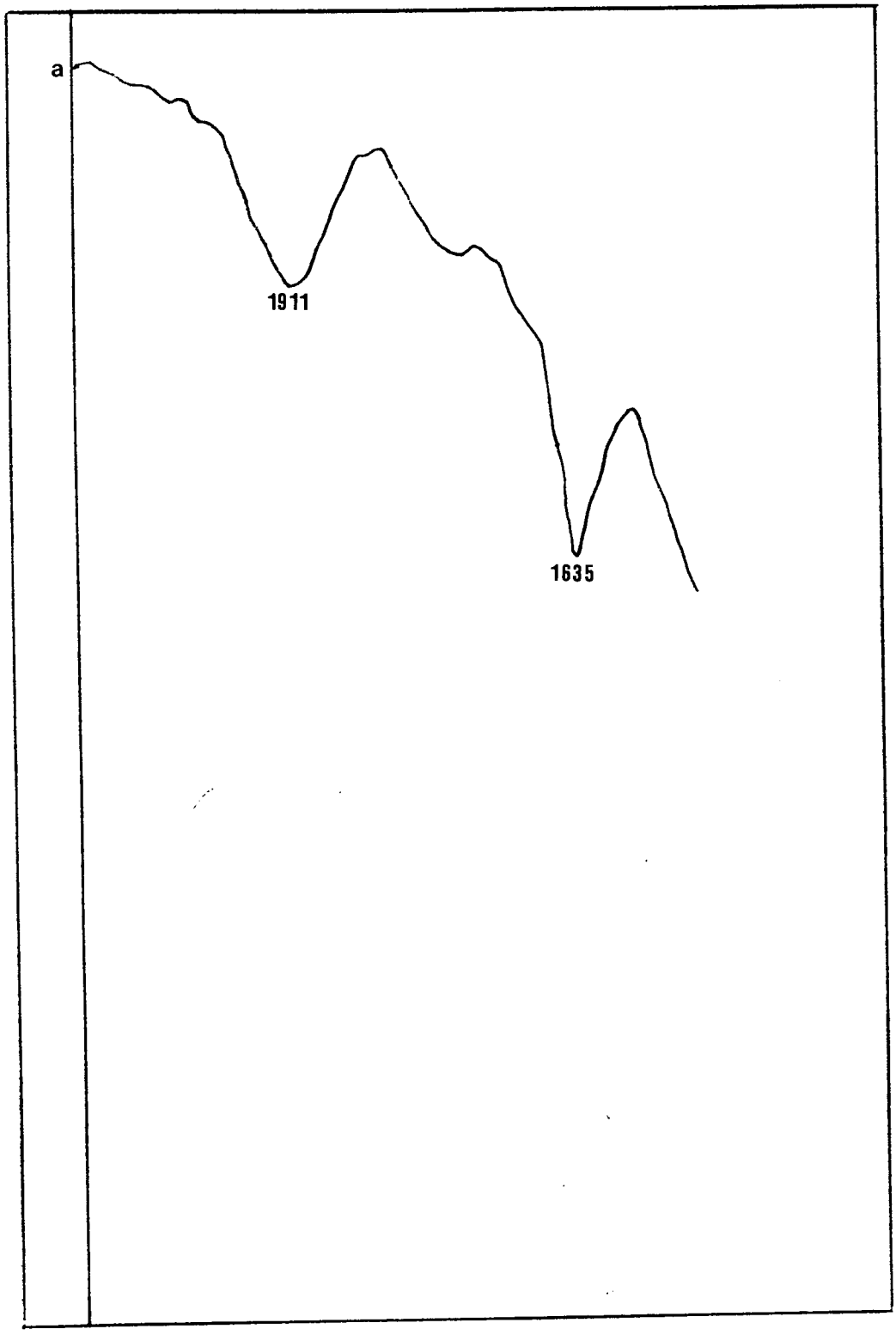


Figure 3.5 the infrared spectra of AMS.

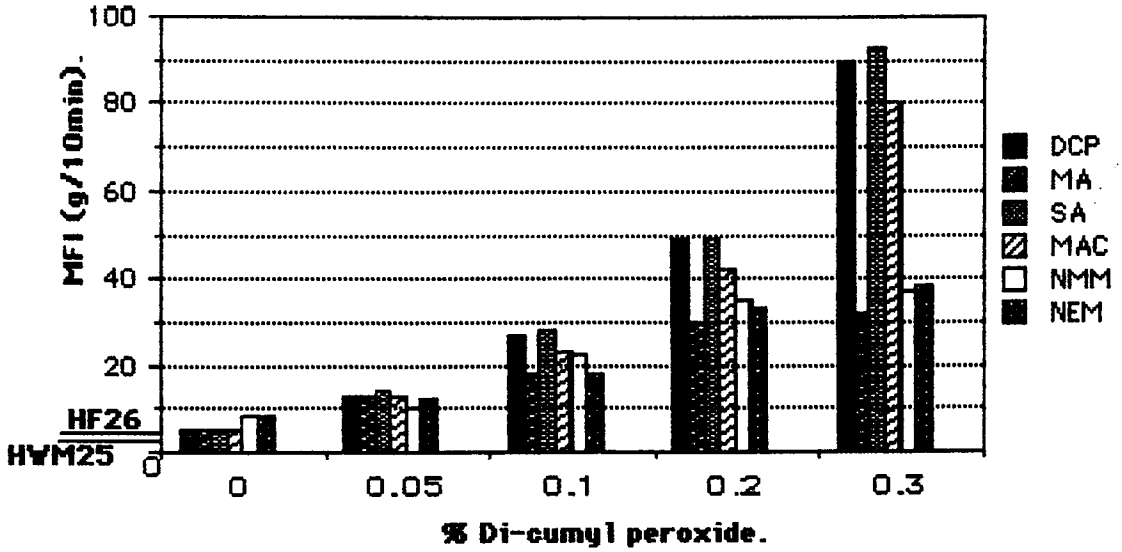


Figure 3.6. MFI measurements (see section 2.4.2.2) of PP (HF26) containing 1% modifiers (see table 3.1) in the presence of variable concentrations of DCP. Processing according to scheme 3.1.

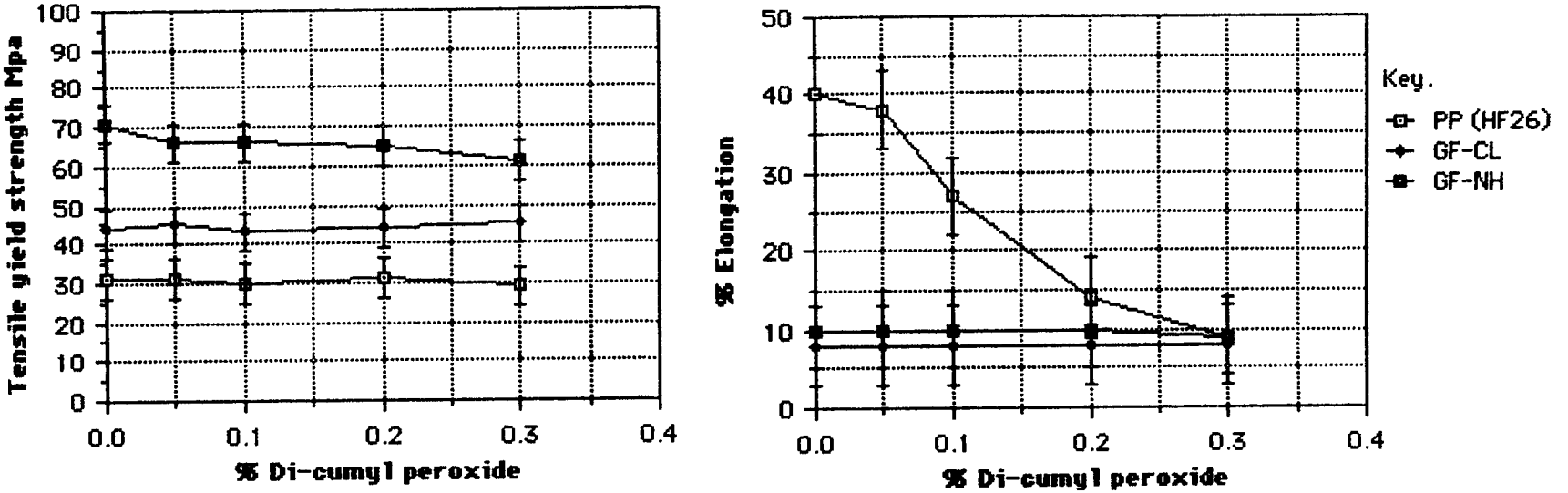


Figure 3.7 Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites processed according to scheme 3.3 with DCP (0-0.3%). No modifier was used in these formulations.

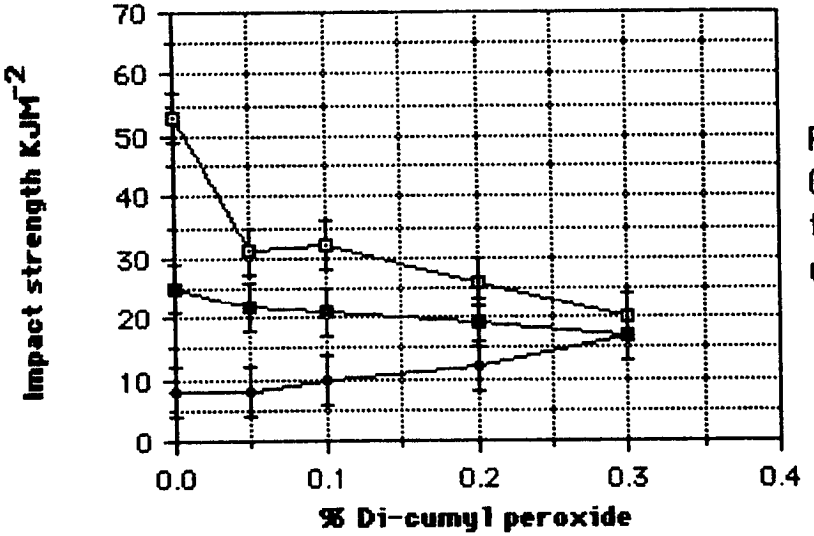


Figure 3.8 The impact strength of PP (HF26) its GF-CL and GF-NH composites processed according to scheme 3.3 with DCP (0-0.3%). No modifier was used in any of these formulations.

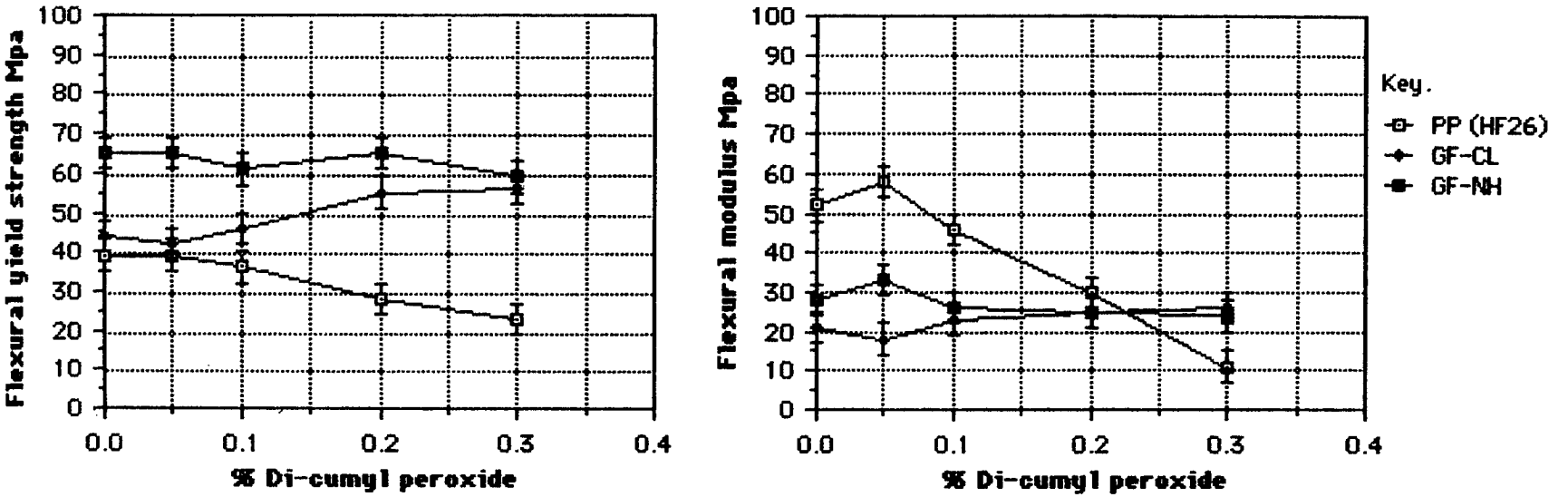


Figure 3.9 Flexural strength and flexural modulus of PP (HF26), its GF-CL and GF-NH composites processed according to scheme 3.3 with DCP (0-0.3%). No modifier was used in any of these formulations.

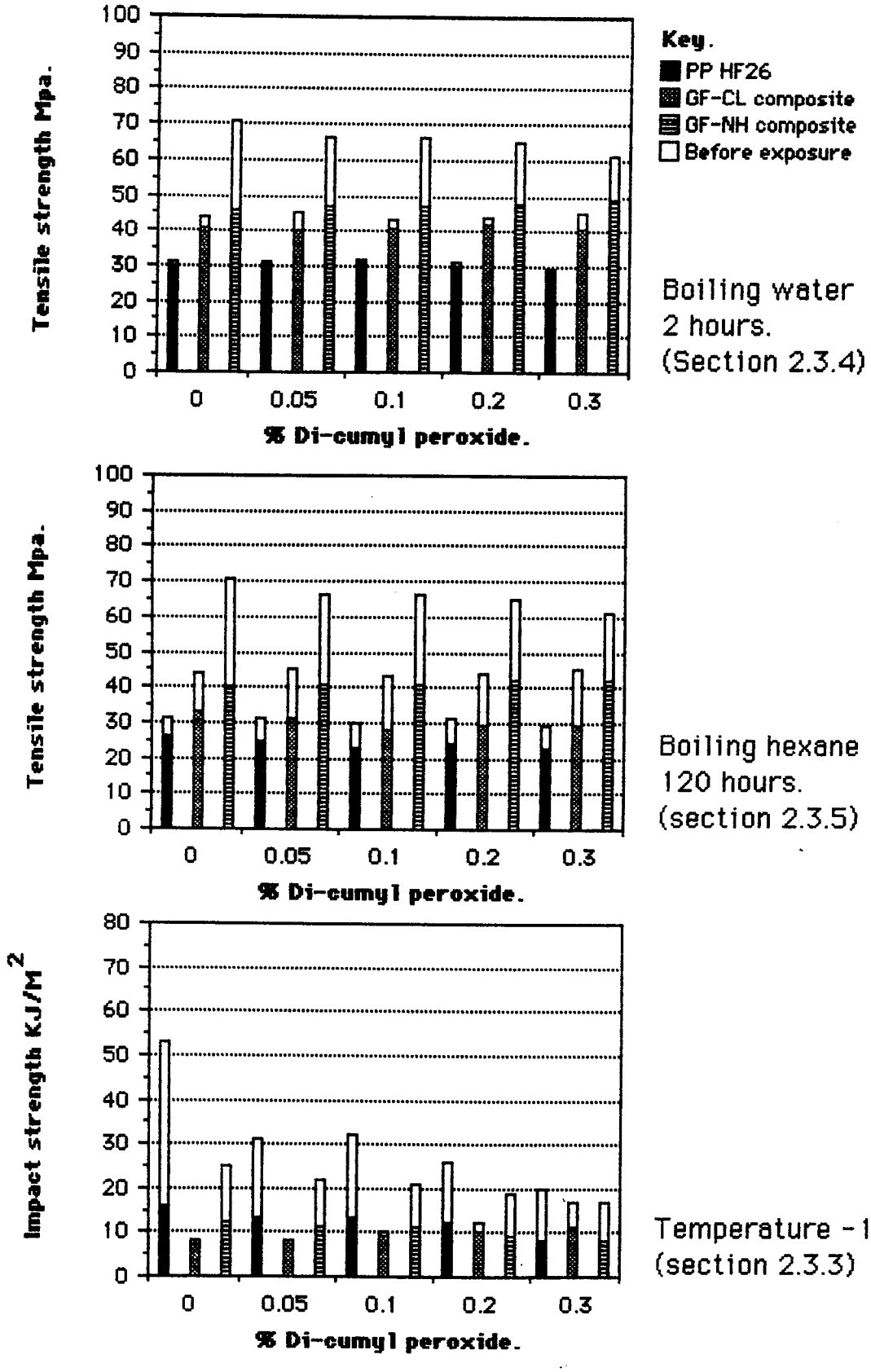


Figure 3.10 The tensile yield strength of PP (HF26), its GF-CL and GF-NH composites processed according to scheme 3.3 with DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 3.2 Mechanical properties of unmodified PP (HF26) containing DCP (0-0.3%) in the absence and presence of GF-CL and GF-NH. The symbol > by an impact result means that some samples did not break when tested and the average quoted is therefore based on those samples which did break.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	31	40	53	39	52
0.05	-	-	31	38	31	39	51
0.1	-	-	30	27	32	36	46
0.2	-	-	31	14	26	28	30
0.3	-	-	29	9	20	23	11
0	30	-	44	8	8	44	11
0.05	30	-	45	8	8	42	21
0.1	30	-	43	8	10	46	18
0.2	30	-	44	8	12	55	23
0.3	30	-	45	8	17	56	25
0	-	30	71	10	25	65	28
0.05	-	30	66	10	22	65	33
0.1	-	30	66	10	21	61	26
0.2	-	30	65	10	19	65	25
0.3	-	30	61	9	17	59	24
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

Table 3.3 Mechanical properties of unmodified PP (HF26) containing DCP (0-0.3%) in the absence and presence of GF-CL and GF-NH and exposed to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at -10°C. The figures in brackets () are the percentage loss in the property from the unexposed samples table 3.2.

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-10°C) KJ/M^2
0	-	-	30 (0%)	26 (-16%)	16 (-70%)
0.05	-	-	31 (0%)	25 (-19%)	13 (-58%)
0.1	-	-	31 (0%)	23 (-23%)	13 (-59%)
0.2	-	-	30 (0%)	24 (-23%)	12 (-54%)
0.3	-	-	29 (0%)	23 (-20%)	8 (-60%)
0	30	-	41 (-7%)	33 (-25%)	8 (0%)
0.05	30	-	40 (-11%)	31 (-31%)	8 (0%)
0.1	30	-	41 (-5%)	28 (-35%)	9 (0%)
0.2	30	-	42 (-5%)	29 (-34%)	10 (0%)
0.3	30	-	41 (-8%)	29 (-35%)	11 (-35%)
0	-	30	46 (-35%)	40 (-43%)	12 (-52%)
0.05	-	30	47 (-29%)	41 (-38%)	11 (-50%)
0.1	-	30	47 (-29%)	41 (-38%)	11 (-48%)
0.2	-	30	48 (-26%)	42 (-35%)	9 (-52%)
0.3	-	30	49 (-20%)	42 (-31%)	8 (-53%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

3.3 Mechanochemical modification of PP (HF26) with Maleic Anhydride (MA) and DCP, the mechanical performance of corresponding glass fibre containing composites.

Figure 3.11 shows the spectra of PP (spectra **a**) and that of PP modified according to scheme 3.1 with 1% MA (spectrum **b**) and various concentrations of DCP (0.1% spectrum **c**, 0.3% spectrum **d**). The addition of 1% MA to the PP led to the formation of a small peak at 1789cm^{-1} (spectrum **b**). As the DCP concentration is progressively increased from 0.1 to 0.3% this peak increases in size, in addition, a new peak is formed at 1863cm^{-1} (see spectrums **c** and **d**). At DCP concentration of 0.3% (spectrum **d**) peaks at 1694cm^{-1} and 1640cm^{-1} also increase. The peaks at 1789cm^{-1} and 1863cm^{-1} are typical of MA (see spectrum E), the 1789cm^{-1} peak being an unresolved combination of the 1792cm^{-1} and 1781cm^{-1} peaks. The MA (spectrum **e**) also possess a peak at 1640cm^{-1} which may be attributed to unsaturation in the MA.

The MFI of MA modified PP samples in the presence of varying concentrations of DCP is shown in figure 3.6. The effect of DCP concentration is to increase the MFI value indicating chain scission.

The effect of DCP concentration on the level of binding of MA (see section 2.4.4.3) is shown in table 3.4. Increasing DCP concentration increases the level of MA binding to PP backbone; a maximum of 50% was found to be unextractable at a DCP concentration of 0.3%.

When PP was modified according to scheme 3.1 with MA (1%), DCP (0.3%) and CLS (1%), to simulate the presence of glass fibres (GF-CL) then the spectrum shown in figure 3.12 **a** was obtained. This shows some similarities to the spectrum of PP modified with MA and DCP only (figure 3.11 **d**) with peaks at 1862cm^{-1}, 1789cm^{-1}, 1694cm^{-1} and 1640 cm^{-1}. However, two additional peaks at 1741cm^{-1} and 1710cm^{-1} are formed which are not due to the MA, DCP, PP or CLS individually. The spectrum of PP modified according to scheme 3.3 with MA (1%), DCP (0.3%) and GF-CL (30%) is shown in figure 3.12 **b**. This spectrum was obtained by forming a sample of the composite into a film (see section 2.4.1) and recording its spectrum on a computer system. The spectrum of an analogous composite but without MA was likewise recorded and subtracted from the first spectra. Thus, the spectrum due to the presence of the glass was eliminated. This spectrum (figure 3.12 **b**) has similarities to that of figure 3.12 **a**.

The reaction products formed when the melt reaction of PP containing MA and CLS is modelled in dodecane (DD) at 175^{0}C (see scheme 3.2) in the absence (figure **a**) and presence (figure **b**) of DCP are shown in figure 3.13. In both figures **a** and **b** the peaks at 1742cm^{-1} and 1710cm^{-1}, previously seen in the PP melt, are present in addition to the

peaks at 1852cm^{-1}, 1793cm^{-1} and 1783cm^{-1} attributed to the presence of MA. The spectrum of CLS (thin film) is shown in figure 3.13 **c**, as can be seen this has no peaks in this region.

Figure 3.14 **a** shows the infrared spectrum of PP modified with MA, DCP and the amino silane coupling agent (AMS). This was done in order to simulate the presence of GF-NH (see scheme 3.1) in modified PP. This spectrum has notable peaks at 1780cm^{-1}, 1703cm^{-1}, 1649cm^{-1} and 1560cm^{-1}. A similar spectrum was obtained when the same conditions were used but without DCP. When the reaction was modelled in dodecane (see scheme 3.2) with MA and AMS, a yellow gel was produced (figure 3.14 **b**). Strong absorptions at 1718cm^{-1}, 1649cm^{-1} and 1572cm^{-1} are observed. When the same reaction is carried out but in the presence of DCP a red solid (figure 3.14 **c**) was produced. This has weaker absorptions at 1778cm^{-1}, 1706cm^{-1}, 1650cm^{-1} and 1560cm^{-1}. This spectra is quite similar to the analogous reaction (figure 3.14 **a**). When DCP was added to the yellow gel (figure 3.14 **b**) and the reaction continued a similar red solid was produced with infrared spectrum similar to that shown in figure 3.14 **c**. The spectrum of a model compound produced when MA and AMS are reacted (see section 2.1.4.5) is shown in figure 3.15 **a**. This possesses strong absorptions at 1713cm^{-1}, 1645cm^{-1} and 1566cm^{-1}. Finally, the spectrum of a composite containing DCP (0.3%), MA (1%) and GF-NH (30%) is shown in figure 3.15 **b**. This spectrum has strong similarities with those discussed previously (figures 3.14 to 3.15).

The effect of MA modification on the mechanical properties of PP (see scheme 3.3) in the absence and presence of glass fibres is shown in figures 3.16 to 3.18. Unfilled PP shows TS, EL and FS which are not significantly different from PP containing the same amount of DCP but no MA (cf table 3.2 and 3.5). The IS and FM of the MA modified system are quite different from the unfilled unmodified PP. The former increases dramatically and shows an increasing trend with increasing DCP concentrations (the reverse of the unmodified polymer system) (cf figures 3.17 and 3.4). The latter is lower than the unfilled unmodified system (cf figures 3.18 and 3.5).

All the properties, except for the FM which was lower were comparable to the commercial HWM25.

In the presence of adverse environments the performance of the unfilled MA modified PP was similar to the unmodified polymer under boiling water conditions and low temperature impact but was much better under hexane exposure (cf table 3.6 and 3.3, figure 3.19).

Except for the TS under boiling water conditions the results obtained were all comparable to the HWM25 when subjected to the same environments.

Comparison of tables 3.3 and 3.6 shown clearly that the GF-CL filled MA modified composite show a much enhanced overall mechanical performance, when compared to the filled unmodified analogues (see also figures 3.16 to 3.18).

Similarly, when the MA modified GF-CL filled system is compared with the commercial composite material (HW60/GR30); it demonstrated overall superior properties in all respects.

This MA modified GF-Cl composite material also performed well under adverse environments (figure 3.19). In all respects the results obtained were superior to the analogous GF-CL filled unmodified composites (cf tables 3.7 and 3.4).

The physical properties of the MA modified GF-NH composite samples on the other hand, (figure 3.16 to 3.18) were surprisingly similar to the analogous GF-NH filled but unmodified samples.

In all respects the MA modified GF-NH composites were not as good as the commercial composite and were certainly inferior to the corresponding GF-CL MA modified samples.

The performance of the MA modified GF-NH systems under aggressive environments is very similar to the corresponding filled but unmodified analogous except for a superior low temperature IS (cf tables 3.7 and 3.4). The IS at $-10^{0}C$ was also superior to the commercial composite (HW60/GR30).

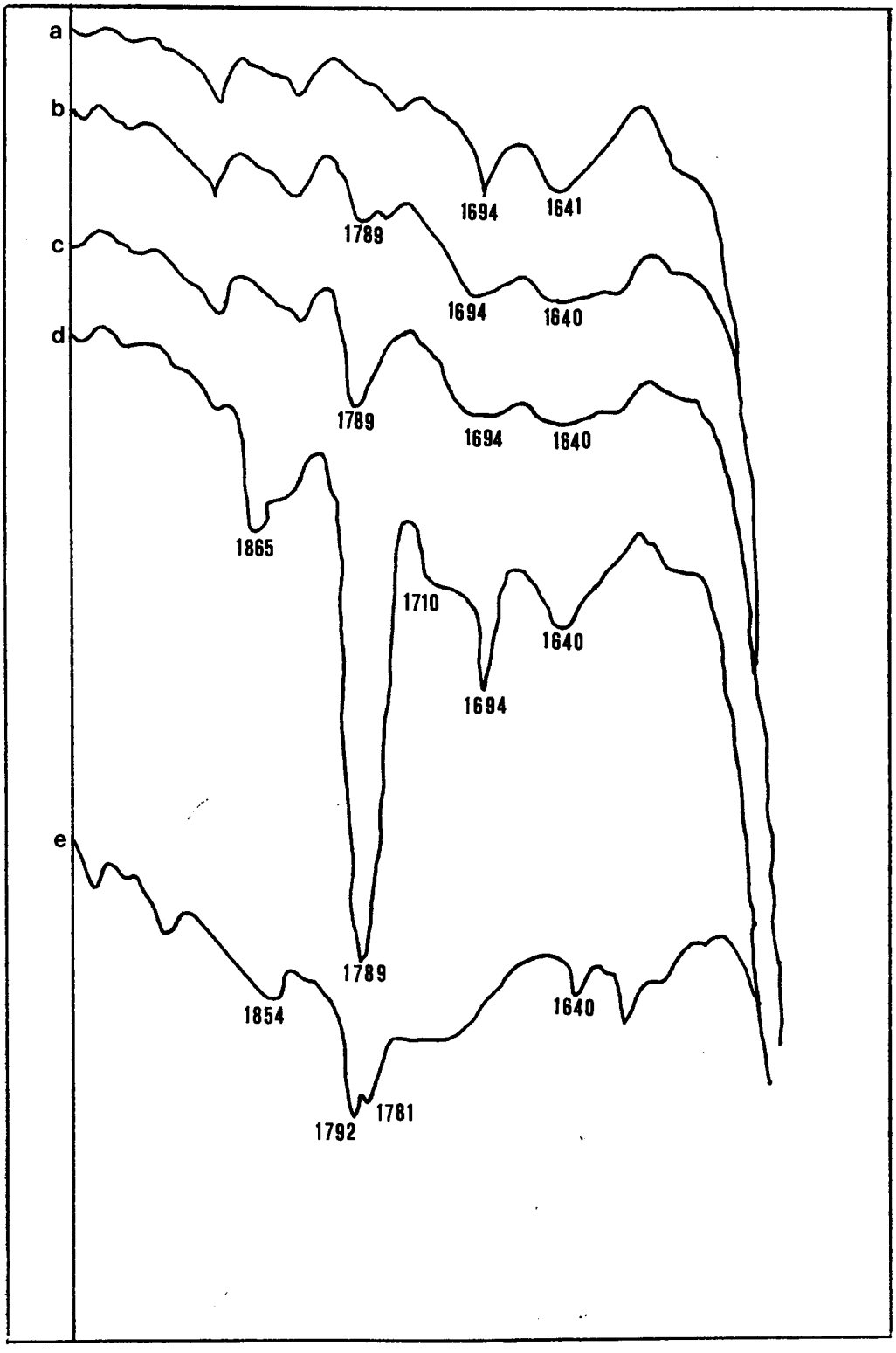


Figure 3.11. **a** = PP, **b** = PP + 1% MA, **c** = PP + 1% MA + 0.1% DCP, **d** = PP + 1% MA + 0.3% DCP, **e** = MA (nujol mull).

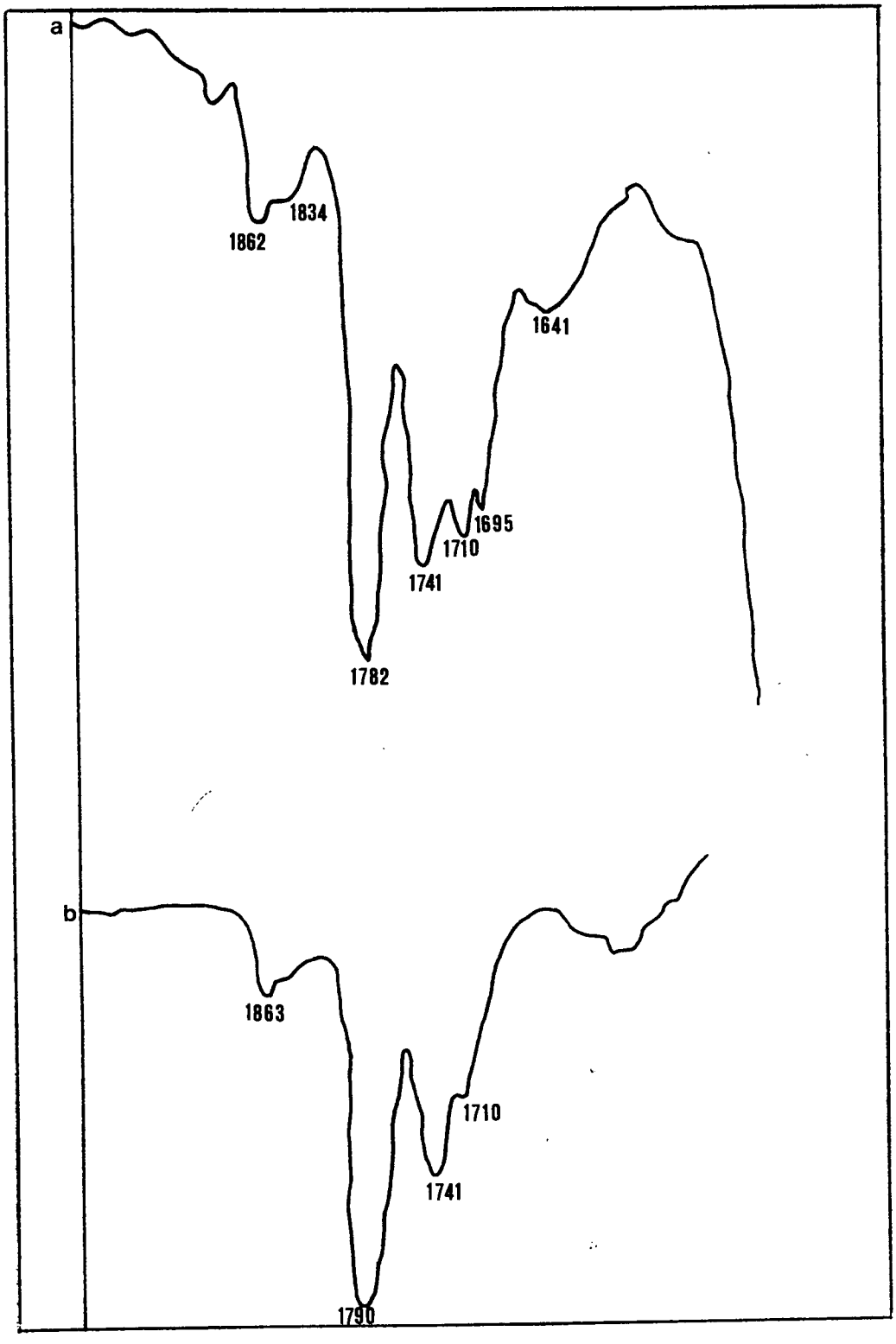


Figure 3.12. **a** = PP + 1% MA + 1% CLS, **b** = PP + 1% MA + 1% CLS + 0.3% DCP

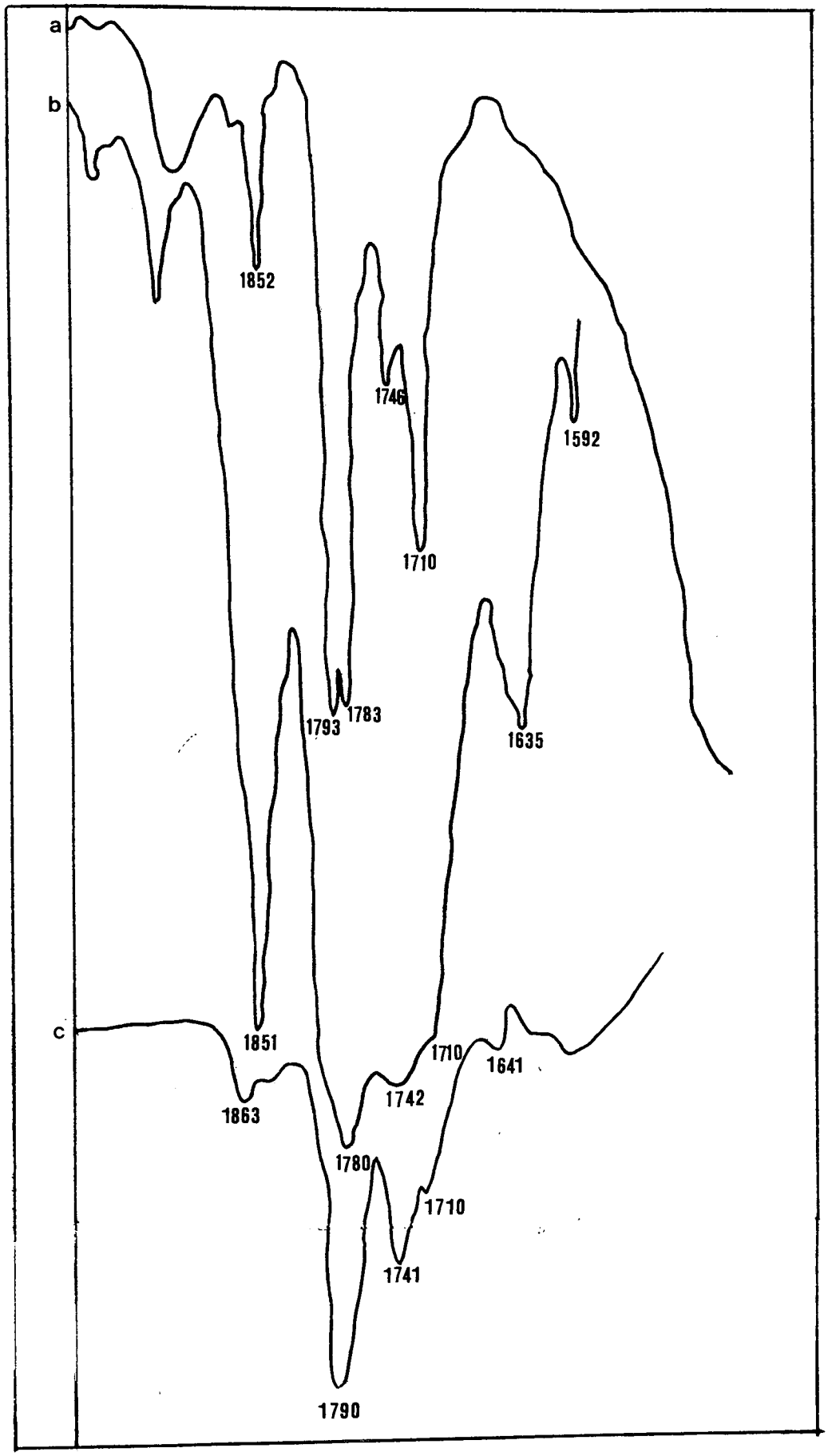


Figure 3.13. **a** = Dodecane + 1% MA + 1% CLS, **b** = Dodecane + 1% MA + 1% CLS + 0.3% DCP, **c** = PP + 1% MA + 0.3% DCP + 30% GF-CL.

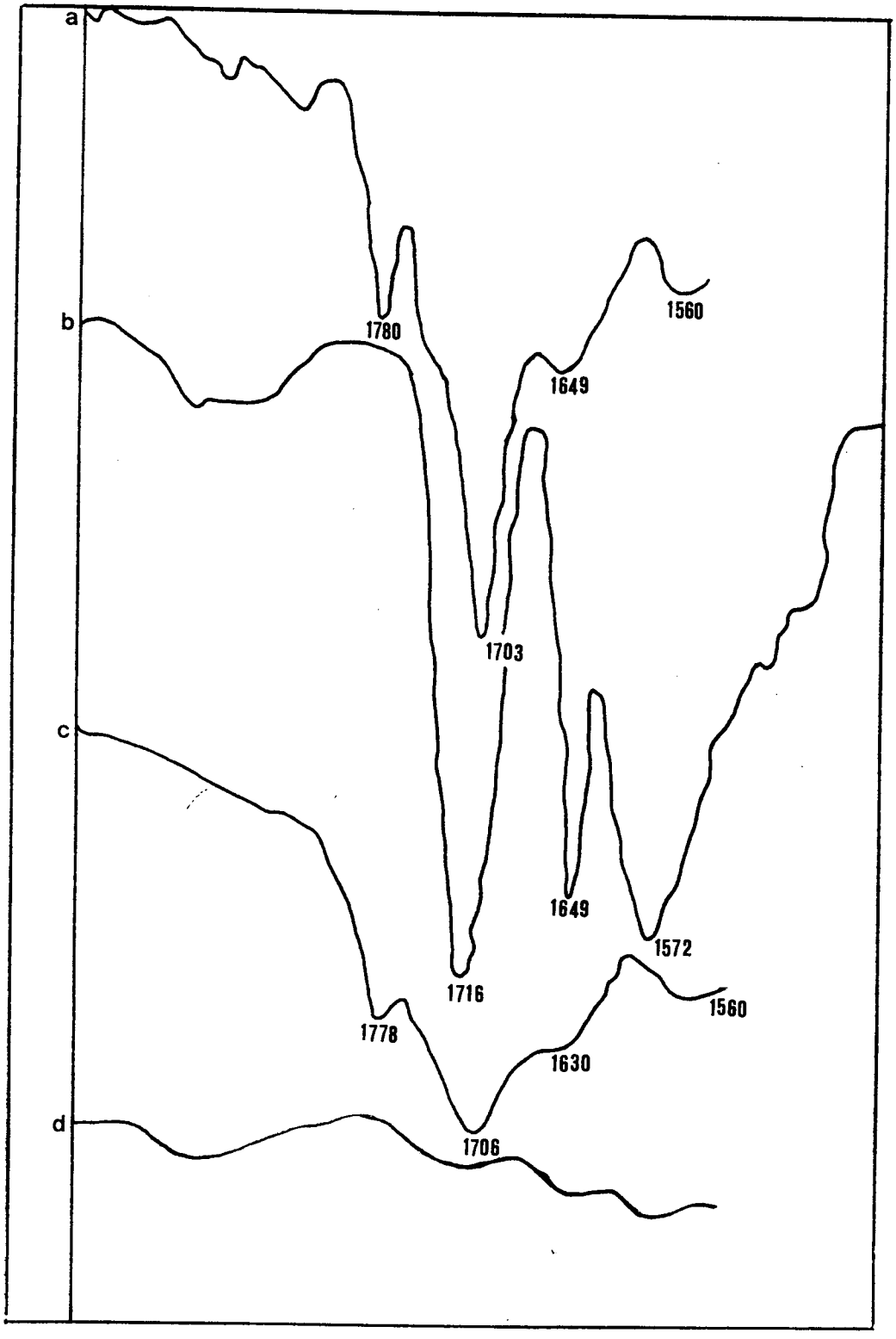


Figure 3.14. **a** = PP + 1% MA + 1% AMS + 0.3% DCP (red solid), **b** = Dodecane + 1% MA + 1% AMS (yellow gel), **c** = Dodecane + 1% MA + 1% AMS + 0.3% DCP (red solid), **d** = AMS (thin film).

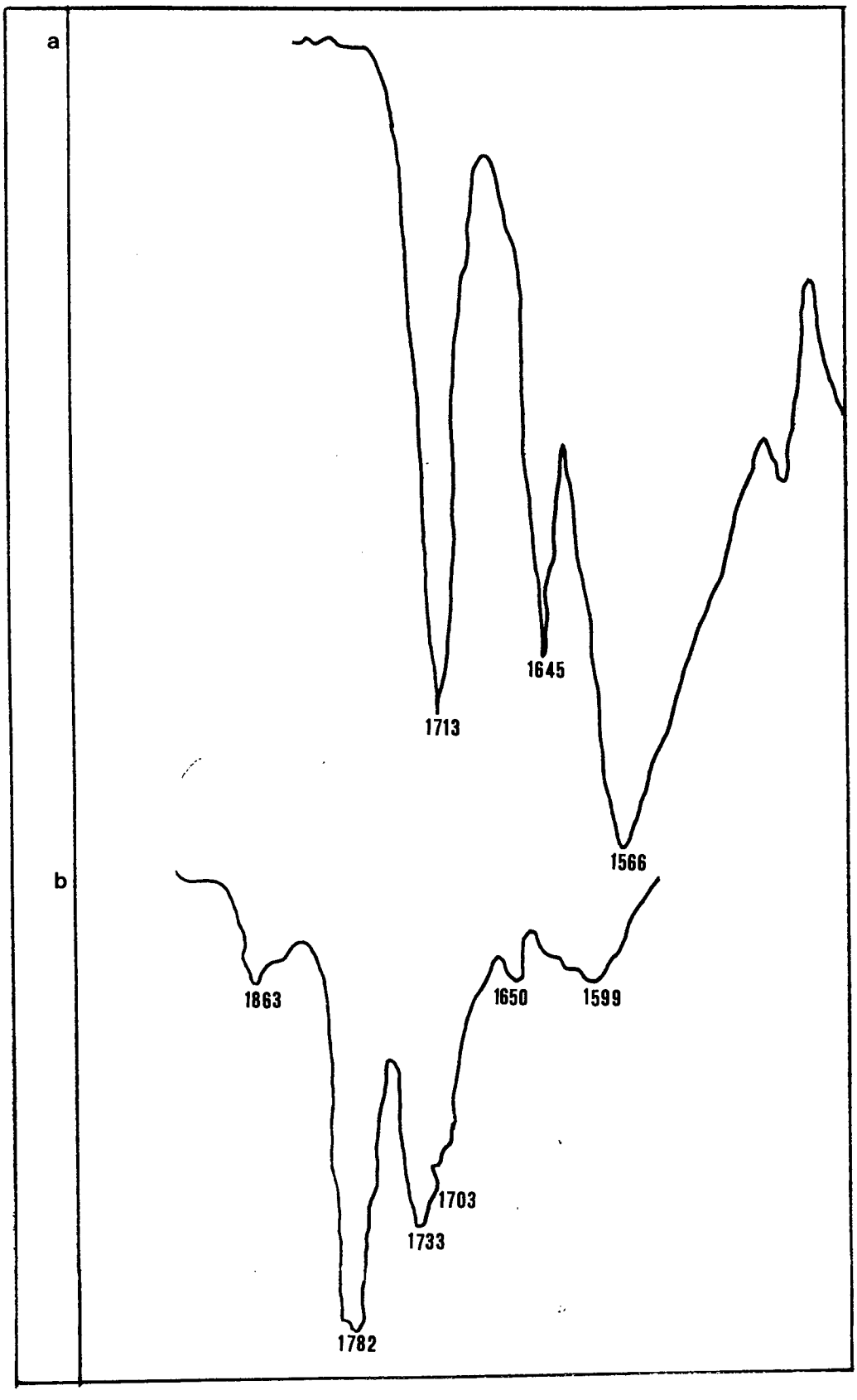


Figure 3.15. **a** = NMA (see section 2.1.4.6) (yellow liquid), **b** = PP + 1% MA + 0.3% DCP + 30% GF-NH.

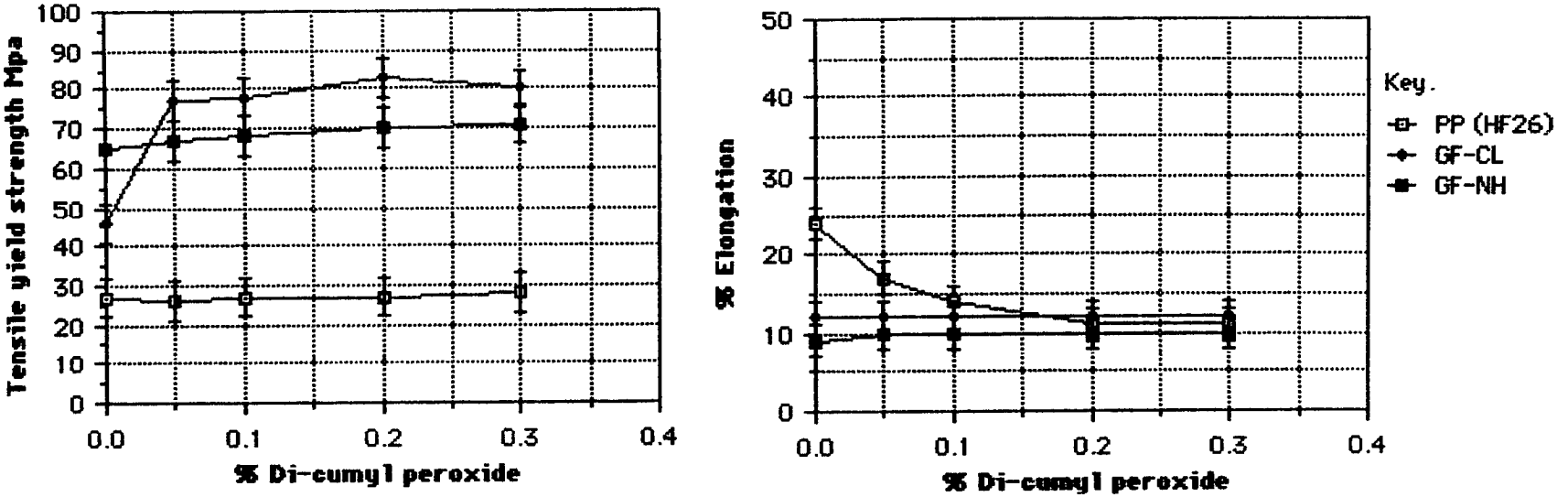


Figure 3.16Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with MA (1%) and DCP (0-0.3%).

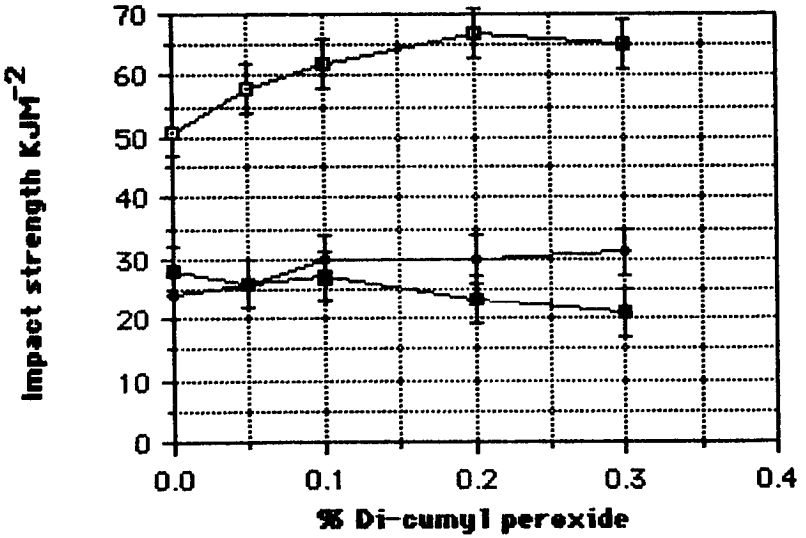


Figure 3.17 Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with MA (1%) and DCP (0-0.3%)

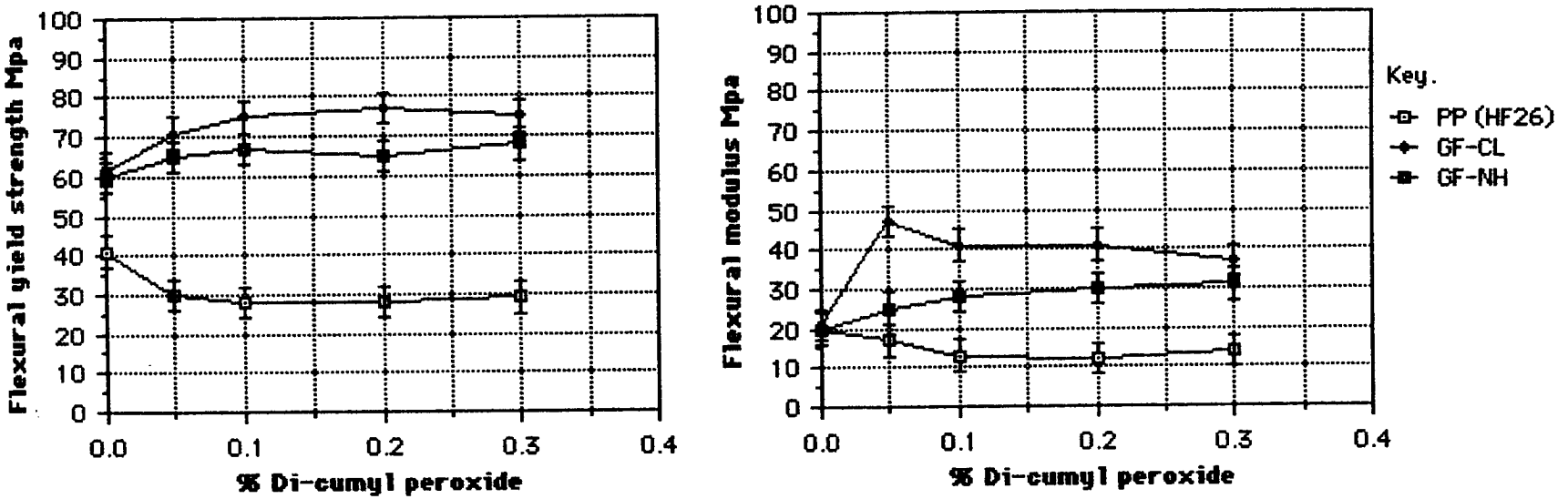


Figure 3.18. Flexural strength and flexural modulus of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with MA (1%) and DCP (0-0.3%).

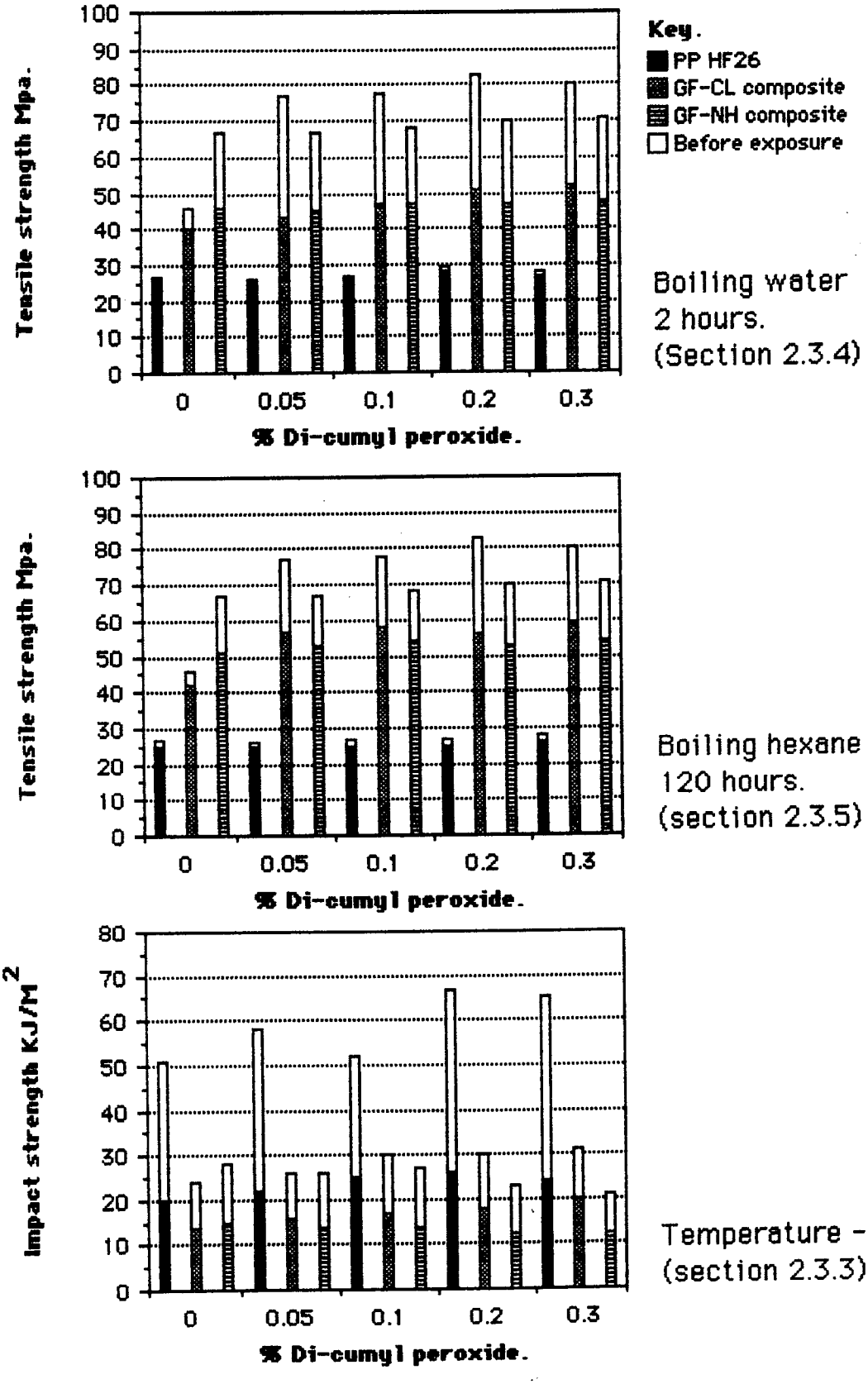


Figure 3.19 Tensile yield strength of PP HF26, its GF-CL and GF-NH composites modified according to scheme 3.3 with MA (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 3.4. The binding of MA (1%) to PP HF26 determined according to section 2.4.4.4

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.89	0.10	10
0.1	1	0.92	0.37	37
0.3	1	0.87	0.53	53
	No of modifier molecules per 10000 PP repeat units.			
0	56	49	5.7	-
0.1	56	51	21	-
0.3	56	48	30	-

Table 3.5 The effect of DCP concentration on the mechanical properties of PP (HF26) modified with MA (1%) (see scheme 3.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those samples which did.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	27	24	51	41	20
0.05	-	-	26	17	58	30	17
0.1	-	-	27	14	>62	28	13
0.2	-	-	27	11	>67	28	12
0.3	-	-	28	11	>65	29	14
0	30	-	46	12	24	62	21
0.05	30	-	77	12	26	71	47
0.1	30	-	78	12	30	75	41
0.2	30	-	83	12	30	77	41
0.3	30	-	80	12	31	75	37
0	-	30	65	9	28	60	20
0.05	-	30	67	10	26	65	25
0.1	-	30	68	10	27	67	28
0.2	-	30	70	10	23	65	30
0.3	-	30	71	10	21	68	31
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

Table 3.6 The effect of adverse environments of boiling water for 2 hours of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with MA (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples table 3.6).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-10°C) KJ/M^2
0	-	-	27 (0%)	25 (-7%)	20 (-61%)
0.05	-	-	26 (0%)	25 (-7%)	22 (-62%)
0.1	-	-	26 (0%)	25 (-15%)	25 (-60%+)
0.2	-	-	28 (0%)	25 (-13%)	26 (-61%+)
0.3	-	-	27 (0%)	26 (-7%)	24 (-63%+)
0	30	-	40 (-13%)	42 (-9%)	14 (-41%)
0.05	30	-	43 (-44%)	57 (-26%)	16 (-38%)
0.1	30	-	47 (-40%)	58 (-34%)	17 (-43%)
0.2	30	-	51 (-38%)	56 (-32%)	18 (-40%)
0.3	30	-	52 (-35%)	59 (-26%)	20 (-36%)
0	-	30	46 (-29%)	51 (-21%)	15 (-46%)
0.05	-	30	45 (-33%)	53 (-21%)	14 (-46%)
0.1	-	30	47 (-31%)	54 (-21%)	14 (-48%)
0.2	-	30	47 (-33%)	53 (-24%)	12 (-48%)
0.3	-	30	48 (-32%)	54 (-24%)	12 (-43%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

3.4 Mechanochemical modification of PP HF26 with Succinic anhydride (SA) and DCP.

Succinic anhydride (SA) was chosen for study for its similarity to MA, however, SA does not possess unsaturation and thus binding to the PP is not expected to take place. Studies of the results obtained with SA may help to elucidate the reactions taking place with the MA.

The spectrum of a nujol mull of SA is shown in figure 3.20 **a**, this has two notable peaks at 1863cm^{-1} and 1785cm^{-1}. The spectrum of PP modified according to scheme 3.1 with SA containing 0, 0.1 and 0.3% DCP are shown in figure 3.20 **b** to 3.20 **d** respectively. These spectra show little sign of the SA peaks but instead strongly resemble the PP after progressive addition of DCP (figure 3.1). The MFI of the SA modified PP is shown in figure 3.6, the results do not differ significantly from those of the unmodified PP.

The percentage binding of the SA was determined (see section 2.4.3, table 3.7), these results show that none of the SA was bound to the PP. This result confirms the results obtained in earlier work (121).

Figure 3.21 shows the infrared spectrum for PP modified according to scheme 3.1 with SA (1%) and CLS (1%) in the presence (**a**) and absence (**b**) of DCP (0.3%). These spectra have peaks at 1893cm^{-1}, 1732cm^{-1}, 1674cm^{-1} and 1600cm-1 and are very similar to the previous spectra in the absence of CLS (figure 3.20 **b** to **d**). When the reaction was modelled in DD at 175^{0}C with SA (1%), DCP (0.3%) and CLS (1%) then the spectrum shown in figure 3.21 **c** was obtained, as can be seen this strongly resembles the nujol mull spectrum of SA (figure 3.20 **a**).

When PP was modified according to scheme 3.1 with SA (1%) and AMS (1%), to simulate the presence of GF-NH then the spectrum shown in figure 3.22 **a** was obtained. When the same reaction was modelled in dodecane at 175^{0}C according to scheme 3.2 then spectrum **b** was obtained. Finally, the spectrum of a model compound produced when SA and AMS were reacted (see section 2.1.4.5) is shown in figure 3.22 **c**. All the spectra (figure 3.22 **a** to **c**) are identical.

The mechanical properties of the SA modified unfilled PP (see scheme 3.3) did not differ significantly from those of the unfilled unmodified PP (cf tables 3.8 and 3.2, (see figures 3.23 to 3.25). Likewise, the properties obtained in the aggressive environments did not differ significantly (cf tables 3.9 and 3.3) (see figure 3.26).

Except for the TS, the mechanical properties of the GF-CL filled SA modified PP (see scheme 3.3), did not differ significantly from those of the corresponding filled unmodified

PP (cf table 3.8 and 3.2), (see figure 3.23 to 3.25). The TS was significantly improved and increased with increasing DCP concentration (cf tables 3.8 and 3.2), (see figure 3.23), the maximum TS obtained was, however, inferior to the commercial composite material (HW60/GR30).

In the aggressive environment the mechanical properties of the SA modified GF-CL filled PP did not differ significantly from those of the analogous filled unmodified samples, (cf tables 3.9 and 3.3), (see figure 3.26).

The IS of the SA modified GF-NH filled composite material (see scheme 3.3) did not differ significantly from that of the analogous filled unmodified PP (cf tables 3.8 and 3.2) (see figure 3.24). On the other hand, the remaining properties, TS, EL, FS and FM were all inferior to the analogous filled unmodified PP (cf tables 3.8 and 3.2) (see figures 3.23 and 3.25). Likewise, the mechanical properties of this composite were all inferior to those of the commercial composite (HW60/GR30).

In the aggressive environments the TS on exposure to boiling water and hexane of the SA modified GF-NH filled composite were inferior to those of the analogous unmodified filled composites (cf tables 3.9 and 3.3) (see figure 3.26). The IS of $-10^{0}C$, however, did not differ significantly. When compared with the commercial composite (HW60/GR30 in these environments the tensile properties of the SA modified composite were inferior (see table 3.9).

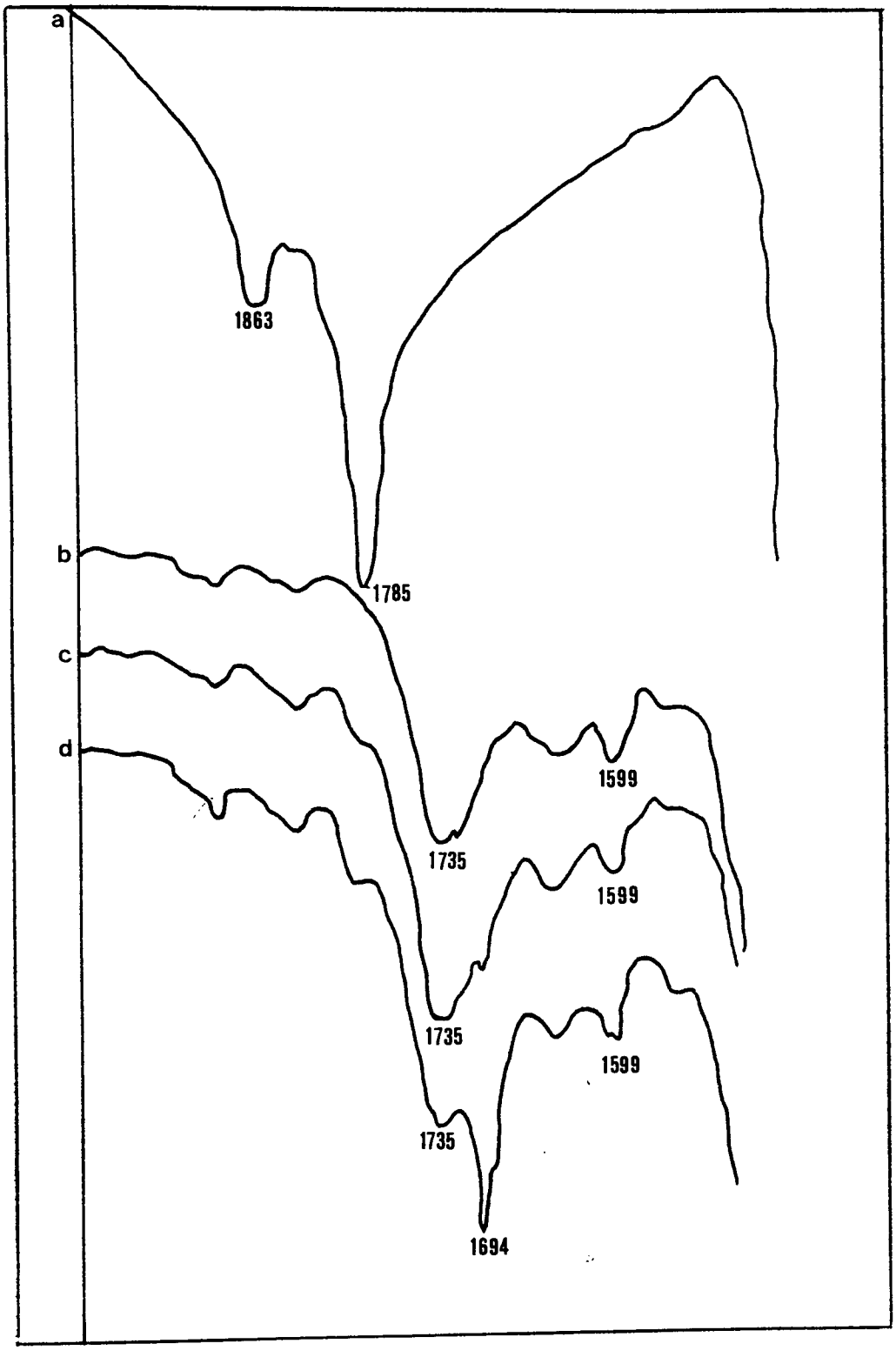


Figure 3.20. **a** = SA (nujol mull). **b** = PP + 1% SA (scheme 3.2). **c** = PP + 0.1% DCP + 1% SA (scheme 3.2). **d** = PP + 0.3% DCP + 1% SA (scheme 3.2)

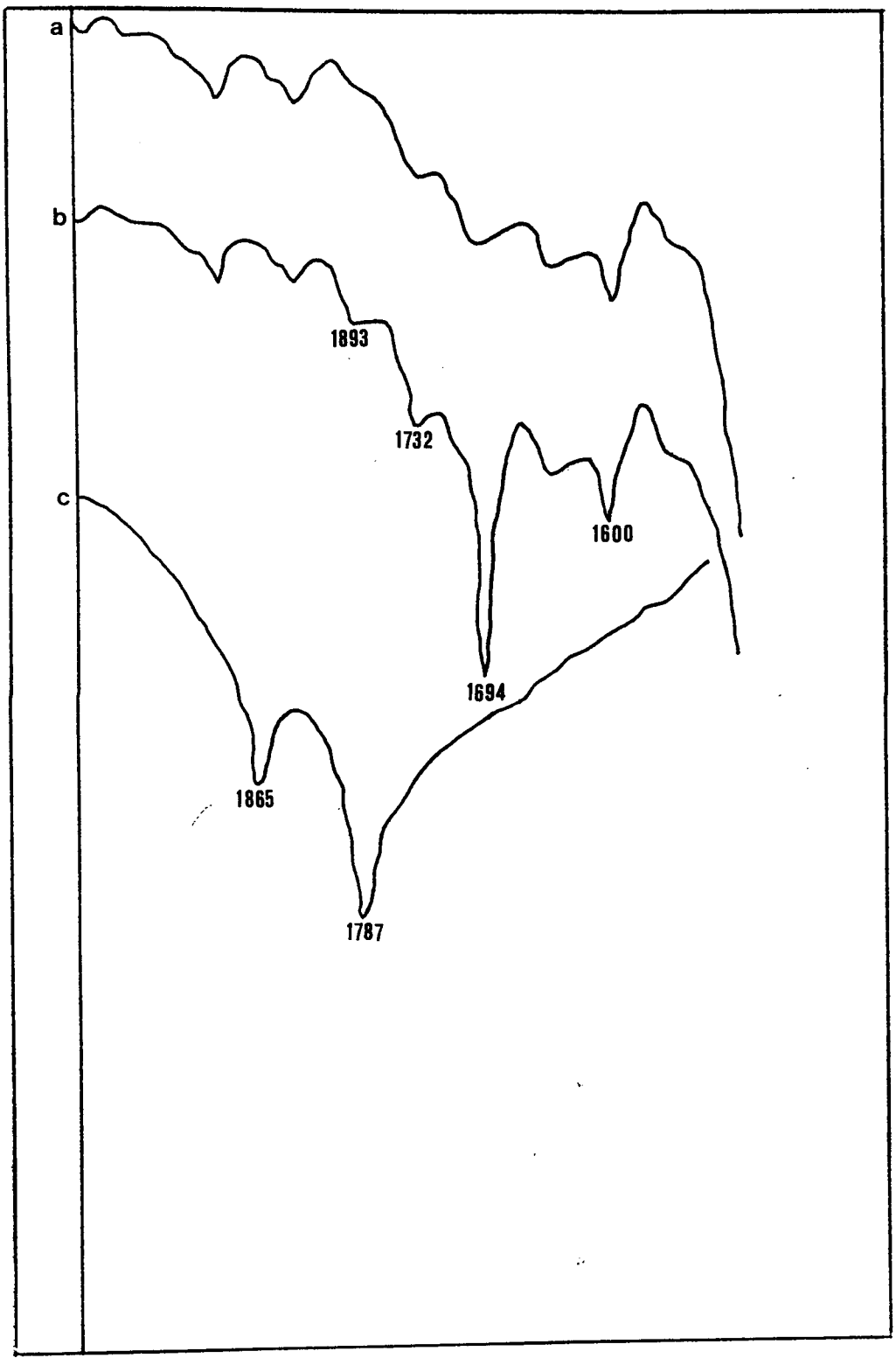


Figure 3.21. **a** = PP + 1% SA + CLS (scheme 3.1). **b** = PP + 0.3% DCP + 1% SA + 1% CLS (scheme 3.1). **c** = dodecane + 0.3% DCP + 1% SA + 1% CLS (scheme 3.2).

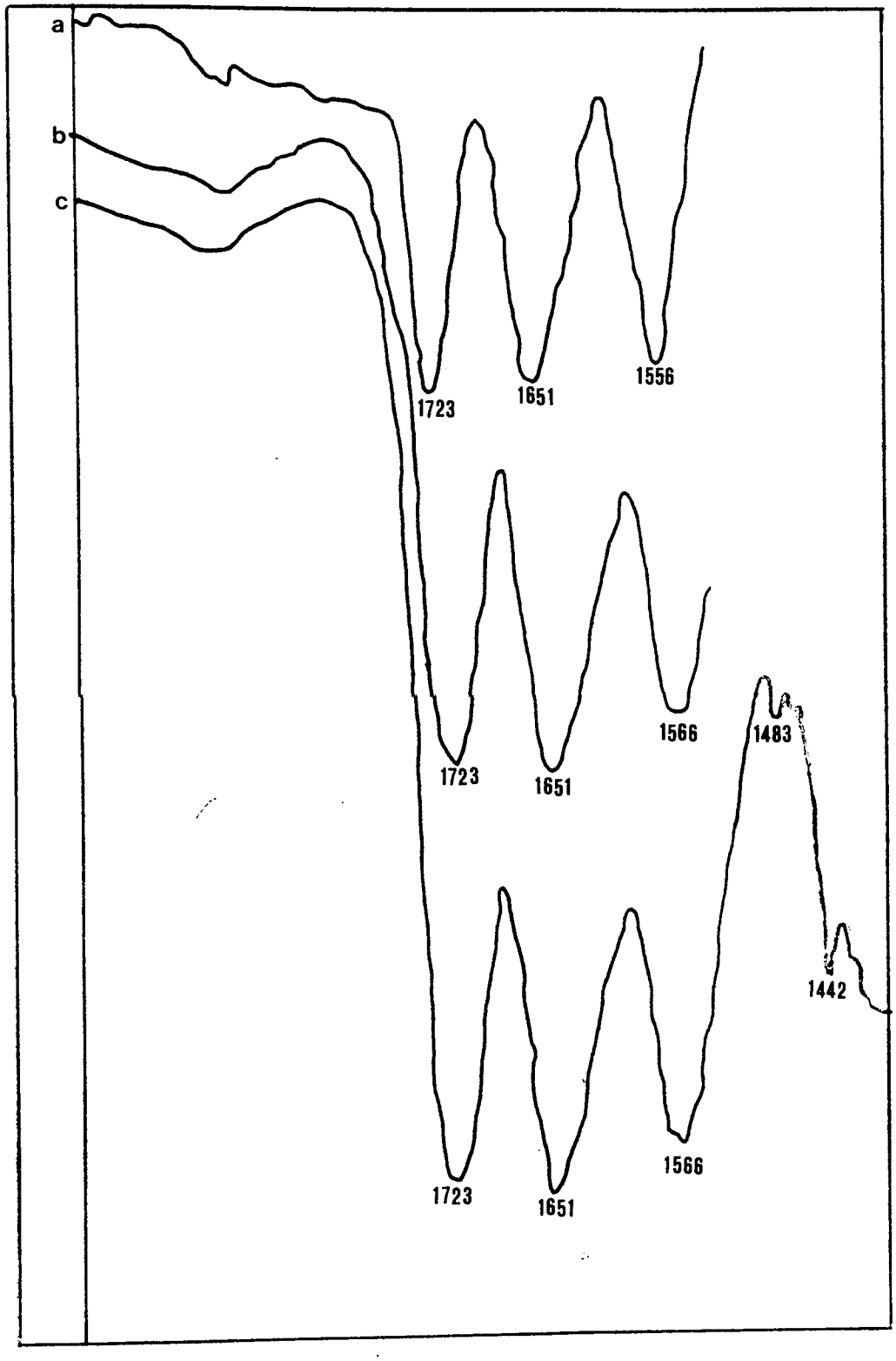
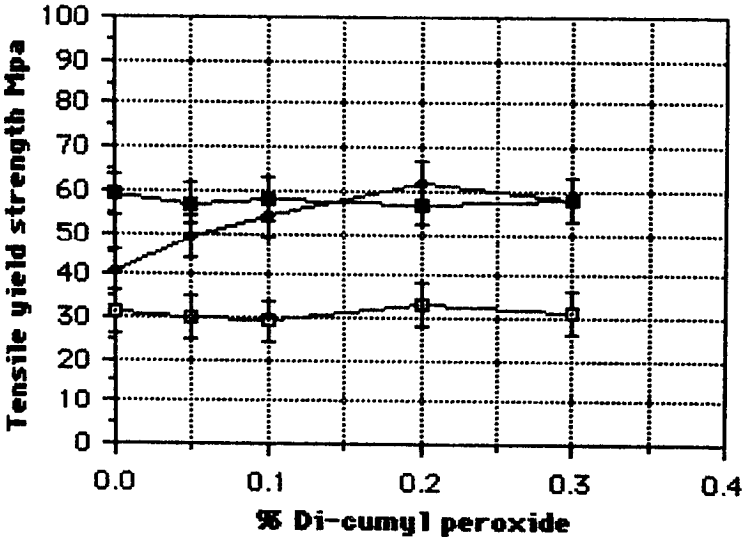


Figure 3.22. **a** = PP + 1% SA + AMS (scheme 3.1). **b** = dodecane + 1% AMS (scheme 3.2). **c** = SSA (section 2.1.4.5)



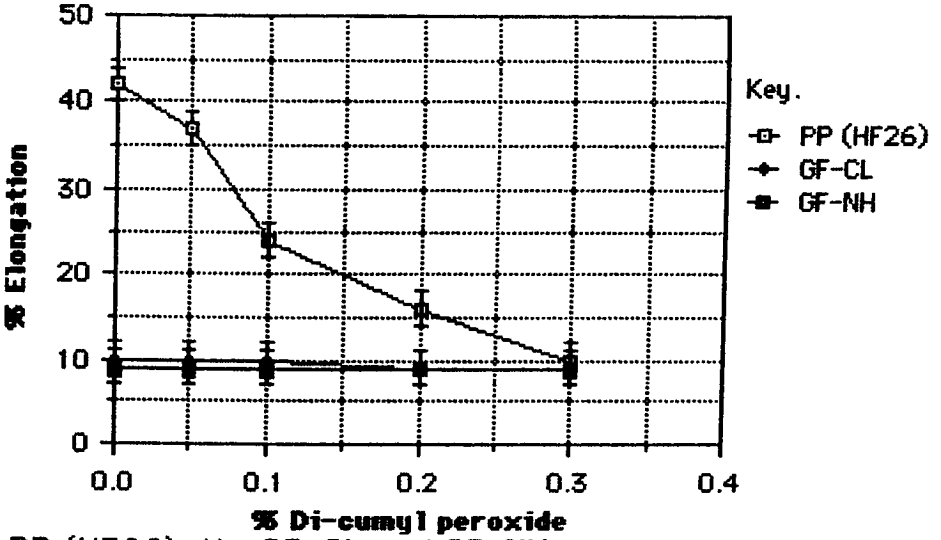


Figure 3.23Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with SA (1%) and DCP (0-0.3%).

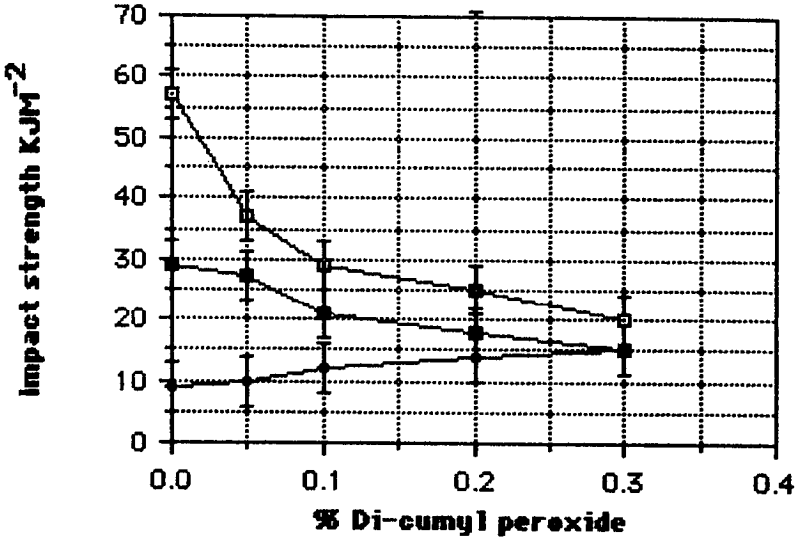


Figure 3.24. Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with SA (1%) and DCP (0-0.3%)

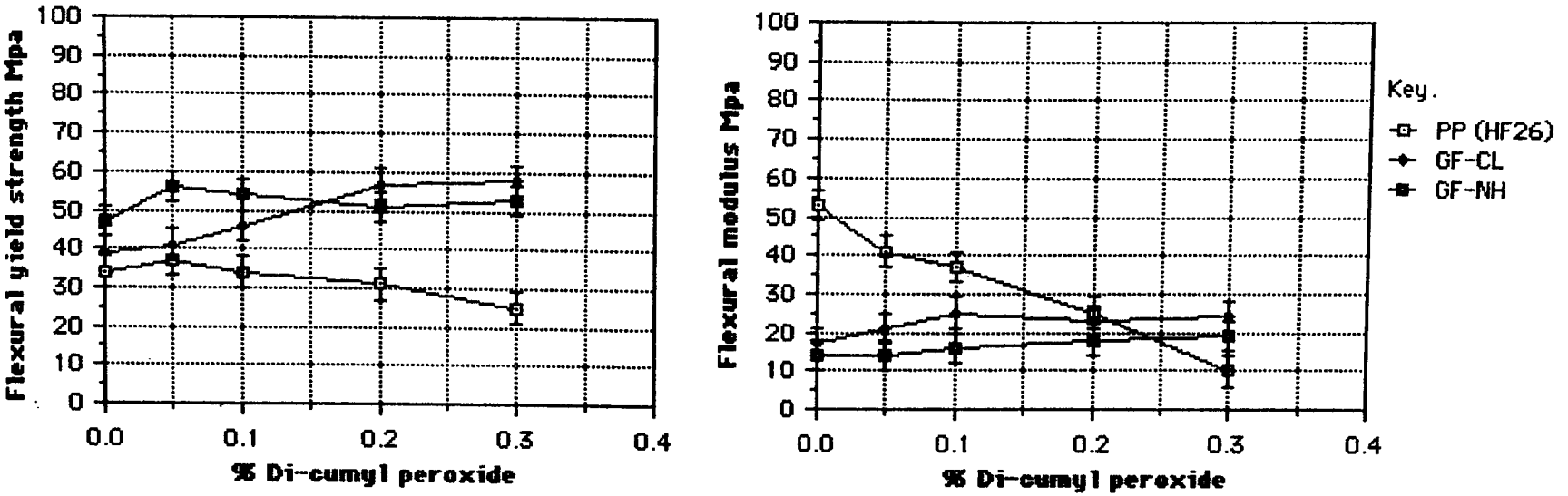


Figure 3.25. Flexural strength and flexural modulus of PP HF26, its GF-CL and GF-NH composites modified according to scheme 3.3 with SA (1%) and DCP (0-0.3%).

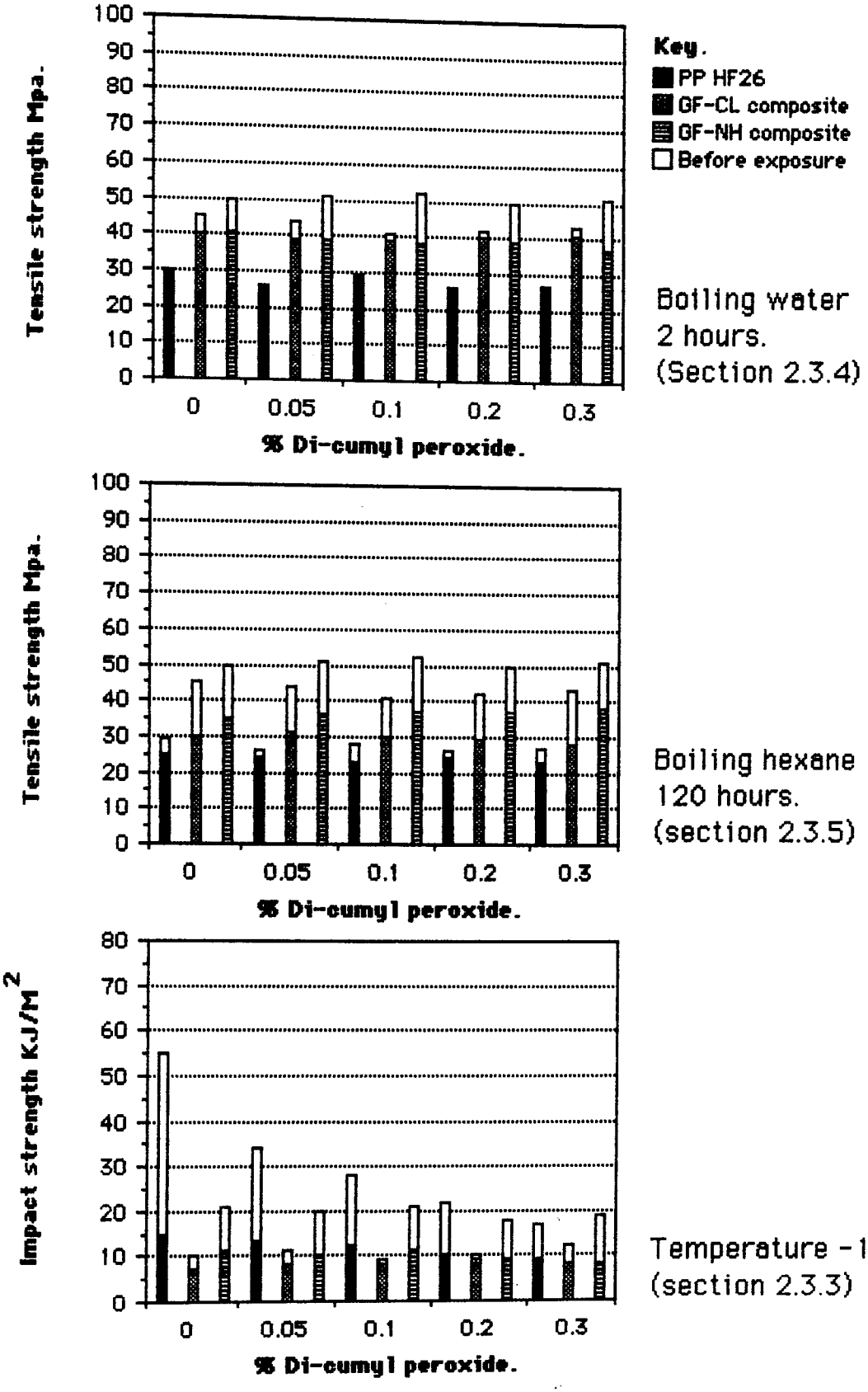


Figure 3.26 Tensile yield strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with SA (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 3.7. The binding of SA (1%) to PP HF26 determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.91	0	0
0.1	1	0.93	0	0
0.3	1	0.86	0	0
	No of modifier molecules per 10000 PP repeat units.			
0	56	51	0	-
0.1	56	42	0	-
0.3	56	48	0	-

Table 3.8 The effect of DCP concentration on the mechanical properties of PP (HF26) modified with SA (1%) (see scheme 3.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those samples which did.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	29	43	55	38	48
0.05	-	-	26	34	34	37	46
0.1	-	-	28	21	28	34	30
0.2	-	-	26	10	22	30	16
0.3	-	-	27	10	17	25	11
0	30	-	45	7	10	47	7
0.05	30	-	44	7	11	45	9
0.1	30	-	41	7	9	42	11
0.2	30	-	42	7	10	40	12
0.3	30	-	43	7	12	44	14
0	-	30	50	7	21	49	20
0.05	-	30	51	7	20	51	21
0.1	-	30	52	7	21	47	16
0.2	-	30	50	7	18	51	16
0.3	-	30	51	7	19	48	15
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

Table 3.9 The effect of adverse environments of boiling water for 2 hours of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with SA (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples table 3.8).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-10°C) KJ/M^2
0	-	-	30 (0%)	25 (-14%)	15 (-73%)
0.05	-	-	26 (0%)	24 (-8%)	13 (-62%)
0.1	-	-	29 (0%)	23 (-18%)	12 (-57%)
0.2	-	-	26 (0%)	24 (-8%)	10 (-54%)
0.3	-	-	26 (0%)	23 (-15%)	9 (-47%)
0	30	-	40 (-11%)	30 (-33%)	7 (-30%)
0.05	30	-	39 (-11%)	31 (-29%)	8 (-27%)
0.1	30	-	39 (-5%)	30 (-27%)	8 (-11%)
0.2	30	-	40 (-5%)	29 (-31%)	9 (-10%)
0.3	30	-	41 (-5%)	28 (-35%)	8 (-33%)
0	-	30	41 (-18%)	35 (-30%)	11 (-47%)
0.05	-	30	39 (-23%)	36 (-29%)	10 (-50%)
0.1	-	30	38 (-27%)	37 (-29%)	11 (-48%)
0.2	-	30	39 (-22%)	37 (-26%)	9 (-50%)
0.3	-	30	37 (-27%)	38 (-25%)	8 (-58%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

3.5 Mechanochemical modification of PP HF26 with Cis-Maleic acid (MAC) and DCP.

Maleic acid (MAC) was chosen for study to help to elucidate the reactions taking place with the MA. It was expected that many of the reactions taking place would be similar to the MA. The mechanical properties have been determined for completeness. The modification of PP with MAC, according to scheme 3.3 was not expected to produce any improvement in the properties.

The infrared spectrum of a nujol mull of MAC is shown in figure 3.27 **a**, this has four notable peaks at $1707cm^{-1}$, $1637cm^{-1}$, $1588cm^{-1}$ and $1567cm^{-1}$. The spectra of PP modified according to scheme 3.1 with MAC 1% in the absence (**b**) and presence of DCP (0.3%) (**c**) are also shown in figure 3.27. These have peaks at $1893cm^{-1}$, $1834cm^{-1}$, $1785cm^{-1}$, $1695cm^{-1}$ and $1641cm^{-1}$. On addition of the DCP the peaks at $1785cm^{-1}$, $1695cm^{-1}$ and $1641cm^{-1}$ increase in size.

The MFI of the MAC modified PP (see scheme 3.1) at DCP concentrations from 0 to 0.3% is shown in figure 3.6. These results do not differ significantly from those obtained with PP at DCP concentrations 0 to 0.3%. The binding studies of MAC modified PP (see scheme 3.1) showed that as expected no MAC was bound to the PP (see table 3.10).

Figure 3.28 shows the infrared spectrum of PP modified with MAC (1%) and CLS (1%) in the absence (**a**) and presence (**b**) of DCP (0.3%). Three notable peaks were observed at $1782cm^{-1}$, $1741cm^{-1}$ and $1695cm^{-1}$.

The infrared spectrum of PP modified with MAC (1%) and AMS (1%) in the absence and presence of DCP (0.3%) are shown in figure 3.28 **c** and **d** respectively. These strongly resemble the spectra of PP modified with MAC (1%) in the absence and presence of DCP (0.3%) see figure 3.27 **b** and **c** respectively.

The physical properties of the MAC modified PP in the absence and presence of GF-Cl and GF-NH were not significantly different from the analogous unmodified material (cf tables 3.11 and 3.2) (see figures 3.29 to 3.31), thus the results were comparable to the unfilled commercial PP (HWM25) and inferior to the commercial composites (HW60/GR30). The mechanical properties of the MAC modified PP in the absence and presence of GF-CL or GF-NH in the adverse environment also did not differ significantly from the analogous unmodified material (cf tables 3.12 and 3.3) (see figure 3.32).

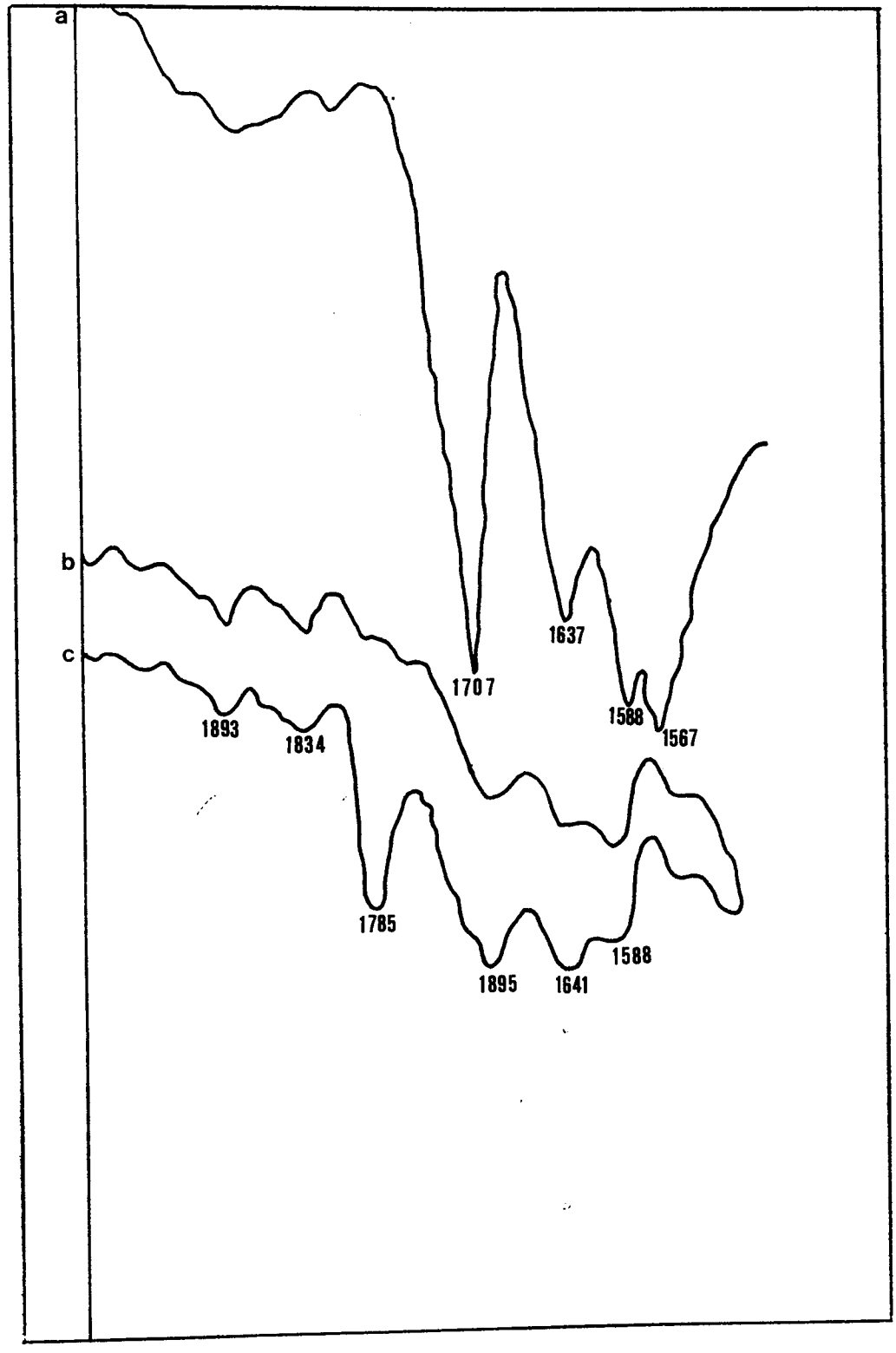


Figure 3.27. **a** = MAC (nujol mull), **b** = PP + 1% MAC, **c** = PP + 1% MAC + 0.3% DCP

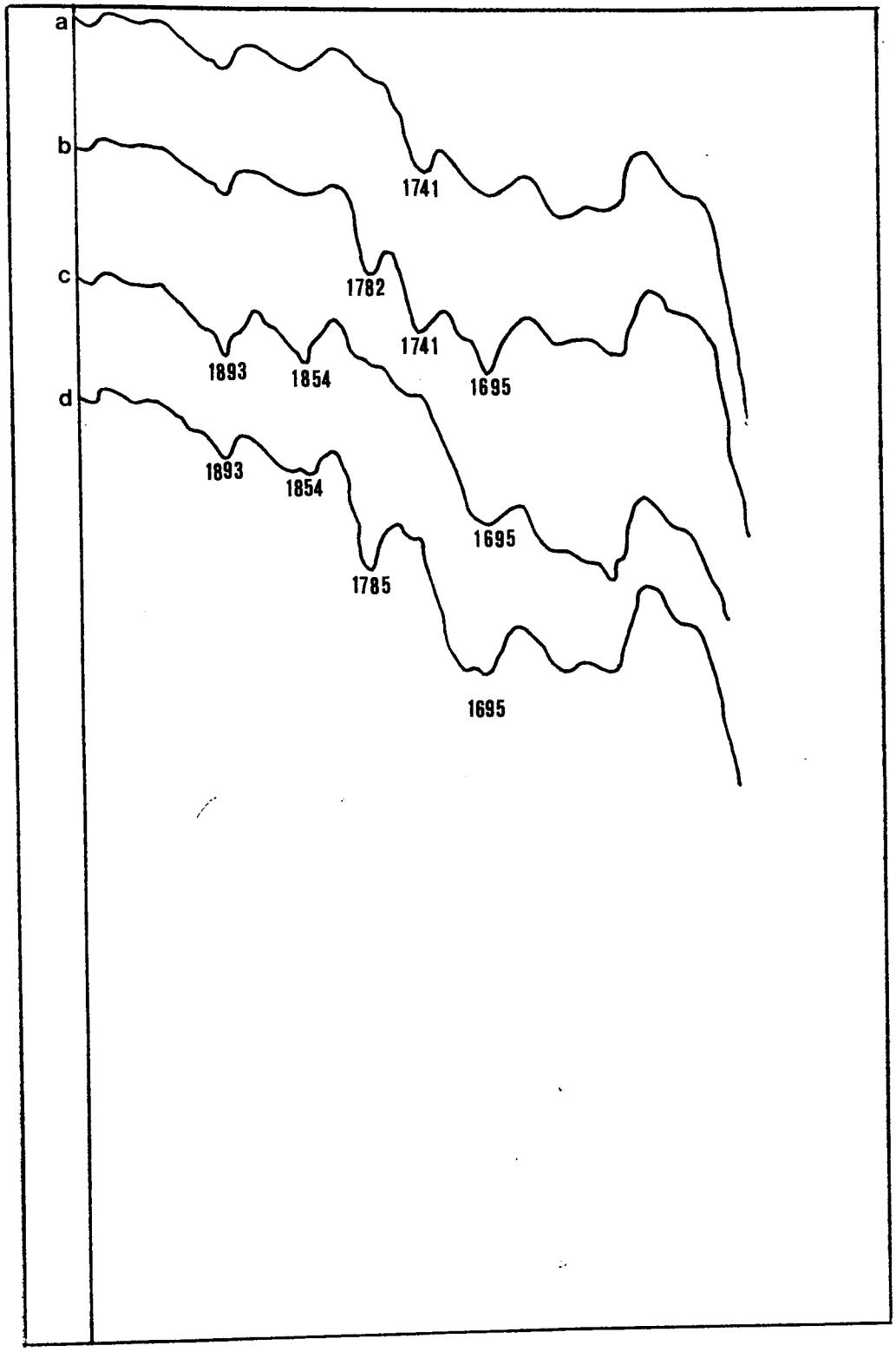
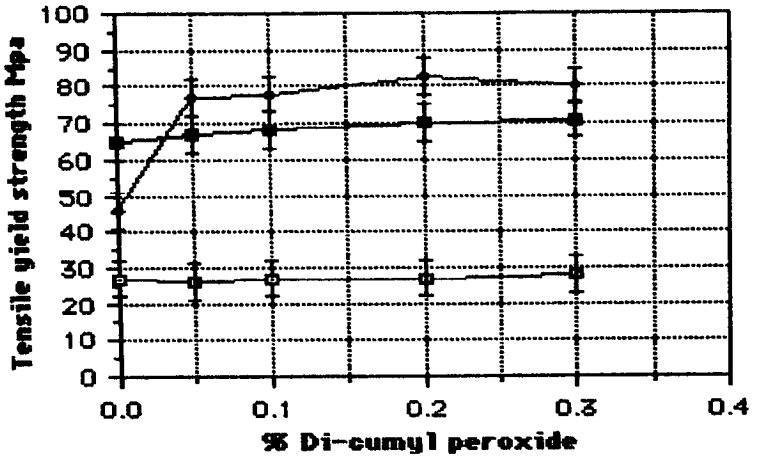


Figure 3.28. **a** = PP + 1% MAC + 1% CLS (scheme 3.1). **b** = PP + 0.3% DCP + 1% MAC + 1% CLS (scheme 3.1). **c** = PP + 1% MAC + 1% AMS (scheme 3.1). **d** = PP + 0.3% DCP + 1% MAC + 1% AMS (scheme 3.1).



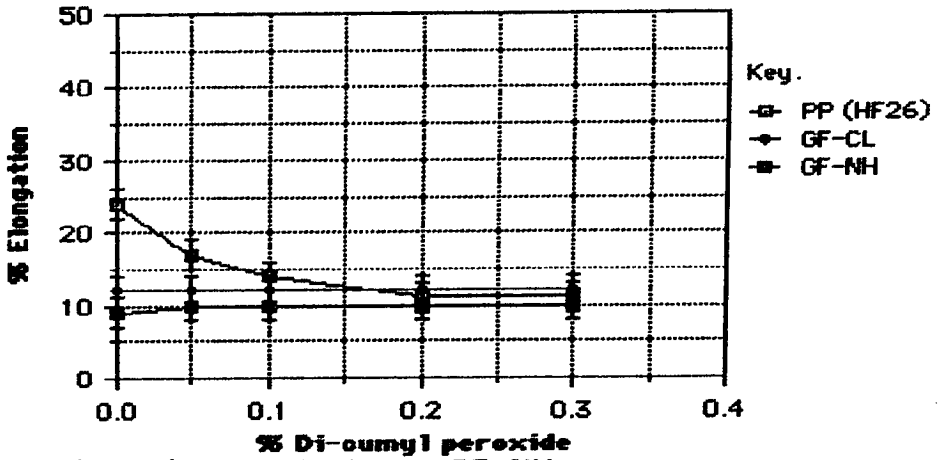


Figure 3.29Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with MAC (1%) and DCP (0-0.3%)

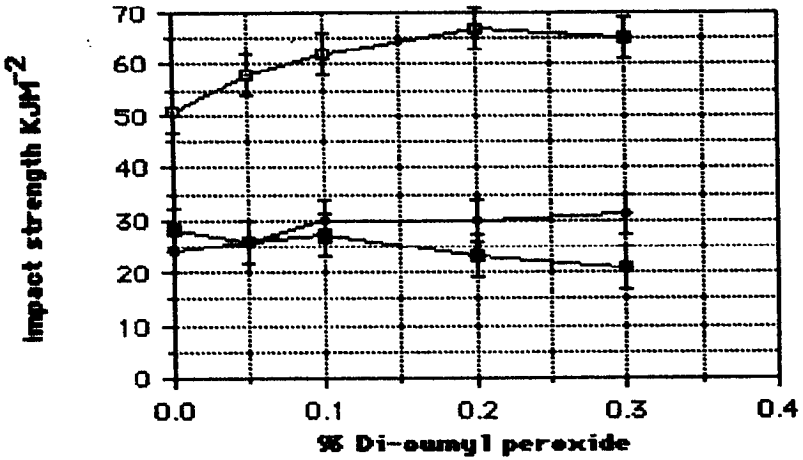


Figure 3.30 Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with MAC (1%) and DCP (0-0.3%)

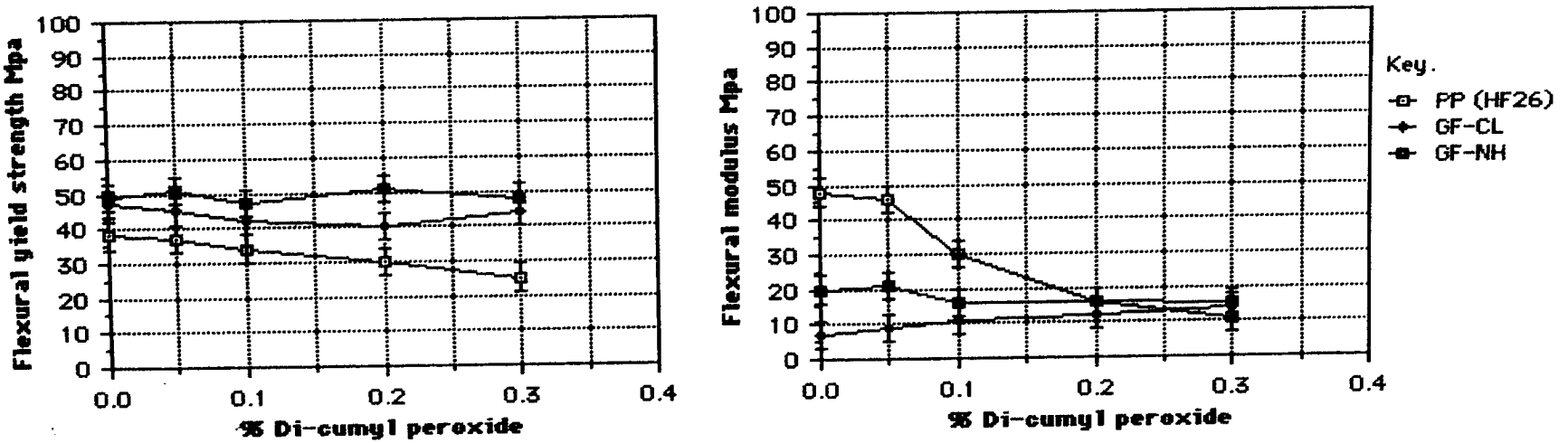


Figure 3.31.Flexural strength and flexural modulus of PP HF26, its GF-CL and GF-NH composites modified according to scheme 3.3 With MAC (1%) and DCP (0-0.3%).

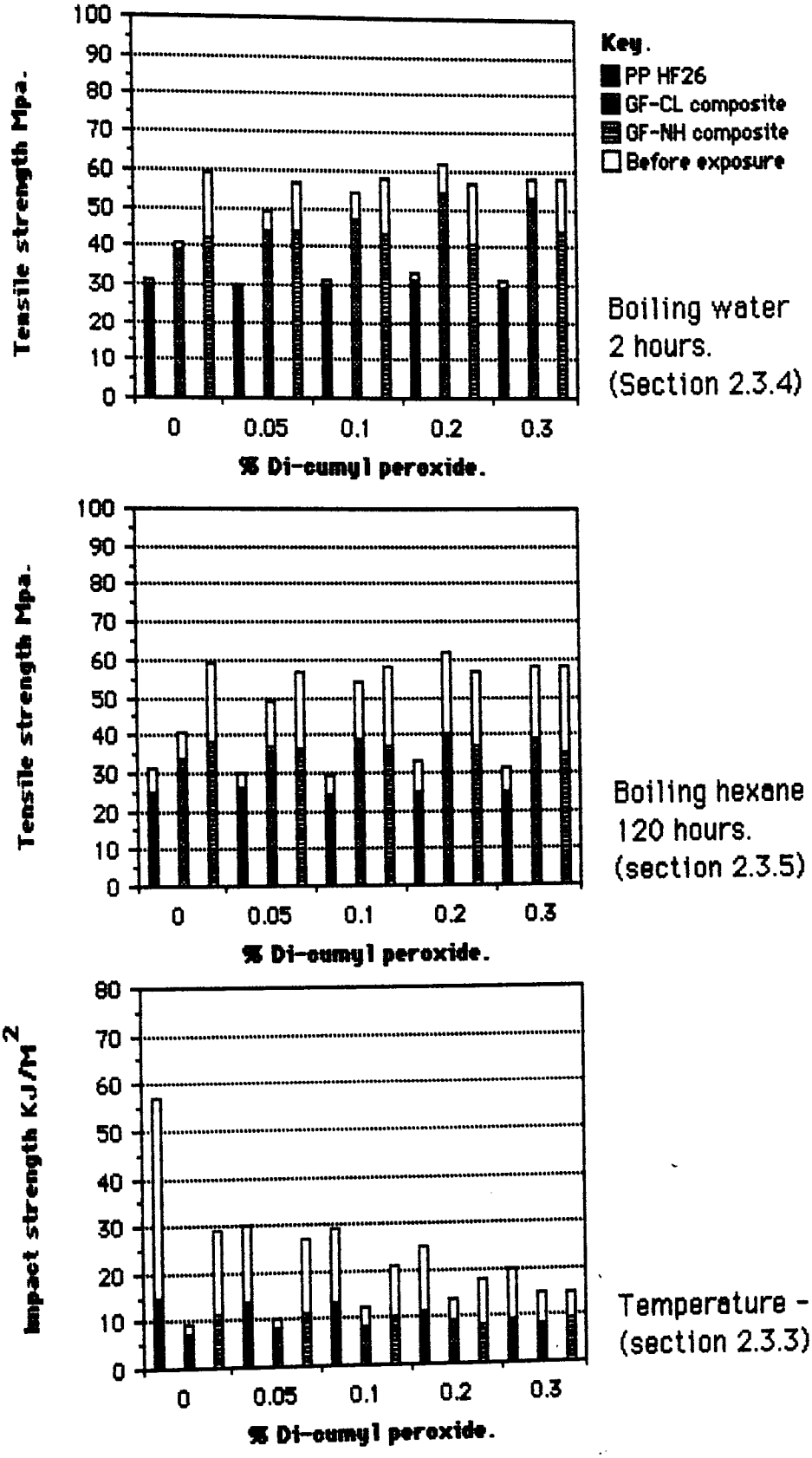


Figure 3.32 Tensile yield strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with MAC (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 3.10. The binding of MAC (1%) to PP (HF26) determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.86	0	0
0.1	1	0.81	0.03	3
0.3	1	0.95	0.12	12
	No of modifier molecules per 10000 PP repeat units.			
0	48	41	0	-
0.1	48	39	1.5	-
0.3	48	45	5.8	-

Table 3.12 The effect of DCP concentration on the mechanical properties of PP (HF26) modified with MA (1%) (see scheme 3.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those samples which did.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	31	42	57	34	53
0.05	-	-	30	37	37	37	41
0.1	-	-	29	24	29	34	37
0.2	-	-	33	16	25	31	25
0.3	-	-	31	10	20	25	10
0	30	-	41	10	9	39	17
0.05	30	-	49	10	10	41	21
0.1	30	-	54	10	12	46	25
0.2	30	-	62	9	14	57	23
0.3	30	-	58	9	15	58	24
0	-	30	59	9	29	47	14
0.05	-	30	57	9	27	56	14
0.1	-	30	58	9	21	54	16
0.2	-	30	57	9	18	51	18
0.3	-	30	58	9	15	53	19
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

Table 3.13 The effect of adverse environments of boiling water for 2 hours of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with MAC (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples table 3.12).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-10°C) KJ/M^2
0	-	-	30 (0%)	25 (-19%)	15 (-74%)
0.05	-	-	30 (0%)	26 (-13%)	14 (-62%)
0.1	-	-	30 (0%)	24 (-17%)	13 (-55%)
0.2	-	-	31 (0%)	25 (-24%)	11 (-56%)
0.3	-	-	29 (0%)	25 (-19%)	9 (-55%)
0	30	-	39 (-5%)	34 (-17%)	7 (-22%)
0.05	30	-	44 (-10%)	37 (-24%)	8 (-20%)
0.1	30	-	47 (-13%)	39 (-27%)	8 (-33%)
0.2	30	-	54 (-13%)	40 (-35%)	9 (-36%)
0.3	30	-	53 (-9%)	39 (-33%)	8 (-46%)
0	-	30	42 (-29%)	38 (-35%)	11 (-62%)
0.05	-	30	44 (-23%)	36 (-37%)	11 (-59%)
0.1	-	30	43 (-26%)	37 (-36%)	10 (-52%)
0.2	-	30	41 (-28%)	37 (-35%)	8 (-55%)
0.3	-	30	44 (-24%)	35 (-39%)	9 (-40%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

3.6 Mechanochemical modification of PP HF26 with N-methylolmaleimide (NMM) and DCP.

N-methylolmaleimide NMM was chosen for study because of its unsaturation (reactivity towards PP) and reactivity via a condensation reaction with amines (103) and thus potential reactivity towards AMS and GF-NH.

The spectra at regions of 2000cm^{-1} to 1400cm^{-1} and 4000cm^{-1} to 3000cm^{-1} for a nujol mull of nmm are shown in figures 3.33 **a** and 3.34 **a** respectively. The main peaks are at 3428cm^{-1}, 3164cm^{-1}, 1775cm^{-1}, 1706cm^{-1} and 1584cm^{-1}. Similarly, the infrared spectra for PP modified according to scheme 3.1 with NMM (1%) in the absence (**b**) and presence of (**c**) 0.3% DCP. Prominent peaks appear at 1775cm^{-1} and 1713cm-1. The spectrum shown in figure 3.33 **d** is that of a red solid produced when the melt reaction of PP containing NMM and DCP is modelled in dodecane according to scheme 3.2; whilst spectrum **e** is that of the corresponding reaction carried out with MAL in place of the NMM. Both these spectra have peaks at 1775cm^{-1} and 1713cm-1. The MFI of the NMM (1%) modified PP (see scheme 3.1) at varying concentrations of DCP (0 to 0.3%) is shown in figure 3.6. As can be seen as the DCP concentrations increases so does the MFI, however, the increase is not a great as when PP was processed with DCP only. The binding studies showed that very high levels of NMM become bound to the PP (up to 100%) with 0.1% DCP, see table 3.14.

The infrared spectra of PP modified with NMM (1%) and CLS (1%) in the absence (**a**) and presence (**b**) of DCP (0.3%) are shown in figure 3.35. Both spectra are very similar and peaks at 1775cm^{-1} and 1713cm^{-1}. The spectrum of a red solid formed when the same reaction is modelled in dodecane (according to scheme 3.2) either with or without DCP is shown in figure 3.35 **c**. All three spectra possess peaks at 1775cm^{-1} and 1713 cm^{-1} though those of **c** are much broader.

The infrared spectra of PP modified according according to scheme 3.1 with NMM (1%) and AMS (1%) in the absence (**a**) and presence (**b**) of DCP (0.3%) are shown in figure 3.36; the product formed (a red solid) when the reaction is modelled in dodecane according to scheme 3.2 is shown in (**c**). All three spectra are very similar to those of of NMM with CLS (cf figures 3.35 and 3.36 **a** to **c**).

The mechanical properties of the NMM modified PP, according to scheme 3.3 are shown is figure 3.37 to 3.39.

The TS, FS and FM of the unfilled NMM modified PP (scheme 3.3) did not differ significantly from those of the unfilled unmodified PP (cf tables 3.15 and 3.3). However, the IS and EL were significantly improved, (cf tables 3.15 and 3.3) (see figure 3.37 and 3.38).

When compared with the unfilled commercial polymer (HWM25) the overall EL was superior, however, the IS was still inferior (see table 3.15). In the aggressive environments the TS in water and hexane did not differ significantly from those of the

analogous modified PP (cf table 3.15 and 3.3). However, the IS at -10°C was significantly improved, (see figure 3.40) and was significantly better than that of the commercial unfilled material (HWM125) at -10°C.

The TS and FS of the NMM modified GF-CL filled composite were superior to those of the analogous filled unmodified material (cf table 3.14 and 3.2), the remaining properties EL, IS and FM were not significantly different (see figure 3.37 to 3.39). The overall properties obtained were similar to those of the commercial composite (see table 3.14). In the aggressive environments the TS after exposure to water and hexane were superior to those of the analogous filled unmodified PP (cf table 3.15 to 3.3) (see figure 3.40). When compared with the commercial composite material (HW60/GR30) the TS in boiling water was inferior whilst the TS in boiling hexane was superior, the IS was not significantly affected (see table 3.15).

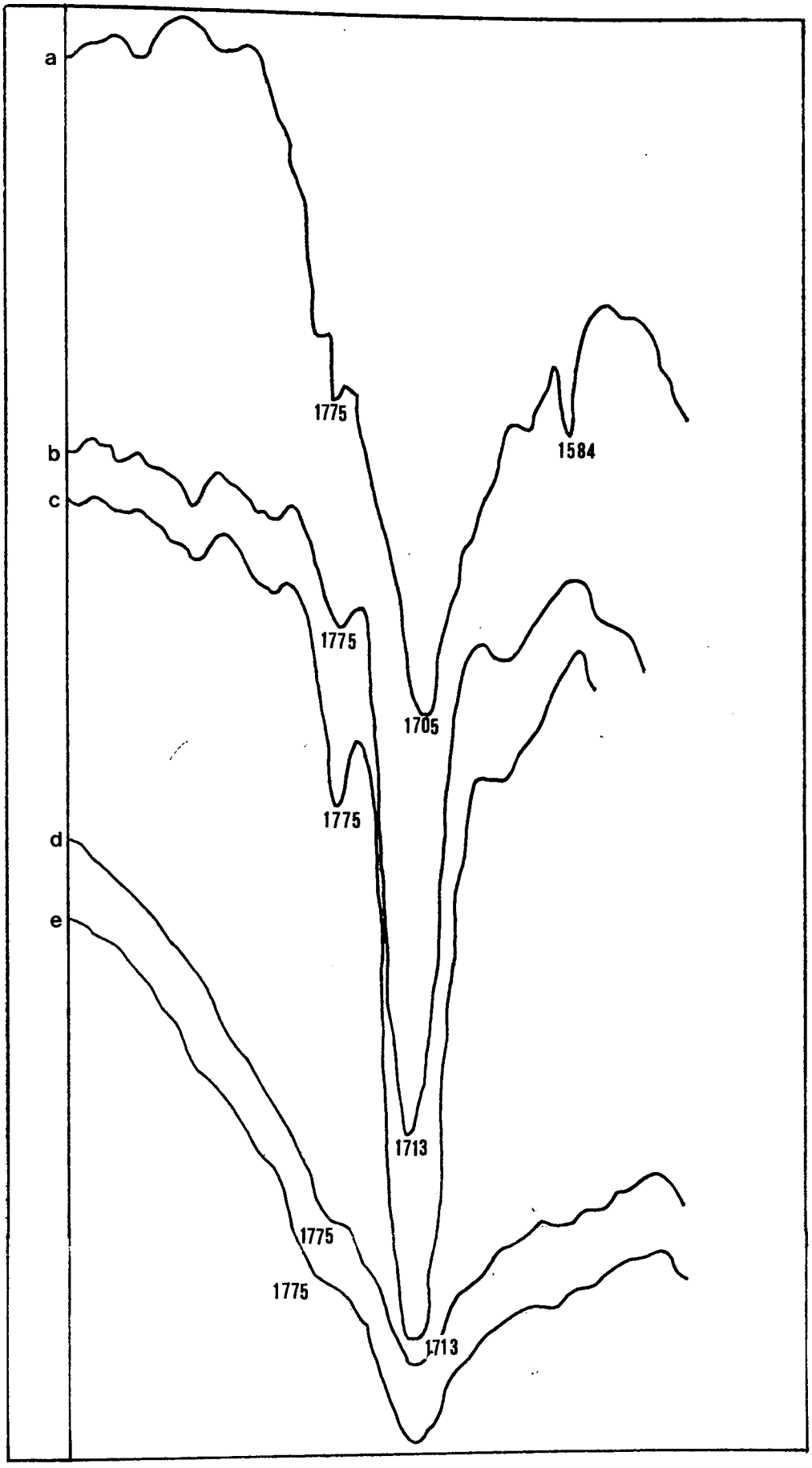


Figure 3.33. **a** = NMM (nujol mull). **b** = PP + 1% NMM (scheme 3.1). **c** = PP + 0.3% DCP + 1% NMM (scheme 3.1). **d** = dodecane + NMM (scheme 3.2), **e** = dodecane + MAL.

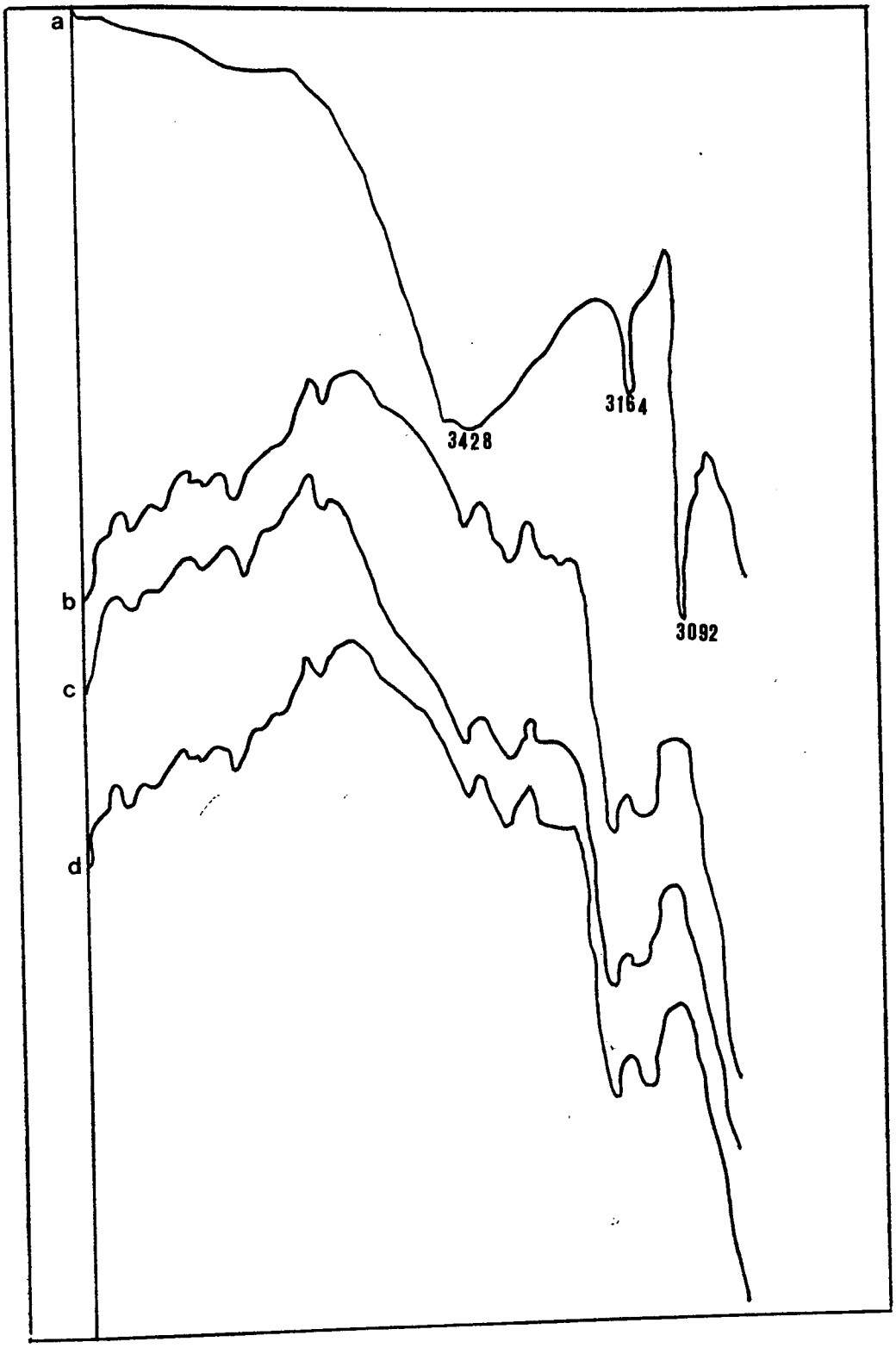


Figure 3.34. **a** = NMM (nujol mull). **b** = PP + 1% NMM (scheme 3.1). **c** = PP + 0.3% DCP + 1% NMM (scheme 3.1). **d** = PP (scheme 3.1)

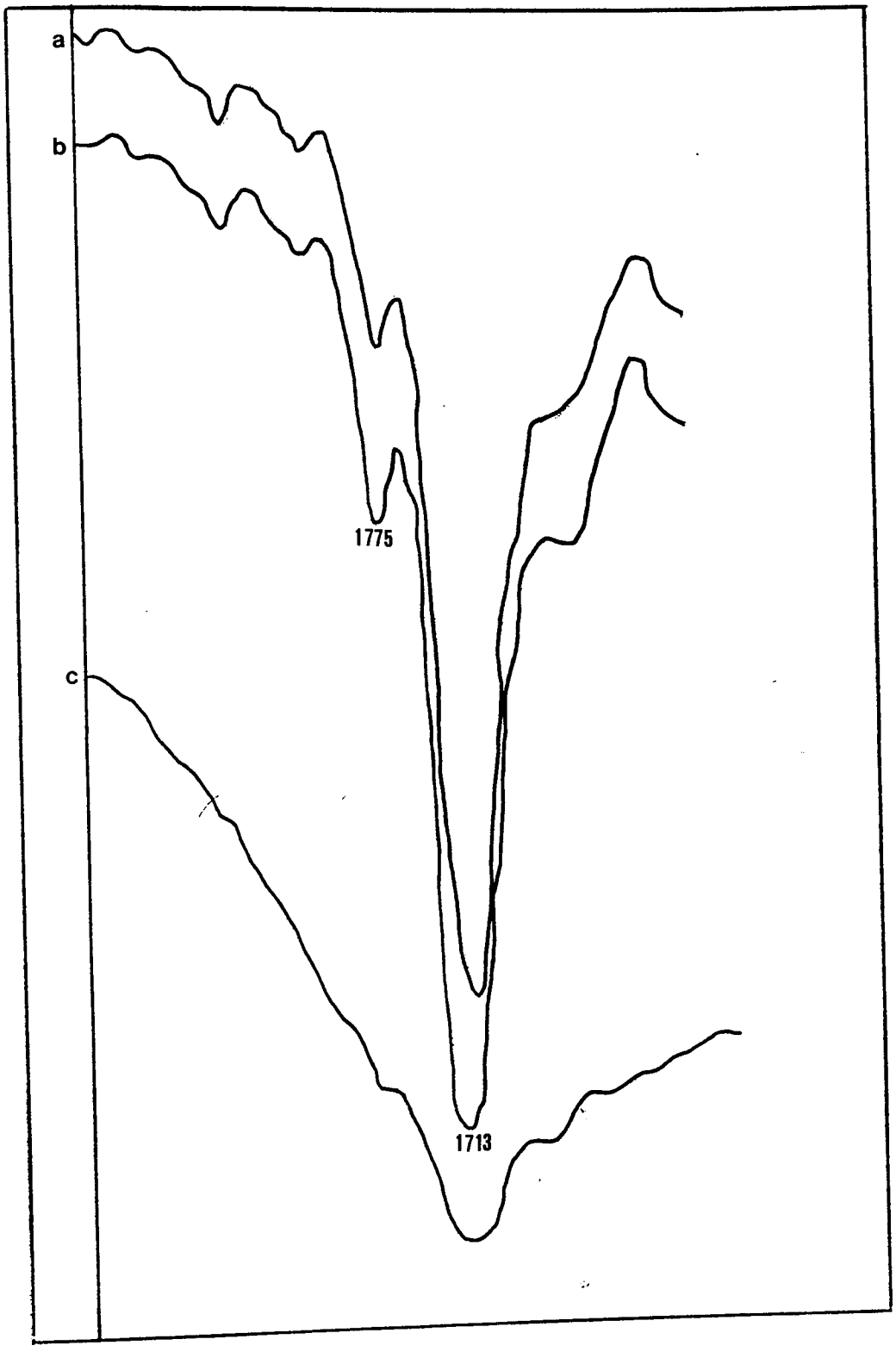


Figure 3.35. **a** = PP + 1% NMM + 1% CLS (scheme 3.1). **b** = PP + 0.3% DCP + 1% NMM + 1% CLS (scheme 3.1). **c** = dodecane + 0.3% DCP + 1% NMM + 1% CLS (scheme 3.1).

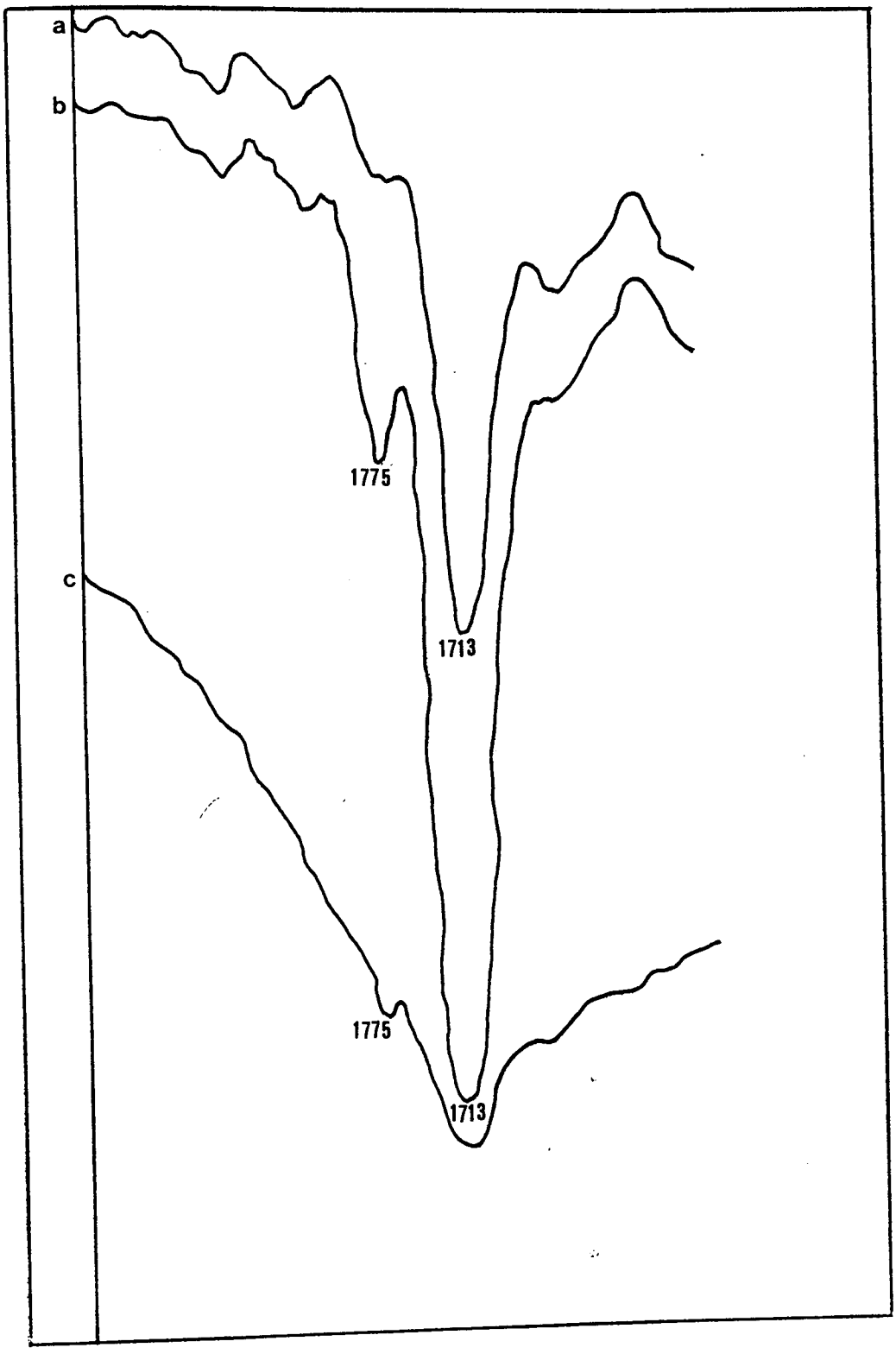
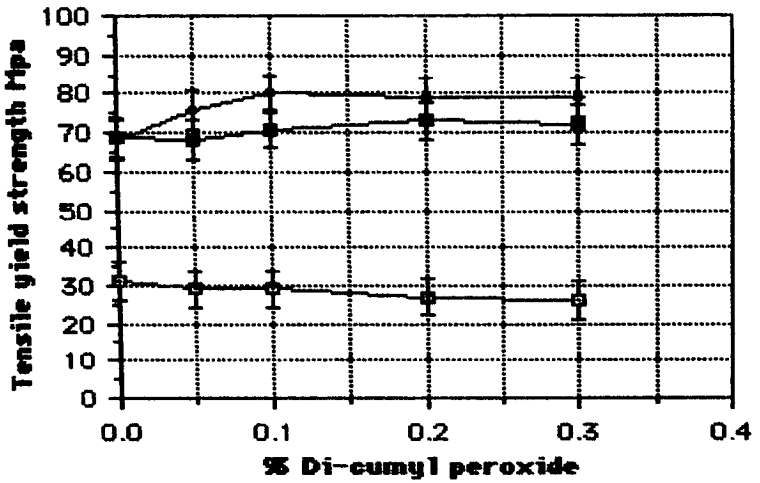


Figure 3.36. **a** = PP + 1% NMM + 1% AMS (scheme 3.1). **b** = PP + 0.3% DCP + 1% NMM + 1% AMS (scheme 3.1). **c** = dodecane + 0.3% DCP + 1% NMM + 1% AMS (scheme 3.2).



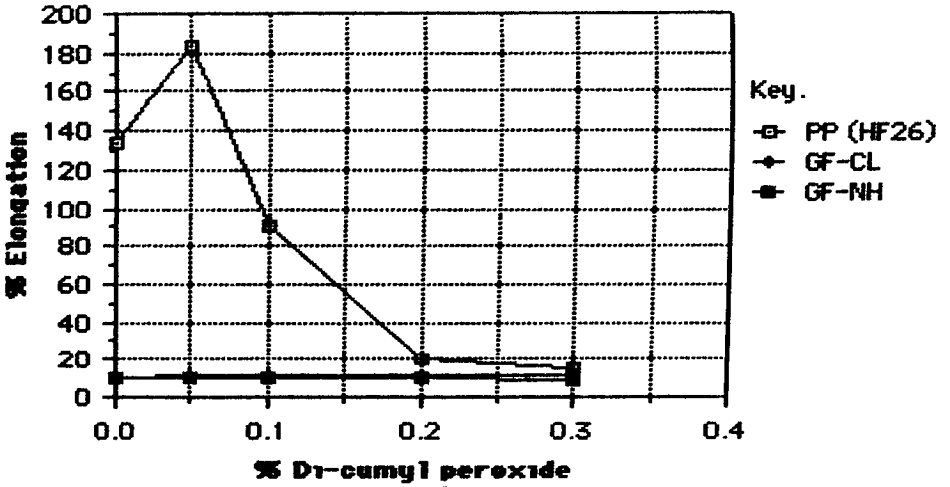


Figure 3.37Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 With NMM (1%) and DCP (0-0.3%)

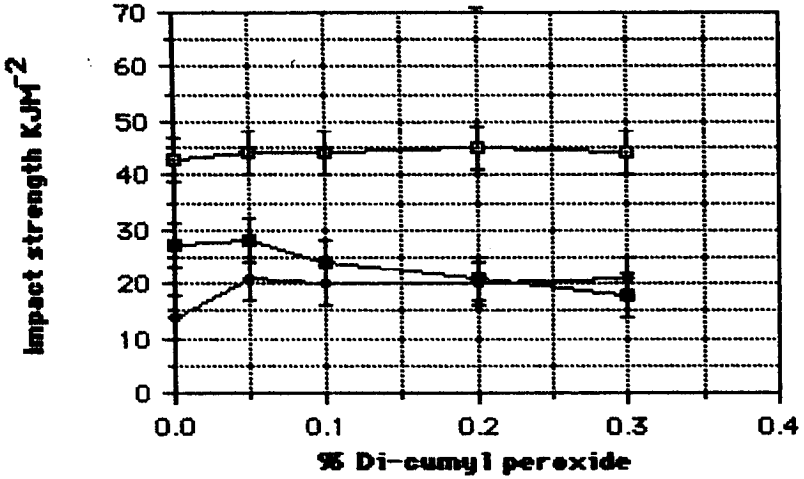


Figure 3.38 Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 With NMM (1%) and DCP (0-0.3%)

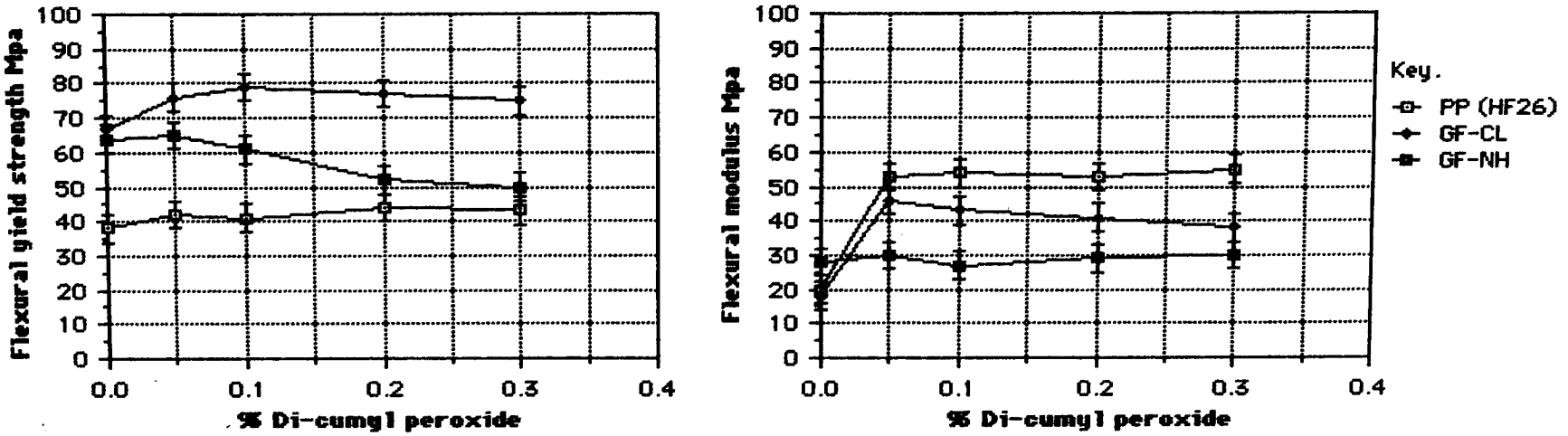


Figure 3.39. Flexural strength and flexural modulus of PP HF26, its GF-CL and GF-NH composites modified according to scheme 3.3 with NMM (1%) and DCP (0-0.3%).

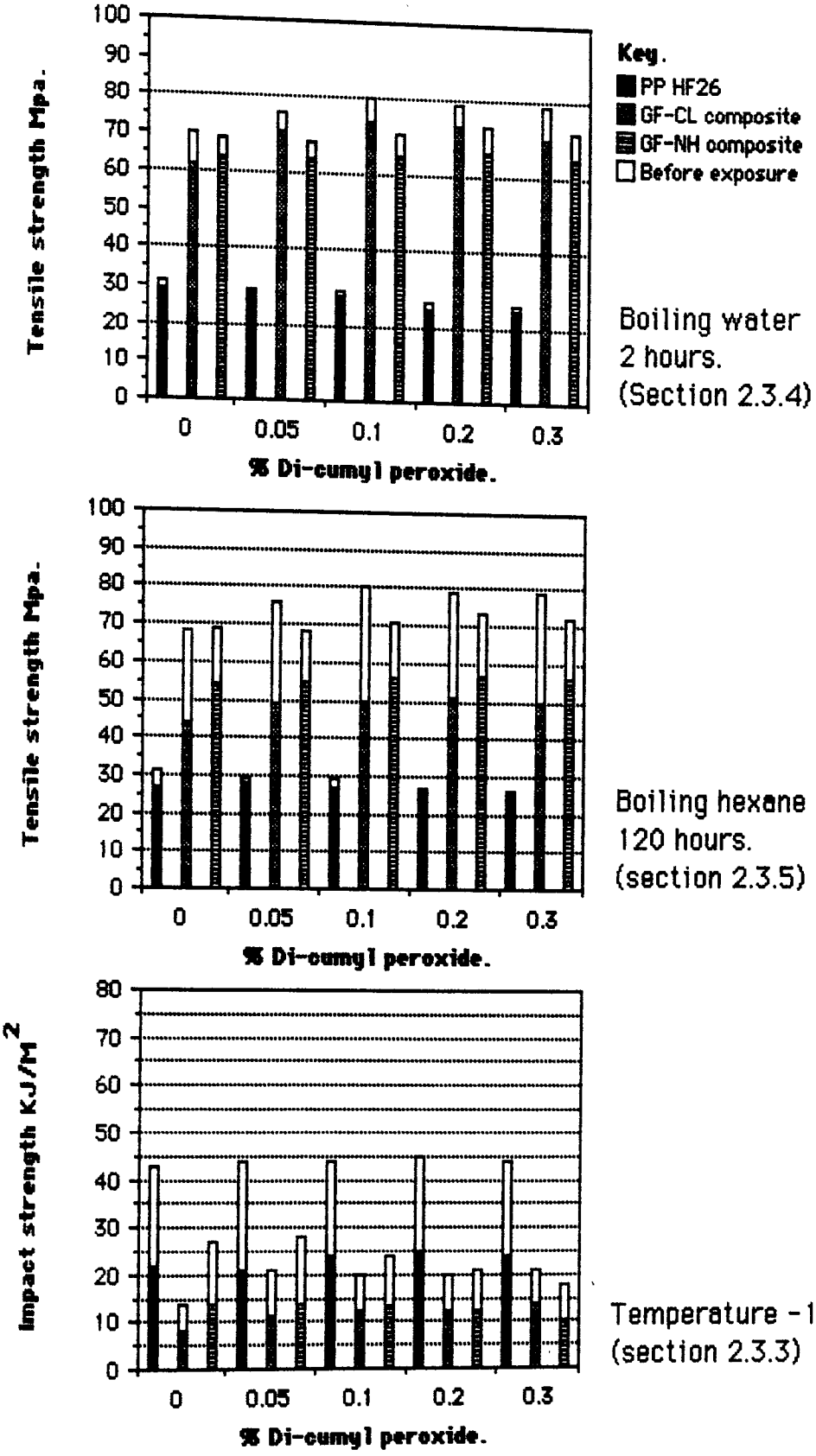


Figure 3.40. The tensile yield strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 with NMM (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 3.13. The binding of NMM (1%) to PP (HF26) determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.97	0.90	90
0.1	1	0.99	0.99	99
0.3	1	1.00	1.00	100
	No of modifier molecules per 10000 PP repeat units.			
0	44	43	39	-
0.1	44	43	43	-
0.3	44	44	44	-

Table 3.14. The effect of DCP concentration on the mechanical properties of PP (HF26) modified with NMM (1%) (see scheme 3.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those samples which did.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	31	134	43	38	20
0.05	-	-	29	183	44	42	53
0.1	-	-	29	91	44	41	54
0.2	-	-	27	20	45	44	53
0.3	-	-	26	15	44	43	55
0	30	-	68	10	14	67	18
0.05	30	-	76	11	21	76	46
0.1	30	-	80	11	20	79	43
0.2	30	-	79	11	20	77	41
0.3	30	-	79	11	21	75	38
0	-	30	69	10	27	64	28
0.05	-	30	68	10	28	65	30
0.1	-	30	71	10	24	61	27
0.2	-	30	73	10	21	52	29
0.3	-	30	72	9	18	50	30
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

Table 3.15 The effect of adverse environments of boiling water for 2 hours of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with NMM (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples table 3.14).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-10°C) KJ/M^2
0	-	-	29 (0%)	27 (-13%)	22 (-49%)
0.05	-	-	29 (0%)	28 (-3%)	21 (-50%)
0.1	-	-	28 (0%)	27 (-7%)	24 (-41%)
0.2	-	-	25 (-7%)	27 (0%)	25 (-43%)
0.3	-	-	25 (-4%)	26 (0%)	24 (-44%)
0	30	-	62 (-8%)	44 (-35%)	8 (-43%)
0.05	30	-	71 (-7%)	49 (-35%)	11 (-48%)
0.1	30	-	74 (-7%)	50 (-37%)	12 (-40%)
0.2	30	-	73 (-7%)	51 (-35%)	12 (-40%)
0.3	30	-	70 (-11%)	50 (-37%)	14 (-33%)
0	-	30	64 (-7%)	54 (-22%)	14 (-48%)
0.05	-	30	64 (-6%)	55 (-19%)	14 (-50%)
0.1	-	30	65 (-8%)	56 (-21%)	13 (-46%)
0.2	-	30	66 (-9%)	57 (-22%)	12 (-43%)
0.3	-	30	65 (-10%)	56 (-22%)	10 (-44%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

3.7 Mechanochemical modification of PP HF26 with N-ethanolmaleimide (NEM) and DCP

The infrared spectrum of PP modified with NEM (1%) (scheme 3.1) in the absence (**a**) and presence (**b**) of DCP (3%) is shown in figure 3.41. Notable peaks were observed at 1744^{-1} and $1708cm^{-1}$ (cf spectrum of a nujol mull of NEM, figure 3.41). When the above melt reaction was modelled in dodecane in the presence or absence of DCP then a white solid with the spectrum shown in figure 3.41**d** was produced. This has two notable peaks at $1744cm^{-1}$ and $1708cm^{-1}$.

The MFI measurements of NEM modified PP containing variable DCP concentrations are shown in figure 3.6 (see scheme 3.1). As can be seen the MFI increases with increasing DCP concentrations, however, the increase is not so great as that obtained with PP modified DCP only. Binding studies of the NEM modified PP are shown in table 3.16, as can be seen the amount of unextractable modifier increases as the DCP concentration increases. The spectrum of PP modified with 1% NEM and 1% CLS in the absence (**a**) and presence of DCP (0.3%) (**b**) are shown in figure 3.42, these have notable peaks at $1744cm^{-1}$ and $1708cm^{-1}$. When the same reaction was modelled in dodecane (see scheme 3.2) the spectrum shown in figure 3.42 **c** was obtained.

The spectrum of PP modified with 1% NEM and 1% CLS in the absence (**a**) and presence (**b**) of DCP (0.3%) are shown in figure 3.43. These have notable peaks at 1744 and 1710cm-1. When this reaction was modelled in dodecane the spectrum figure 3.43 **c** was obtained.

The mechanical properties of PP modified with NEM 1% in the absence and presence of glass fibres are summarised in table 3.17, figures 3.4 4 to 3.46. Only the TS of the unfilled modified PP was not significantly improved when compared with the analogous unfilled unmodified PP (cf tables 3.17 and 3.2). Overall the mechanical properties obtained were equal or superior to those of the unfilled commercial PP (HWM25). In the aggressive environments the results obtained with the modified PP did not differ significantly from those of the analogous unfilled unmodified PP (cf table 3.18 and 3.3) (see figure 3.47).

Overall the mechanical properties of the NEM (1%) modified GF-CL and GF-NH filled composite material did not differ significantly from those of the analogous filled unmodified composites (cf tables 3.18 and 3.3).

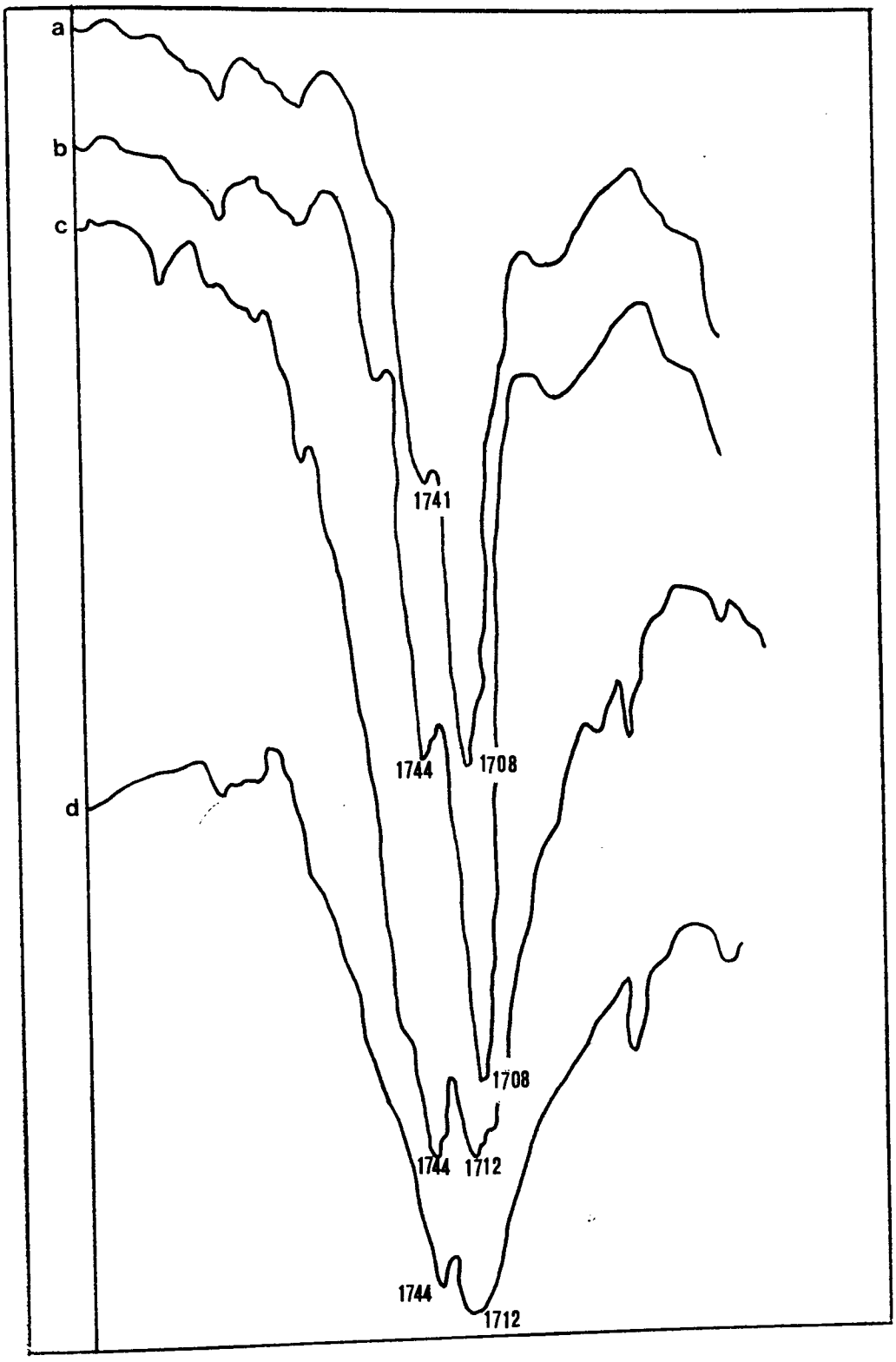


Figure 3.41. **a** = PP + NEM (scheme 3.1). **b** = PP + 0.3% DCP + 1% NEM. **c** = NEM (nujol mull). **d** = dodecane + 0.3% DCP + 1% NEM (scheme 3.2)

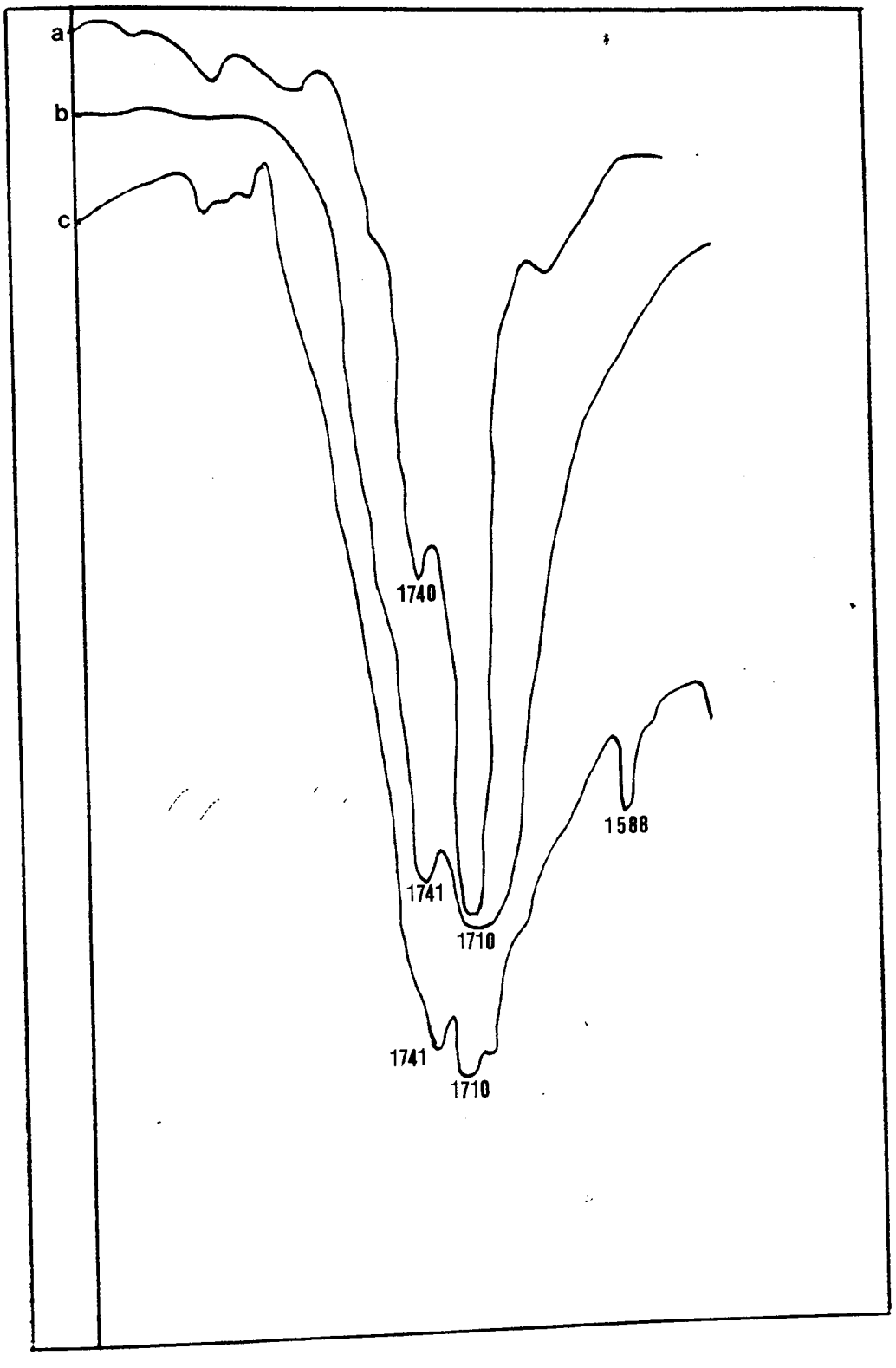


Figure 3.42. **a** = PP + 1% NEM + 1% CLS (scheme 3.1)., **b** = PP + 1% NEM + 1%CLS + 0.3% DCP, **c** = dodecane + 1% NEM + 1% CLS

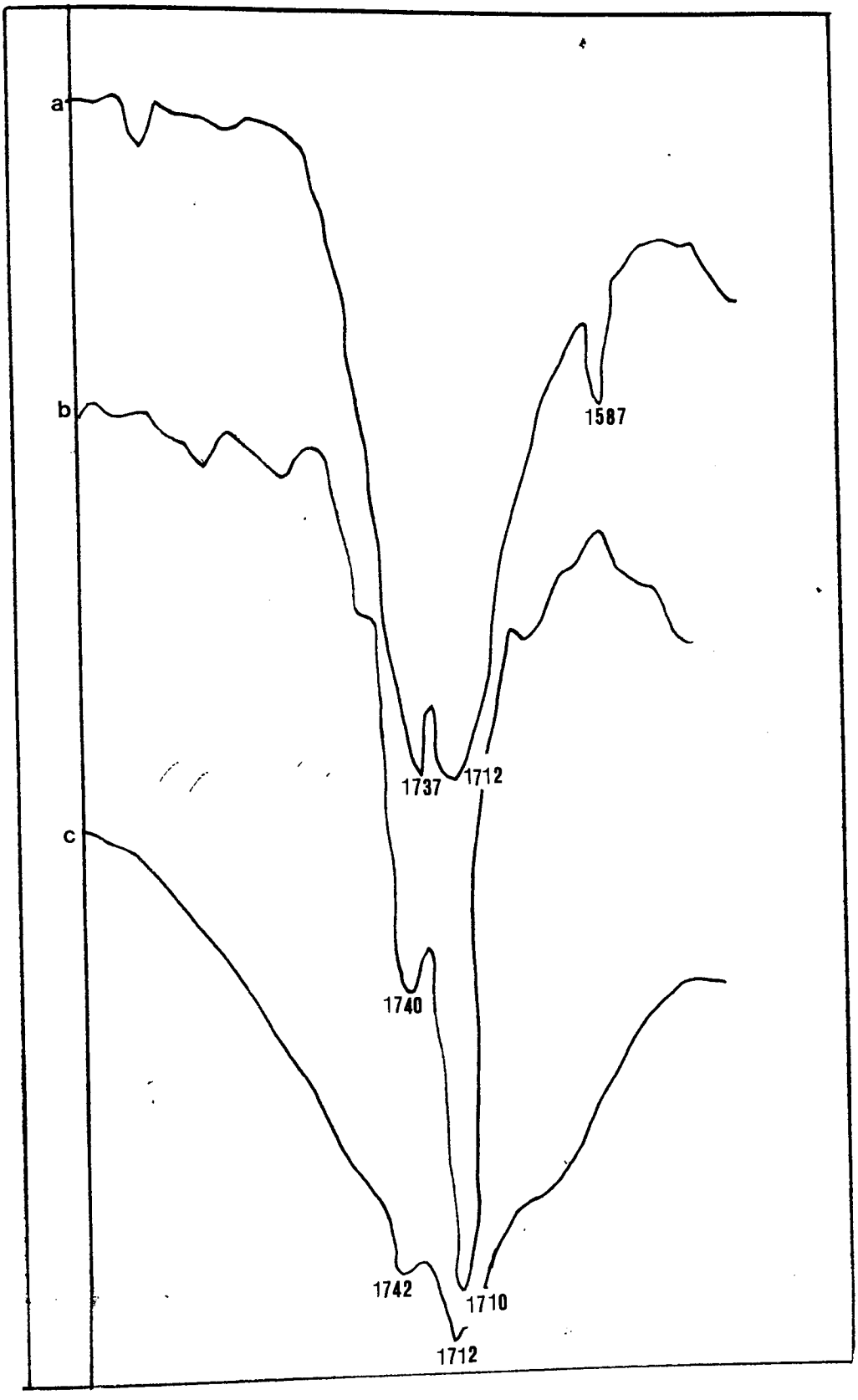


Figure 3.43. **a** = PP + 1% NEM + 1% AMS (scheme 3.1)., **b** = PP + 1% NEM + 1%AMS + 0.3% DCP, **c** = dodecane + 1% NEM + 1% AMS

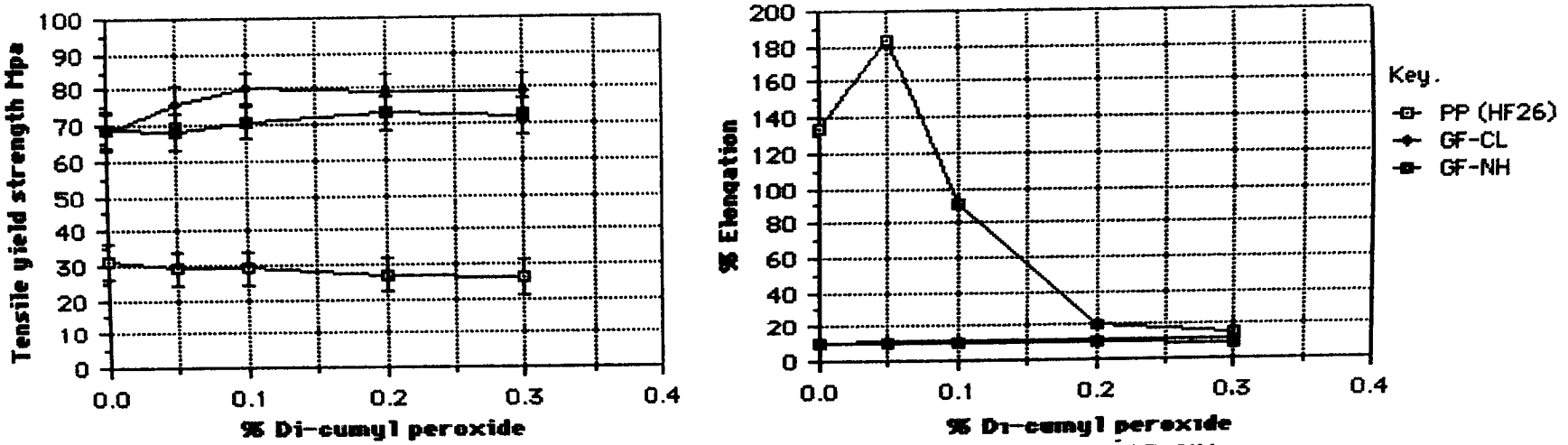


Figure 3.44Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 With NEM (1%) and DCP (0-0.3%)

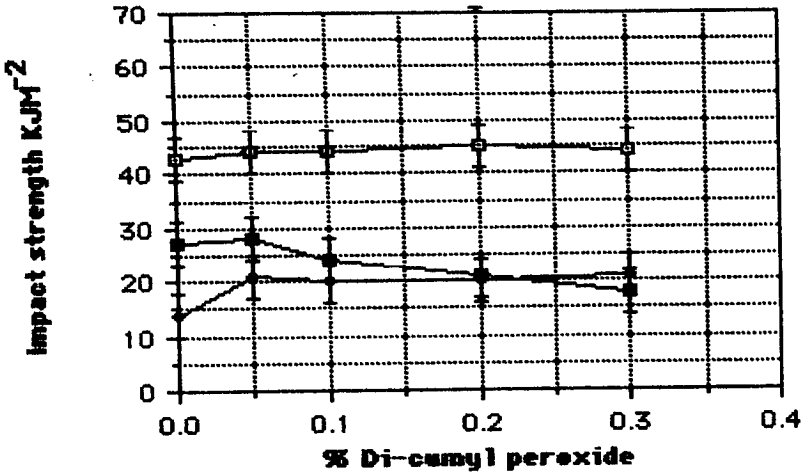


Figure 3.45 Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 3.3 With NEM (1%) and DCP (0-0.3%)

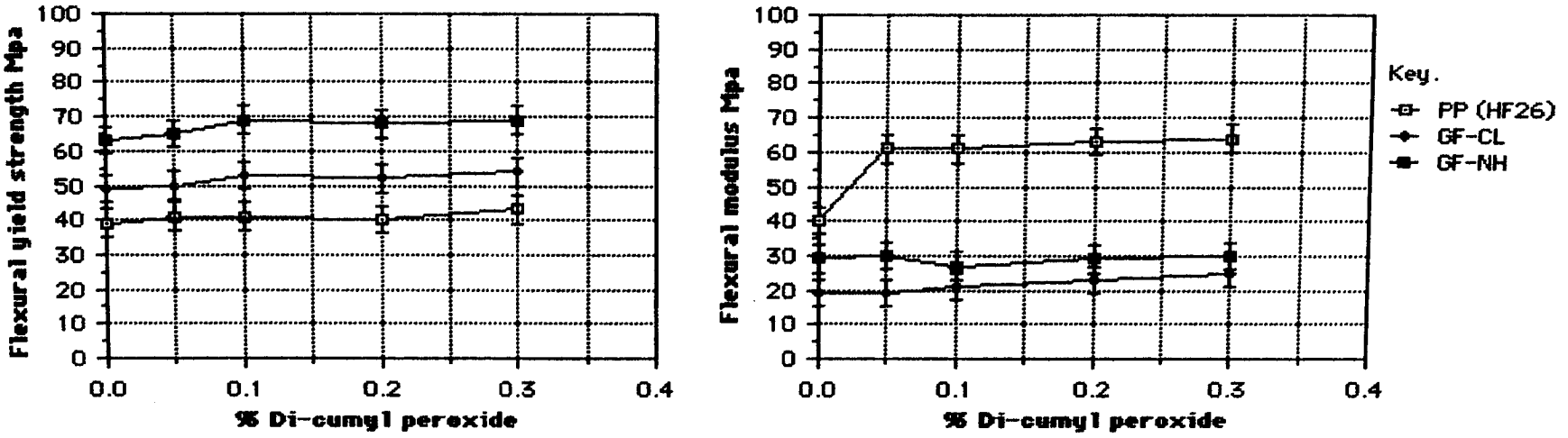


Figure 3.46. Flexural strength and flexural modulus of PP HF26, its GF-CL and GF-NH composites modified according to scheme 3.3 with NEM (1%) and DCP (0-0.3%).

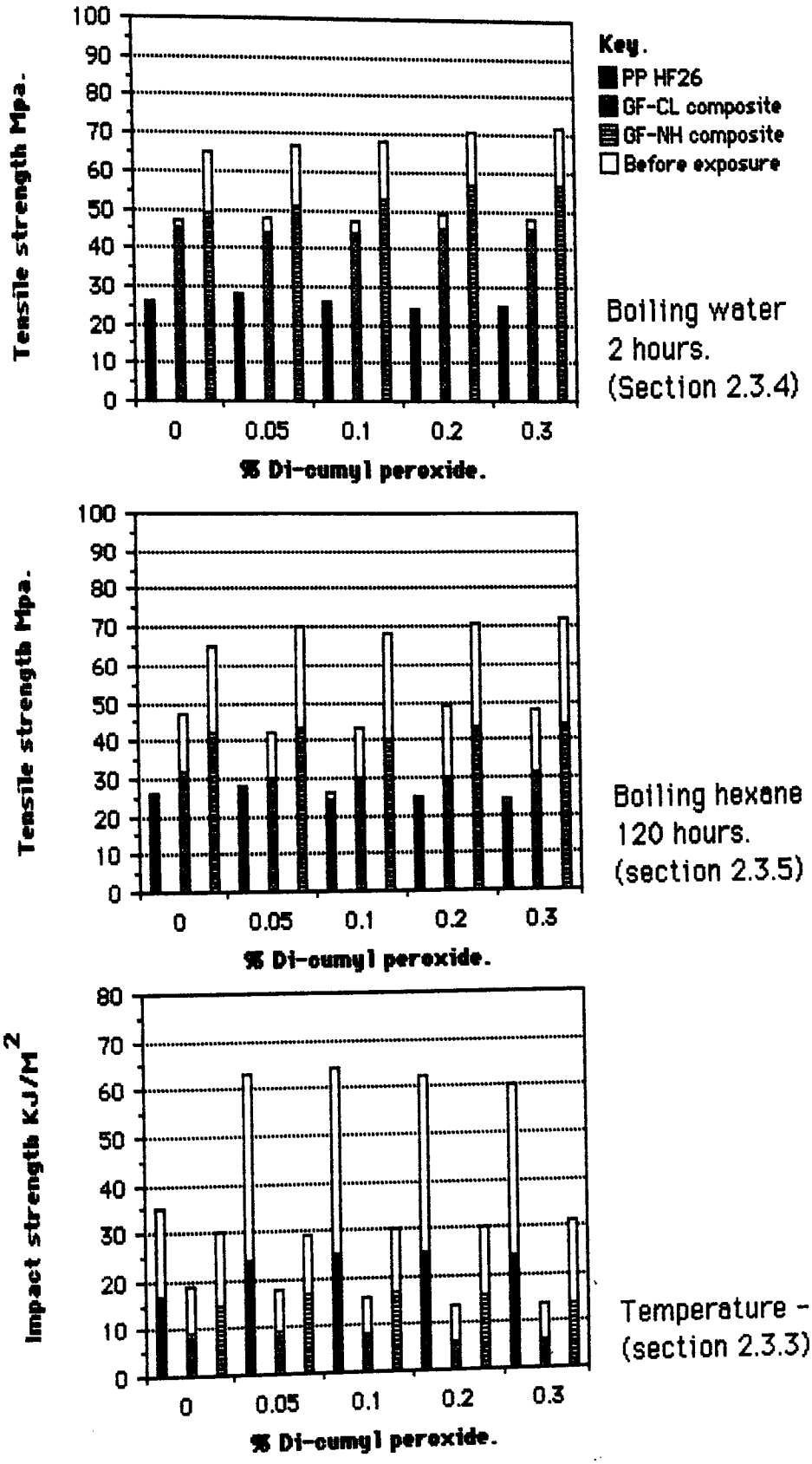


Figure 3.47 The tensile yield strength of PP HF26, its GF-CL and GF-NH composites modified according to scheme 3.3 with NEM (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 3.16. The binding of NEM (1%) to PP (HF26) determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.94	0.05	5
0.1	1	0.92	0.45	45
0.3	1	0.91	0.50	50
	No of modifier molecules per 10000 PP repeat units.			
0	39	36	2	-
0.1	39	36	17	-
0.3	39	35	20	-

Table 3.17. The effect of DCP concentration on the mechanical properties of PP (HF26) modified with NEM (1%) (see scheme 3.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those samples which did.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	26	152	35	39	40
0.05	-	-	28	294	63	41	61
0.1	-	-	26	229	>64	41	61
0.2	-	-	25	121	>62	40	63
0.3	-	-	24	10	>60	43	64
0	30	-	47	8	19	49	19
0.05	30	-	48	8	18	50	19
0.1	30	-	47	8	16	53	21
0.2	30	-	49	8	14	52	23
0.3	30	-	48	8	14	54	25
0	-	30	65	10	28	63	29
0.05	-	30	67	10	29	65	30
0.1	-	30	68	10	30	69	27
0.2	-	30	71	10	30	68	29
0.3	-	30	72	10	31	69	30
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

Table 3.18. The effect of adverse environments of boiling water for 2 hours of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with NEM (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples table 3.17).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-10°C) KJ/M^2
0	-	-	25 (-4%)	25 (-4%)	17 (-51%)
0.05	-	-	28 (0%)	27 (-4%)	24 (-62%)
0.1	-	-	26 (0%)	24 (-8%)	25 (-61%+)
0.2	-	-	24 (0%)	24 (-4%)	25 (-60%+)
0.3	-	-	24 (0%)	23 (-4%)	24 (-60%+)
0	30	-	45 (-4%)	32 (-32%)	9 (-53%)
0.05	30	-	44 (-8%)	30 (-37%0	9 (-50%)
0.1	30	-	44 (-6%)	30 (-36%)	8 (-50%)
0.2	30	-	45 (-8%)	30 (-39%)	6 (-57%)
0.3	30	-	45 (-6%)	31 (-35%)	6 (-57%)
0	-	30	49 (-25%)	42 (-35%)	15 (-46%)
0.05	-	30	51 (-24%)	43 (-36%)	17 (-41%)
0.1	-	30	53 (-22%)	40 (-41%)	17 (-43%)
0.2	-	30	57 (-20%)	43 (-39%)	16 (-46%)
0.3	-	30	57 (-21%)	44 (-39%)	14 (-55%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

3.8 Discussion

3.8.1 General effect of DCP and glass addition to PP HF26

From the results it is clear that the principal chemical effect of adding DCP to PP is to cause degradation, this is indicated by the growing carboxyl peak at 1710cm^{-1} (see figure 3.1) and the increasing MFI (see figure 3.6). In general, when the unfilled unmodified PP was compared with the unfilled commercial PP (HWM25) then their mechanical properties were similar (see table 3.3). This similarity extends to the mechanical properties in adverse environments. The mechanism for the attack of DCP radicals on PP is shown in figure 3.48. The attack of radicals occurs mainly at the tertiary carbon atom in the main chain to generate macro alkyl radicals (A). In the absence of a modifier the macro alkyl radicals disproportionate, reducing the PP molecular weight (B). The rate of disproportionation has been shown to be proportional to the initial DCP concentration and melt processing temperature (B).

For unmodified PP homogenization with GF-CL gave inferior properties to PP homogenisation with GF-NH (see table 3.3, figures 3.7 to 3.9). For the glass filled PP the general effects of the glass addition were to increase the TS and FS and to reduce the EL, IS and FM (see table 3.3, figure 3.7 to 3.9). These results were to be expected since the glass fibres have greater tensile properties than the PP but in general poorer impact and EL.

3.8.2 The properties of the modified unfilled PP HF26.

In general, the modifiers used in this study (see table 3.1) were not expected to significantly affect the properties of the PP HF26. However, in the case of the MA modified PP the IS was significantly impaired (see figure 3.17) whilst with the NMM (see figures 3.37 and 3.38) and NEM modified (see figures 3.44 and 4.45) PP both IS and EL were significantly improved. The MA modified PP system has been investigated previously using identical processing conditions and equipment but the PP used was HF22 (C). This work did not show any significant benefit of MA modification or unfilled PP. One factor which all three modifiers have in common is that they all bind to PP to a high degree (at least 50%).

The binding of MA to PP has been extensively investigated. The reaction takes place via macro alkyl radicals (see figure 3.48) in the presence of MA these radicals do not disproportionate but add preferentially to the MA (B, D, E). A general mechanism for these reactions is shown in figure 3.49. It has been assumed that the unsaturated modified NMM and NEM bind via the same mechanism. Evidence for the modifiers requiring unsaturation for binding can be found in the fact that SA did not bind to the PP (see table 3.8). Spectroscopic evidence for the binding of MA to the PP can be seen in figure 3.11(**c**, **d**). The

absorption of the peak at 1789cm^{-1} assigned to the carbonyl group of MA increases with the DCP concentration but differs slightly from that of free MA(E). Also in spectra 3.11 **c-d** a peak at 1694cm^{-1} can be seen, this also increases in with the DCP concentration. This has been attributed to the presence of MAC. A possible scheme to account for the formation of MAC is shown in figure 3.50. During the modification reaction there are several stages when MAC could be formed; in the initial premixing stage when all the modifiers are weighed and mixed hydrolysis of MA could occur. In scheme 3.3 further hydrolysis could occur as the material sits in the hopper prior to mixing. During mixing some steam is generated from water which condenses on the cold polymer (the unsaturated PP is stored at -10°C to retard degradation). This steam may hydrolyse either bound or unbound MA. Interestingly, when MAC was used as a modifier there is spectroscopic evidence (see figure 3.21) that some of the MAC is converted to MA, this is suggested by the formation of a peak at 1785cm^{-1}. This suggests that the hydrolysis of MA in these melt reactions is reversible.

In the case of NMM binding to PP it has been assumed that the general binding reaction is identical to that of MA (see figure 3.49). However, the structure of the NMM appears to be significantly altered during the melt reactions. NMM itself is a white crystalline solid with a distinct hydroxyl absorption at 3428cm^{-1}. However, in the melt reactions a red colour is observed (see figure 3.33). Likewise, when the melt reactions are modelled in dodecane a red solid is formed, this red solid has no absorption at 1428cm^{-1} but appears identical to a red solid obtained when Maleimide, the precursor to NMM, was melt processed. A possible scheme to account for these results is shown in figure 3.51. A earlier study employing MAL as a modifier and using identical processing conditions has been carried out (F). The properties of unfilled PP were not assessed but high levels of binding up to 83% were observed (F). The NEM binds to the PP without any loss of the hydroxyl absorption and no red colouration of the polymer is observed (see figure 3.41 **d**), again the scheme suggested for its binding to PP is that of MA (see figure 3.49).

It has been noted previously that the three highly bound modifiers MA, NMM and NEM produced changes in the IS and EL of the unfilled PP. These modifiers could be viewed as converting the PP to a branched co-polymer and it may be expected that such a co-polymer will have different properties.

3.8.3 The properties of the modified GF-CL filled PP.

Only two modifiers MA and NMM enhanced the properties of the GF-CL composite. Both these modifiers were characterised by high degrees of binding. In the case of the MA modified PP the spectroscopic evidence indicates the formation of an ester (see figure 3.21 **a, b**) with a peak at 1741cm^{-1} there is also evidence for carboxylic acid (1695cm^{-1}) and

unreacted anhydride ($1782cm^{-1}$). The same compound as is formed in the model melt reactions (scheme 3.1 and 3.2) is clearly formed in the actual composite (cf figures 3.12 **a** and **b**). In the model reactions there are a number of ways in which GF-CL and MA could form an ester, see figure 3.52, compounds A and B would result from hydrolysis of the CLS whilst compound C is the result of a reaction between CLS and an carboxylic acid. With the glass fibre one would not expect compound A and B to be formed so it must be compound C which is formed (see figure 3.12 **b**). Thus, the proposed binding between GF-CL and MA modified PP is shown in figure 3.53. Thus one would expect to see infrared absorption due to an ester and carboxylic acid and this is what is observed. Further evidence can be seen in the fact that MAC (see figure 3.28 **b**) produce similar absorptions when melt processed with CLS, that is, $1741cm^{-1}$ and $1695cm^{-1}$.

The reactions between NMM and CLS are complicated by the apparent breakdown of the NMM to MAL. Previously, MAL has been shown to enhance the mechanical properties of GF-CL filled PP [F], however, no reaction scheme was proposed. Under the conditions of the melt processing reactions it may be possible for a condensation reaction between MAL and CLS to take place (see figure 3.54), there is, however, no direct spectroscopic evidence to support this. It appears, however, that the imide ring does remain unbroken, this is shown by the carboxyl absorptions at $1713cm^{-1}$ and $1775cm^{-1}$ remaining unchanged.

3.8.4 The properties of modified GF-NH filled PP.

The modifiers studied in this chapter were mainly chosen for their potential reactivity towards the amino silane coupled glass fibre (GF-NH). It must be remembered that unmodified PP filled with GF-NH had mechanical properties close to but inferior to the commercial composite (HW60/GR30) (see table 3.3). Thus, there is potential for exceeding the performance of the commercial composite.

Earlier work had been carried out on GF-NH filled on MA modified PP [C] as a result the reaction scheme shown in figure 3.55 was proposed [H]. However, the peaks observed and used to support the proposed reaction scheme were at $1694cm^{-1}$ and $1710cm^{-1}$, that is, those observed with GF-CL. When the melt reaction of MA and AMS was modelled peaks at $1787cm^{-1}$ (attributed to unreacted MA), $1703cm^{-1}$ (carboxylic acid) $1649cm^{-1}$ (attributed to unsaturated acid) and $1572cm^{-1}$ (attributed to amide) were observed (see figure 3.14 **a**). These same absorptions were observed when the reaction was modelled in dodecane (see figure 3.14 **c**) and for a model compound synthesis from MA and AMS (see section 2.1.44). This model compound has a structure very close to that of the proposed reactive product shown in figure 3.55. Further evidence for the reaction shown in figure 3.55 being the one taking place with the glass fibres (GF-NH) can be seen in the spectrum

figure 3.15B. In this case the peaks are slightly shifted, probable due to binding of the MA to the PP. Yet more evidence for this ring opening reaction taking place in the melt can be seen in the spectroscopic studies of SA and AMS (see figure 3.22 **a** to **c**) clearly have the same compound is found in the melt (**a**), dodecane solution (**b**) and in synthesis **c** (see section 2.1.4.5). This is a ring opened compound analogous to that obtained with MA (see figure 3.5.6).

Despite this clear evidence for a chemical bond between fibre and polymer the mechanical properties of the modified PP GF-NH filled composite are disappointing. There was no significant change in the properties, this suggests a maximum value of the interfacial shear strength (see section 1.3) above which no one further enhancement or properties can be achieved. In this context it is interesting to note that maximum values obtained with the GF-CL filled MA modified PP were better than those of the GF-NH filled polymer. Only in the aggressive environments did MA modification of GF-NH filled PP prove to have any advantage, the TS after exposure in boiling hexane was better for the modified as opposed to the unmodified PP (cf table 3.4 and 3.6). Such improved resistance to solvents was the objective of other studies detailed in section 1.5.

The objective behind modifying PP with NMM and then blending with GF-NH fibres was to establish a chemical bond via a condensation reaction reported for NMM[103]. This reaction is shown in generalised form in figure 3.57, this reaction was found to take place in the test tube between NMM and AMS (see section 2.1.4.6). However, in the melt the NMM has been found to decompose and this reaction between NMM and AMS was not observed. No significant enhancement of mechanical properties were seen.

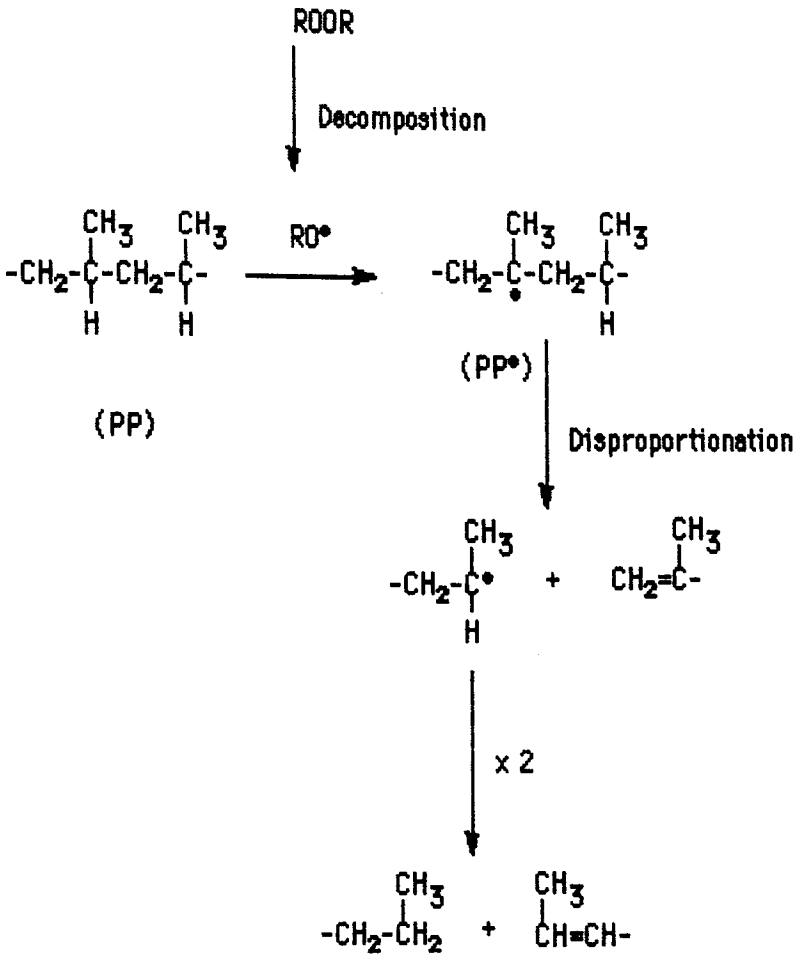


Figure 3.48. Mechanism for the attack of peroxide radicals on PP.

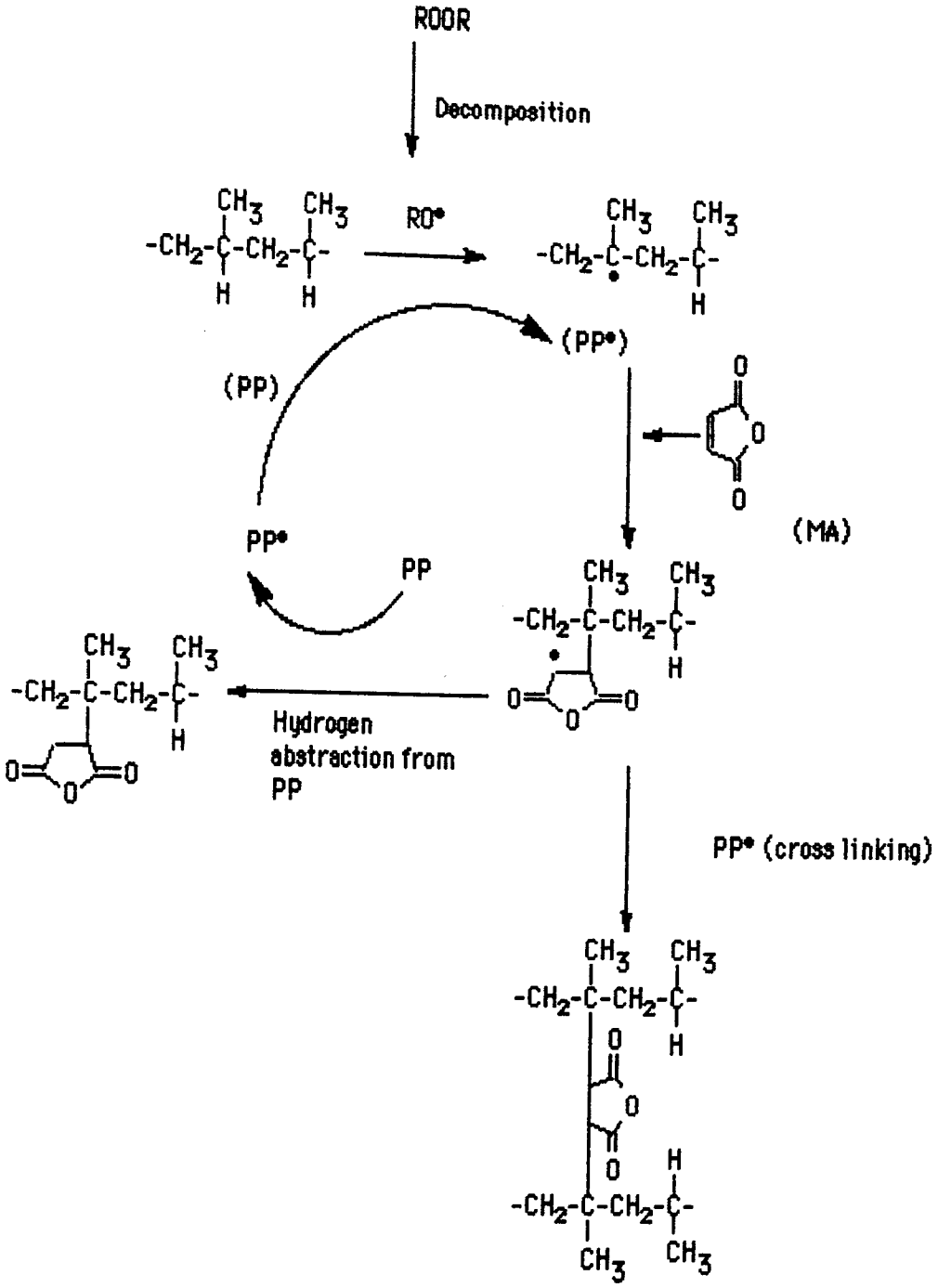


Figure 3.49. Mechanism for the mechanochemical modification of PP with MA.

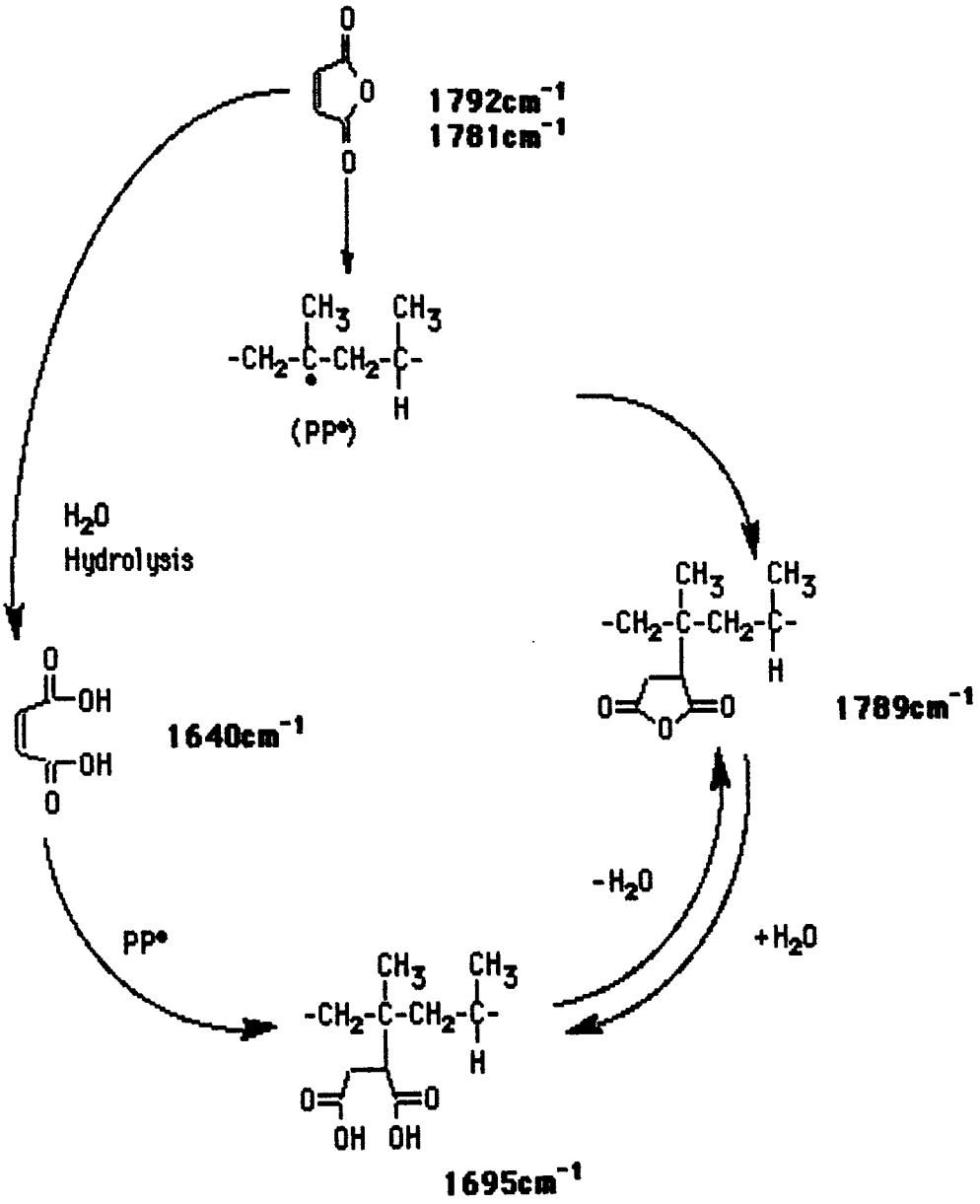


Figure 3.50. Proposed mechanism for the formation of MAC during the mechanochemical modification of PP with MA. Figures in bold are the wave numbers of the associated carbonyl groups.

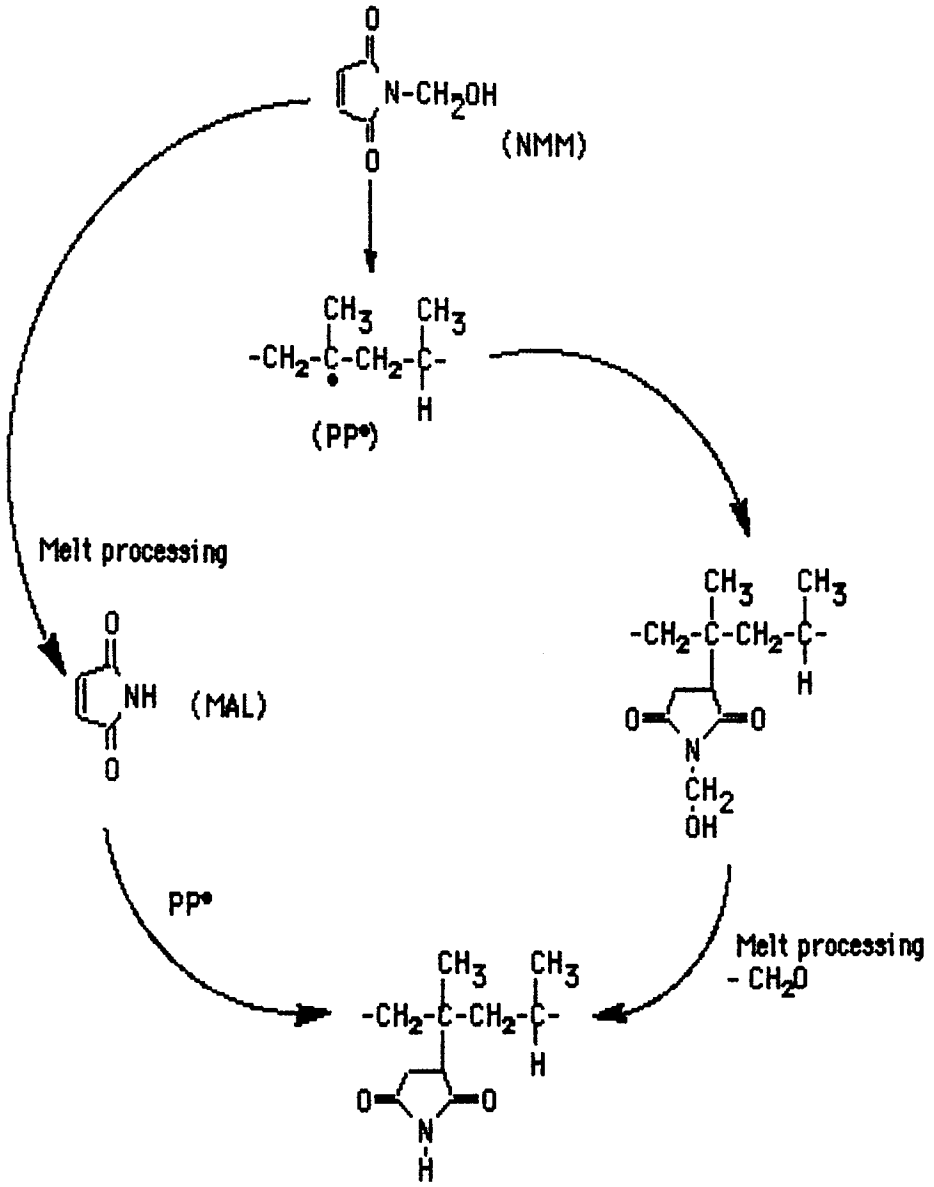


Figure 3.51. Proposed mechanism for the formation of MAL during the mechanochemical modification of PP with NMM.

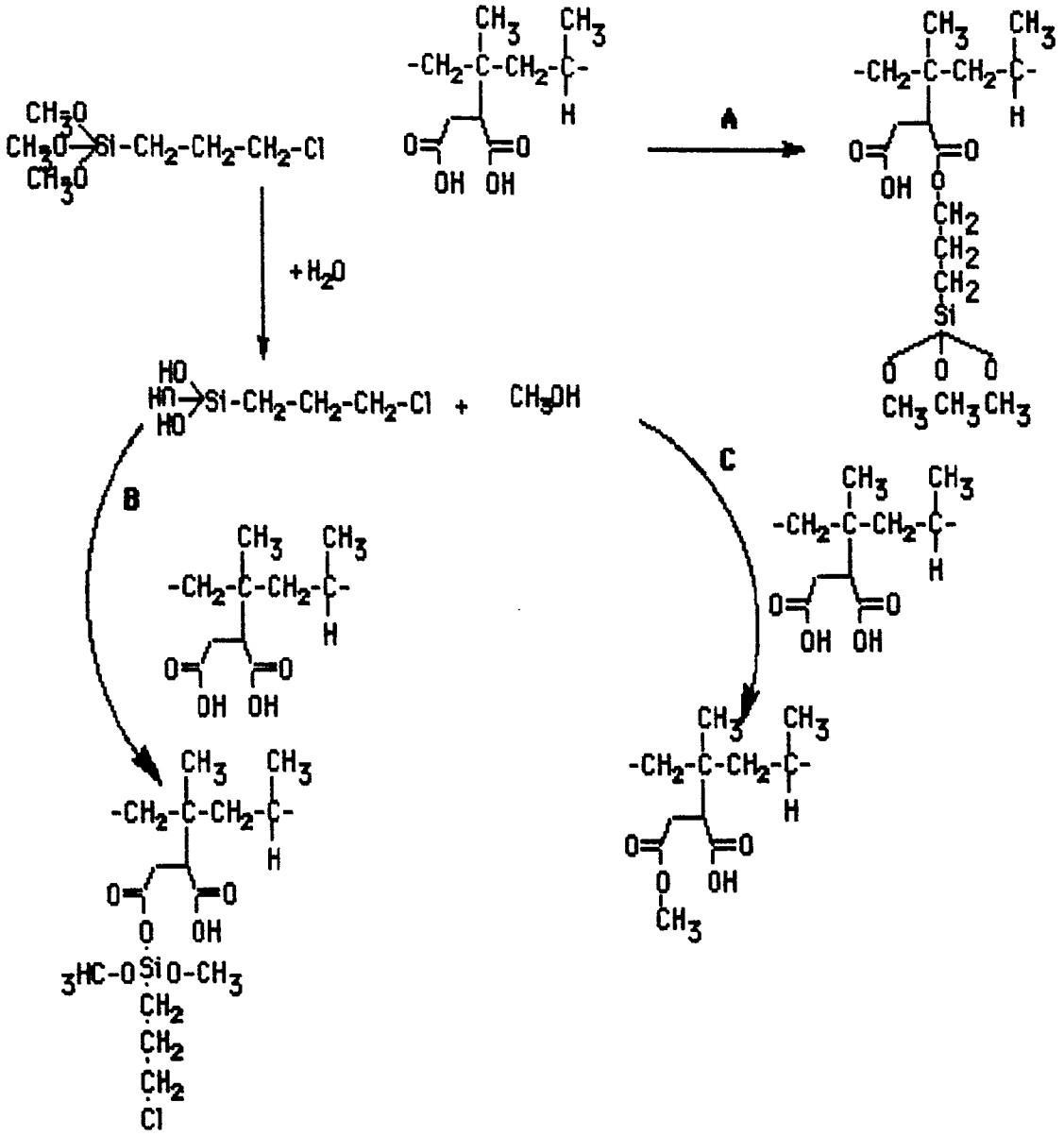
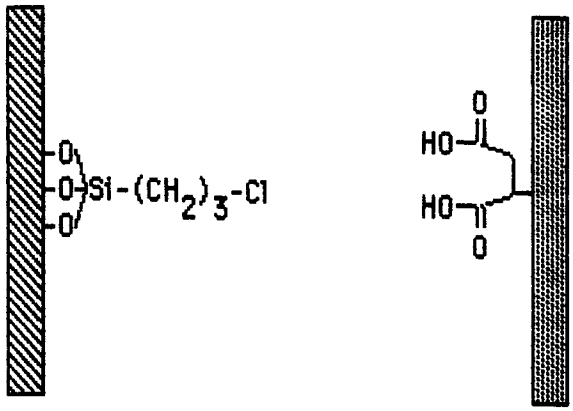


Figure 3.52. Possible reactions between MA and CLS to form an ester.



Chlorosilane coupled glass fibre.

MAC bound to PP

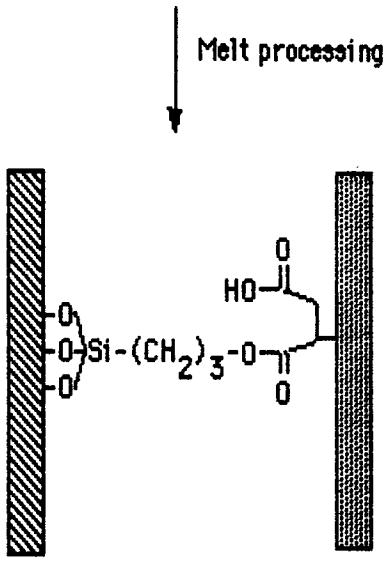


Figure 3.53. Proposed bonding between MA modified PP and chloro silane coupled glass fibres.

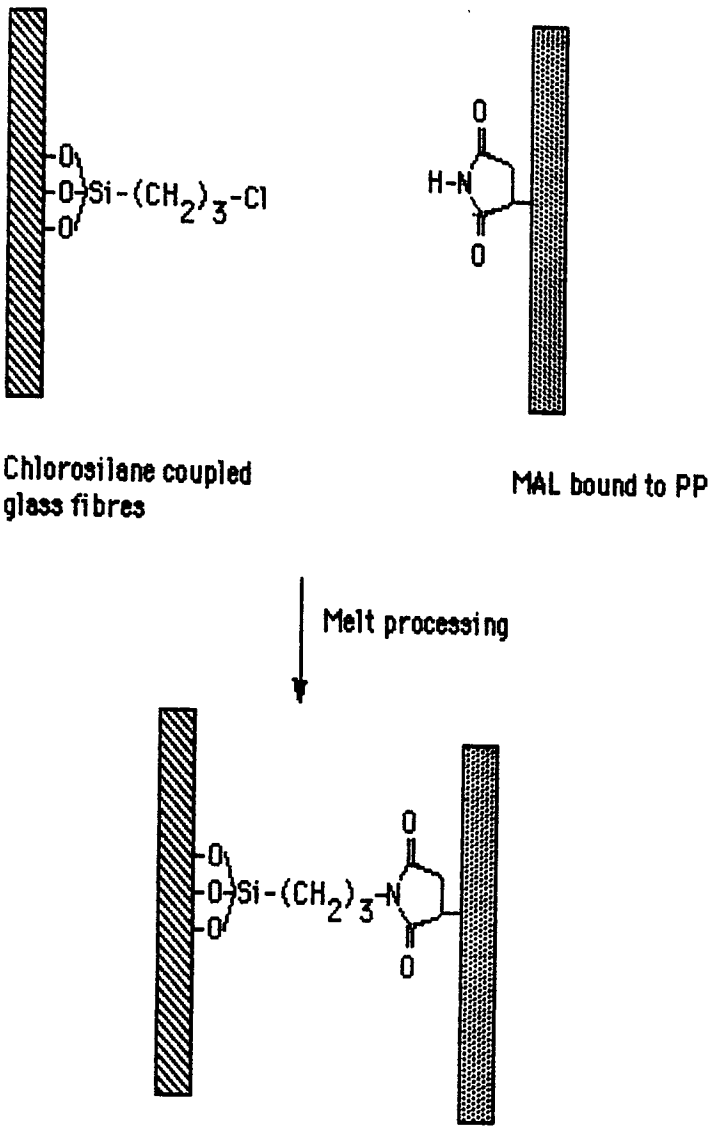


Figure 3.54. proposed reaction between PP bound MAL and chloro silane coupled glass fibres.

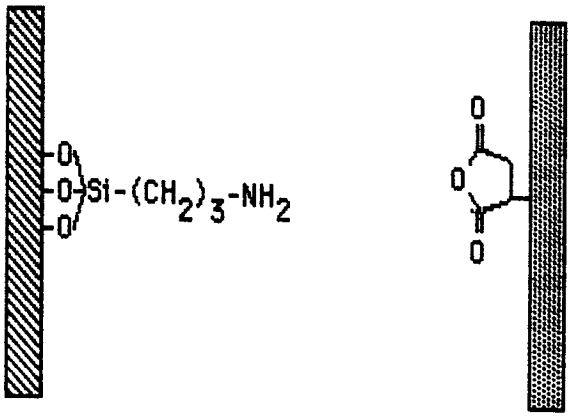


Figure 3.55. proposed reaction between PP bound MA and amino silane coupled glass fibres.

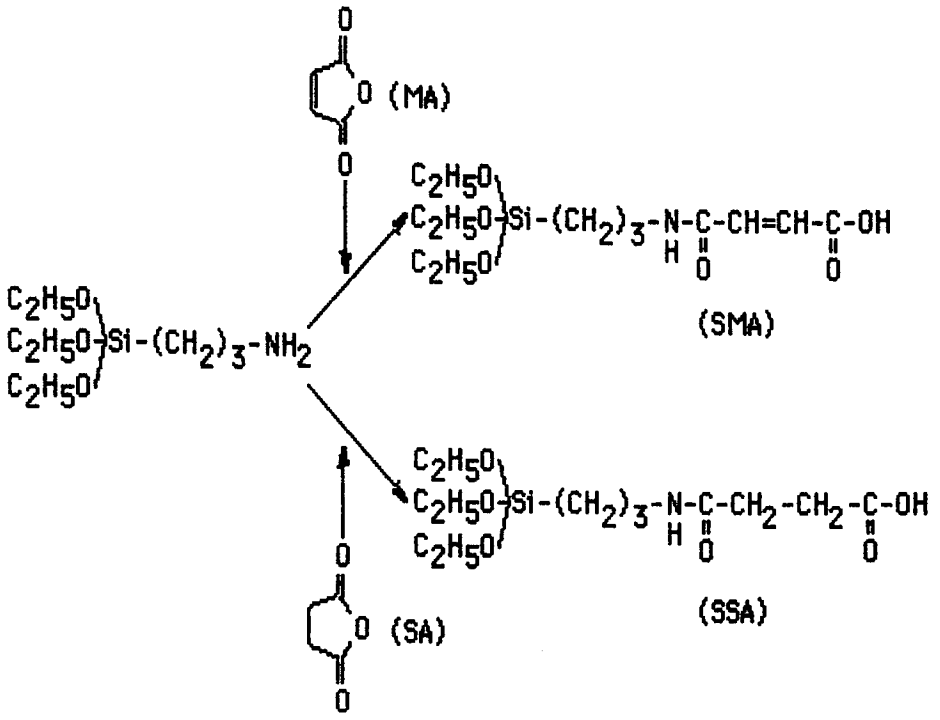


Figure 3.56. Reactions between AMS and MA or SA.

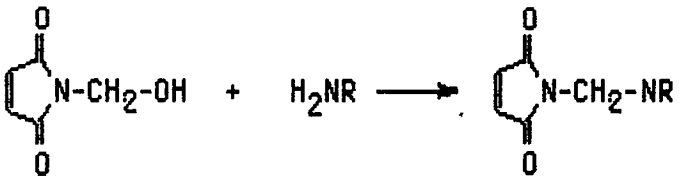


Figure 3.57. Reaction between NMM and an amine.

Chapter 4
The mechanochemical modification of polypropylene with 2-allylamino-4,6-dichloro-1,3,5-triazine and related triazines.

4.1 Outline and Plan

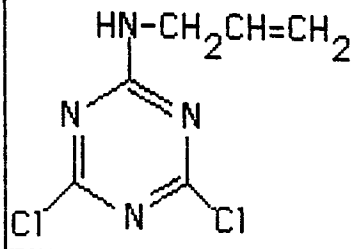
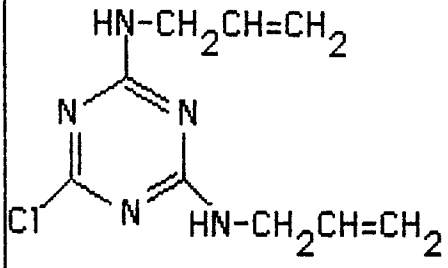
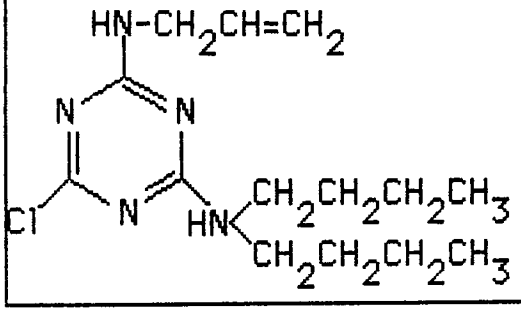
The main objective of the study described in this chapter is to enhance the mechanical properties of glass fibre PP composites by reactive processing the PP with the modifiers (table 4.1). The modifiers were chosen for the same reasons as those described in Chapter 3 (see section 3.1). In the case of the modifiers described in this chapter the reactivity to PP (unsaturation) was provided by the allyl group while reactivity to the AMS coupled glass fibres was provided by the chloro groups on the triazine ring. The melt reactions of the modifiers (table 4.1) were modelled in PP (see scheme 4.1) and in dodecane (see scheme 4.2). Composites for mechanical property determinations were prepared as shown in scheme 4.3. As in Chapter 3 the results obtained are compared with those of the unmodified PP and the commercial polymers HWM25 and HW60/GR30.

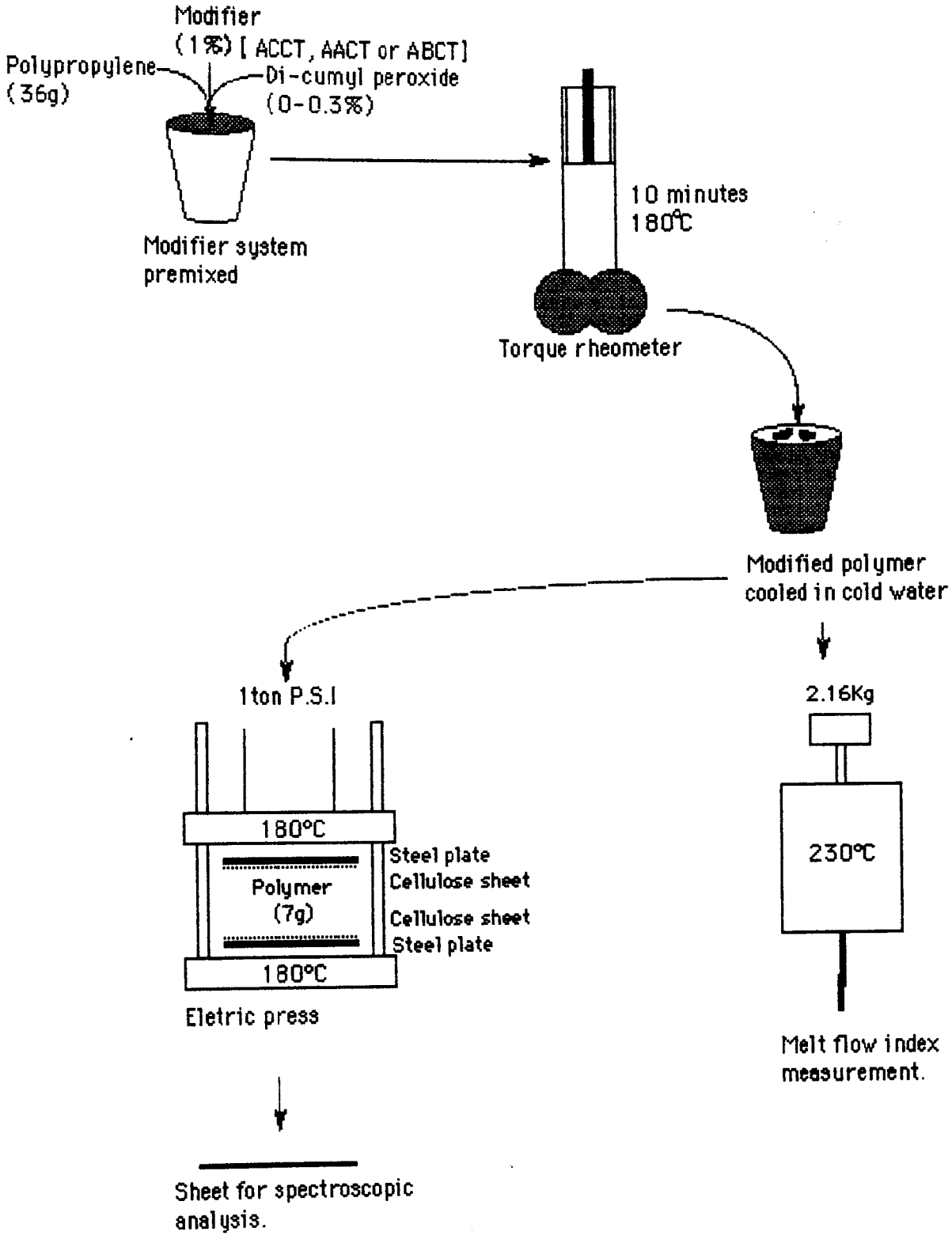
2-allylamino-4,6-dichloro-1,3,5-triazine (AACT) was chosen for study since it possesses unsaturation via the allylamino group and two chloro groups which can potentially react with an amine.

2-chloro-4,6-diallylamino-1,3,6-triazine (AACT) was chosen for study since it possesses two groups which can react with PP and one chloro group for reaction with an amine.

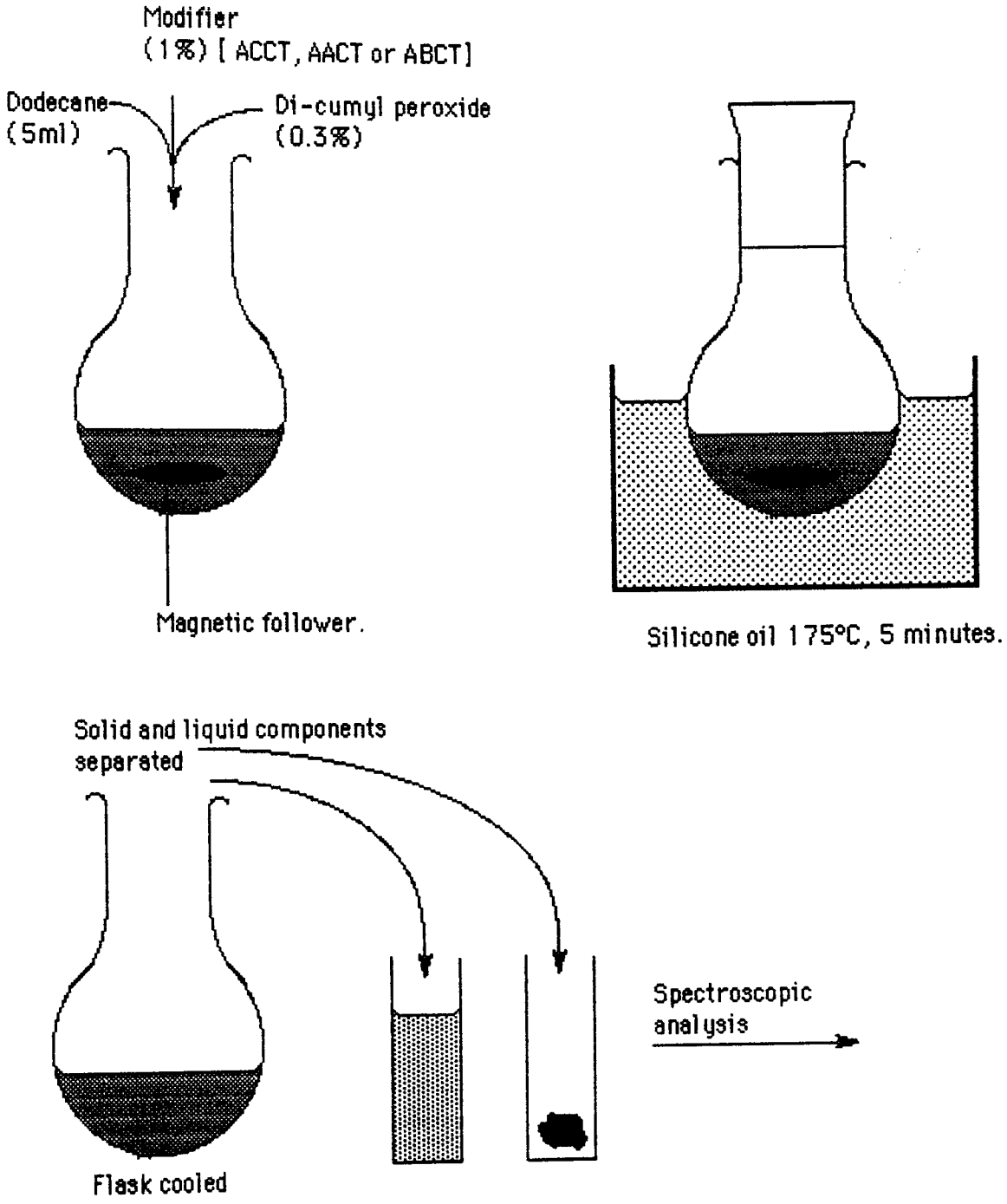
2-allylamino-4 chloro-6-dibutylamino-1,3,5-triazine (ABCT) was chosen for study to assess the effect of only one chloro group on the reativity towards amines. The other group being blocked by the dibutylamine group.

Table 4.1 Modifiers discussed in chapter 4.

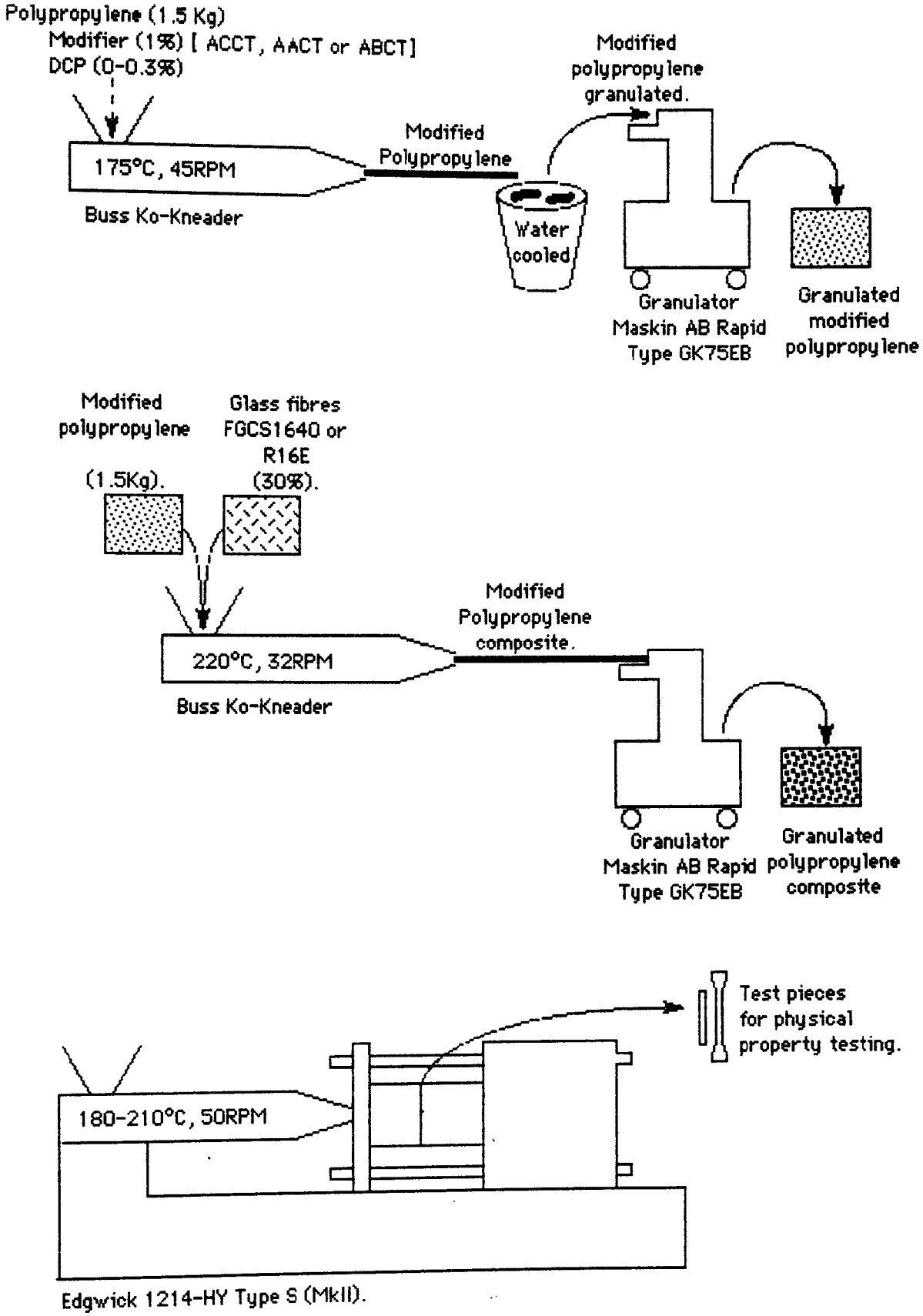
Structure	Name
	2-allylamino-4,6-dichloro-1,3,5-triazine. (ACCT).
	2-chloro-4,6-diallylamino-1,3,5-triazine. (AACT)
	2-allylamino-4-chloro-6-dibutylamino-1,3,5-triazine. (ABCT)



Scheme 4.1. The mechanochemical modification of PP to produce samples for MFI and spectroscopic studies.



Scheme 4.2. The solution modelling of mechanochemical reactions.



Scheme 4.3. Mechanochemical modification of PP with the modifiers table 4.1 and glass fibres GF-CL or GF-NH to produce samples for mechanical property testing.

4.2 Mechanochemical modification of PP with 2-allylamino-4,6-dichloro-1,3,5-triazine (ACCT) and DCP.

The infrared spectrum from 1400cm^{-1} to 2000cm^{-1} of ACCT (nujol mull) is shown in figure 4.1**a**. This has notable peaks at 1753cm^{-1}, 1643cm^{-1}, 1641cm^{-1} and 1553cm^{-1}. When PP was melt processed with ACCT (1%) in the absence (**b**) and presence (**c**) of DCP (0.3%) then the spectra shown in figure 4.1 were obtained. The MFI results for the PP modified with the modifiers table 4.1 are shown in figure 4.2. As can be seen for the ACCT (1%) modified PP (see scheme 4.1) the MFI differ little for that of unmodified PP. The binding studies of ACCT modified PP are shown in table 4.2, these show that no ACCT is bound to the PP.

When PP was modified with ACCT (1%) DCP (0.3%) and CLS (1%) to simulate the presence of the glass fibres GF-CL then the spectra shown in figure 4.3 **a** was obtained. When the same reaction was modelled in dodecane (see scheme 4.2) then the spectrum (**b**) was obtained. Both spectra **a** and **b** appear to be identical and are very similar to the melt reaction spectra in the absence of CLS (figure 4.1 **b** and **c**).

The spectra of the melt reaction ACCT (1%), DCP (0.3%) and AMS (1%) with PP (see scheme 3.1) is shown in figure 4.3 **c**, whilst the corresponding reaction in dodecane (see scheme 4.2) is shown in **d**. Both spectra **c** and **d** have notable peaks at 1714cm^{-1}, 1633cm^{-1} and 1566cm^{-1} and appear identical.

The mechanical properties of the unfilled ACCT (1%) modified PP (see table 4.3, figure 4.4 to 4.6) did not differ significantly from those of the analogous unfilled unmodified PP either in the normal (see tables 3.3 and 4.3) or aggressive environments (cf tables 3.4 and 4.4) (see figure 4.6).

Only the TS of the GF-CL filled ACCT (1%), modified PP (scheme 4.3) (see figure 4.4) differed significantly for the analgous filled unmodified PP (cf tables 3.3 and 4.3). The overall TS was, however, still inferior to the commercial composite material (HW60/GR30) (see table 4.4). In the aggressive environments the results obtained did not differ significantly from those of the analogous filled unmodified PP (cf tables 3.4 and 4.4) (see figure 4.7).

The mechanical properties of the GF-NH filled ACCT (1%) modified PP did not differ significantly from those of the analgous filled unmodified PP in either normal (cf tables 3.3 and 4.3) (see figures 4.4 to 4.6) or in the aggressive environments (cf tables 3.4 and 4.4) (see figure 4.7).

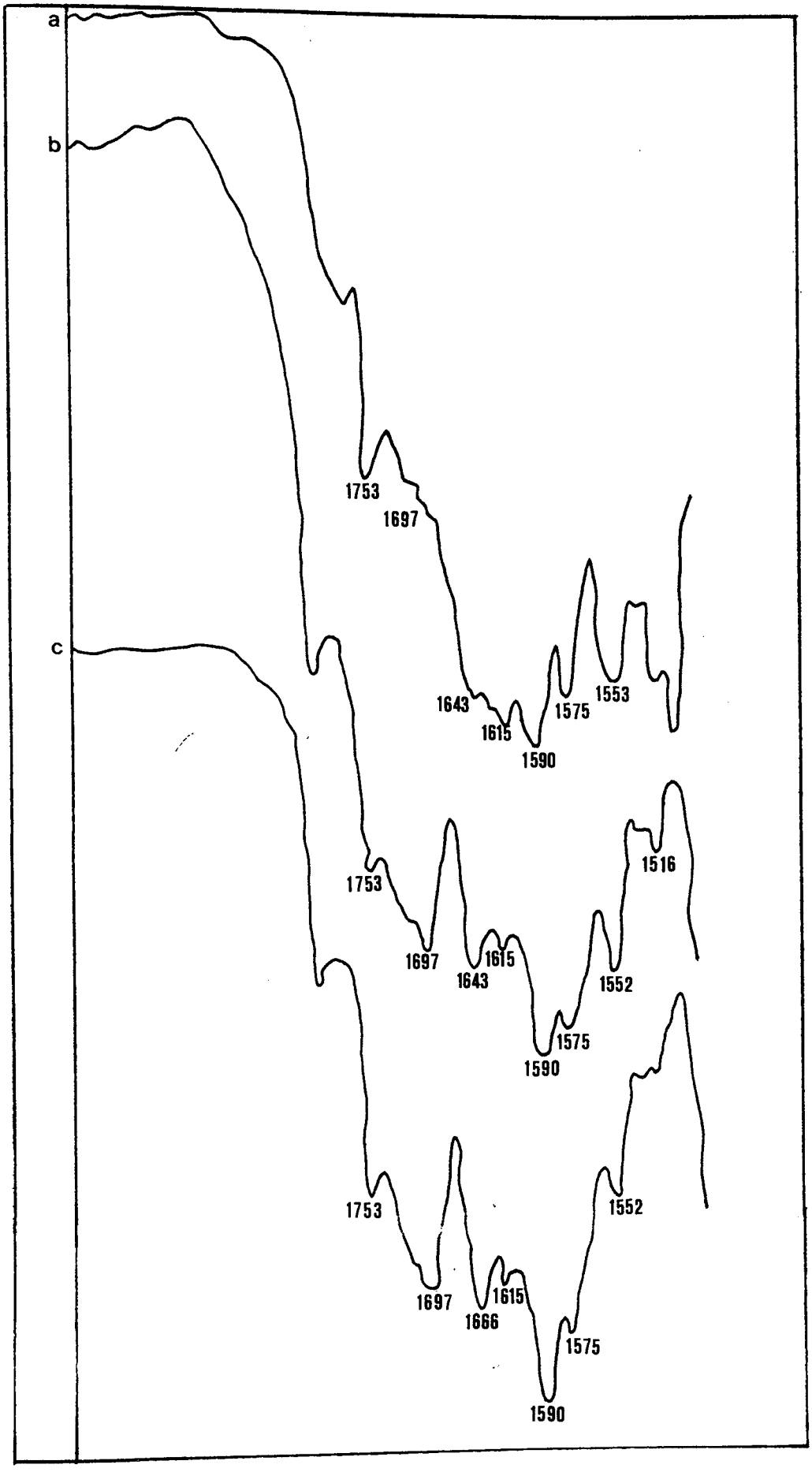


Figure 4.1. **a** = ACCT (nujol mull), **b** = PP + 1% ACCT, **c** = PP + 1% ACCT + 0.3% DCP.

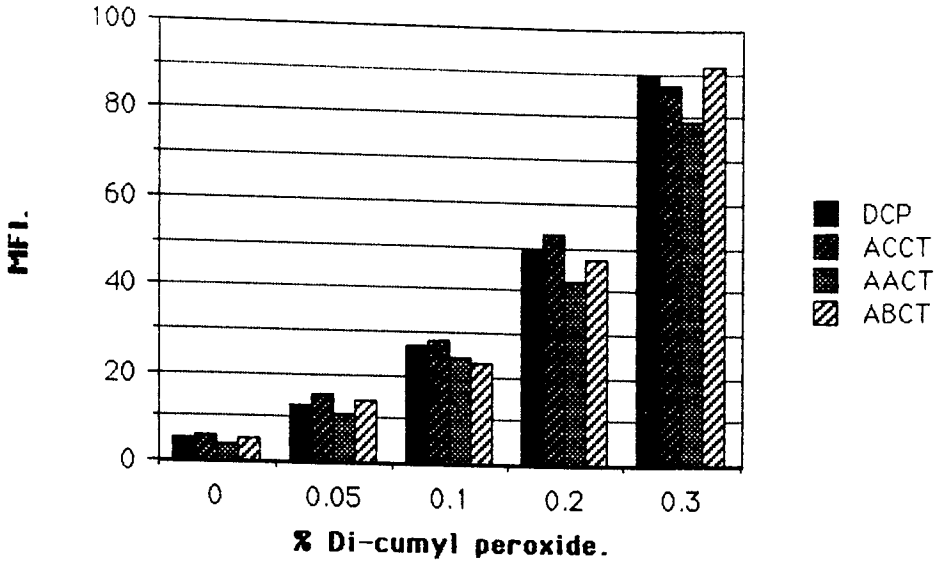


Figure 4.2 MFi measurements (see section 2.4.2.2) of PP (HF26) containing 1% modifiers (see table 4.1) in the presence of variable concentrations of DCP. procesing according to scheme 4.1.

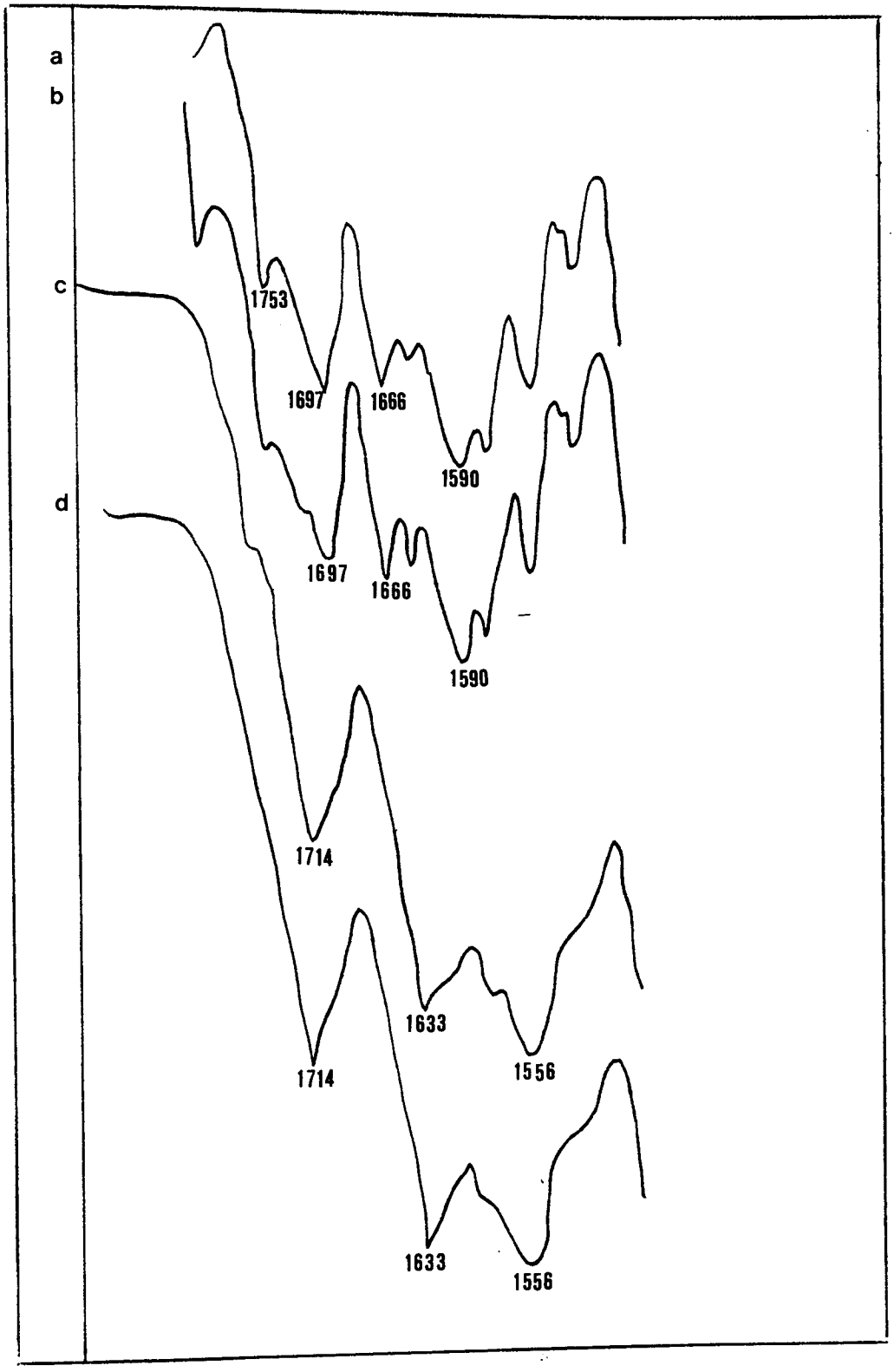
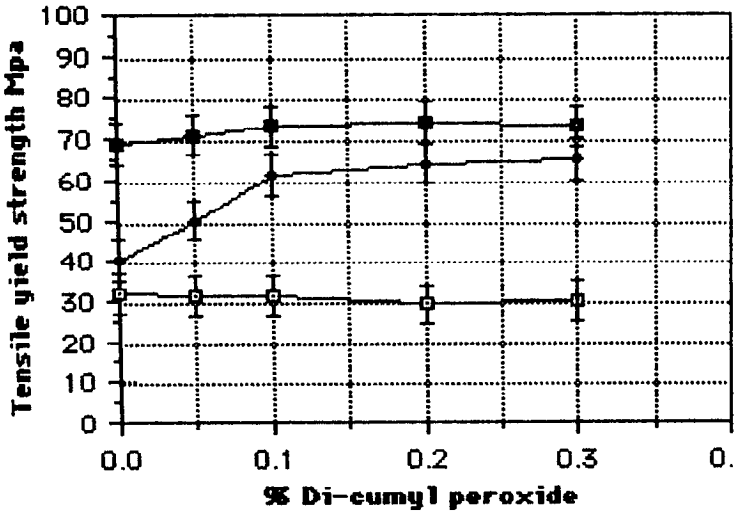


Figure 4.3. **a** = PP + 1% ACCT + 0.3% DCP + 1% CLS, **b** = dodecane + 1% ACCT + 0.3% DCP + 1% CLS, **c** = PP + 1% ACCT + 0.3% DCP + 1% AMS, **d** = dodecane + 1% ACCT + 0.3% DCP + 1% AMS.



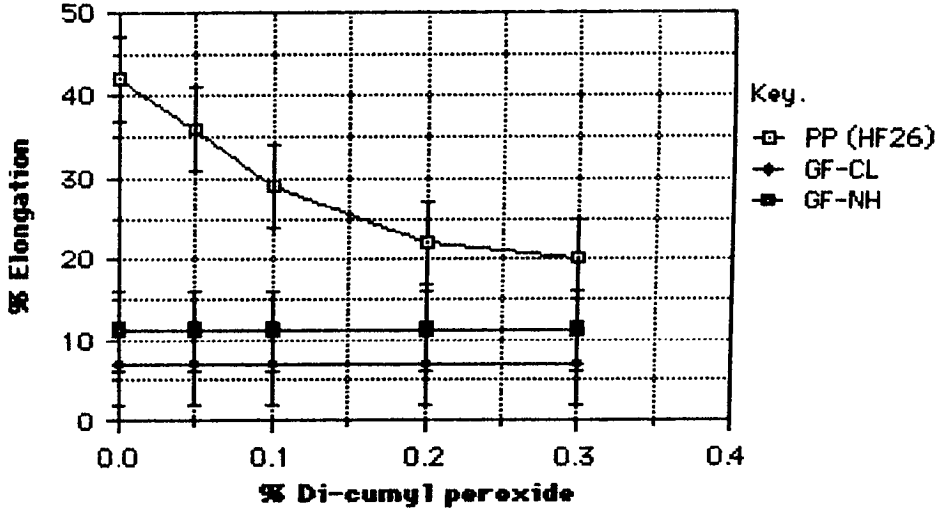


Figure 4.4. Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with ACCT (1%) and DCP (0-0.3%).

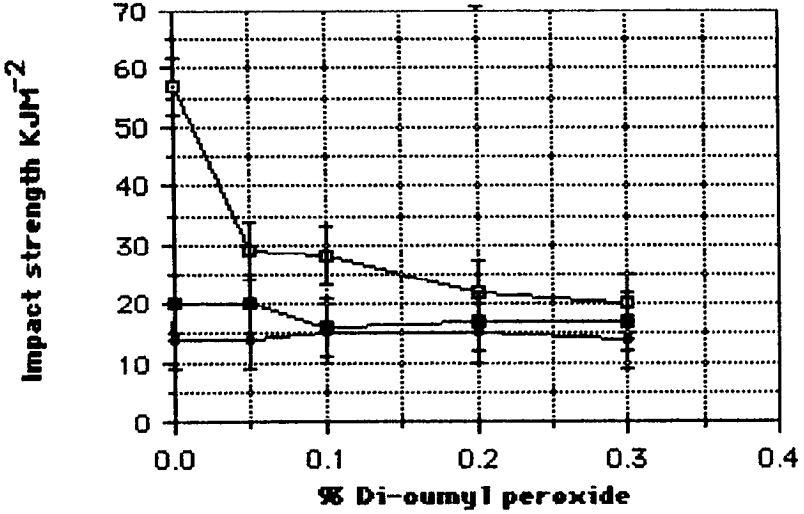


Figure 4.5. Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with ACCT (1%) and DCP (0-0.3%).

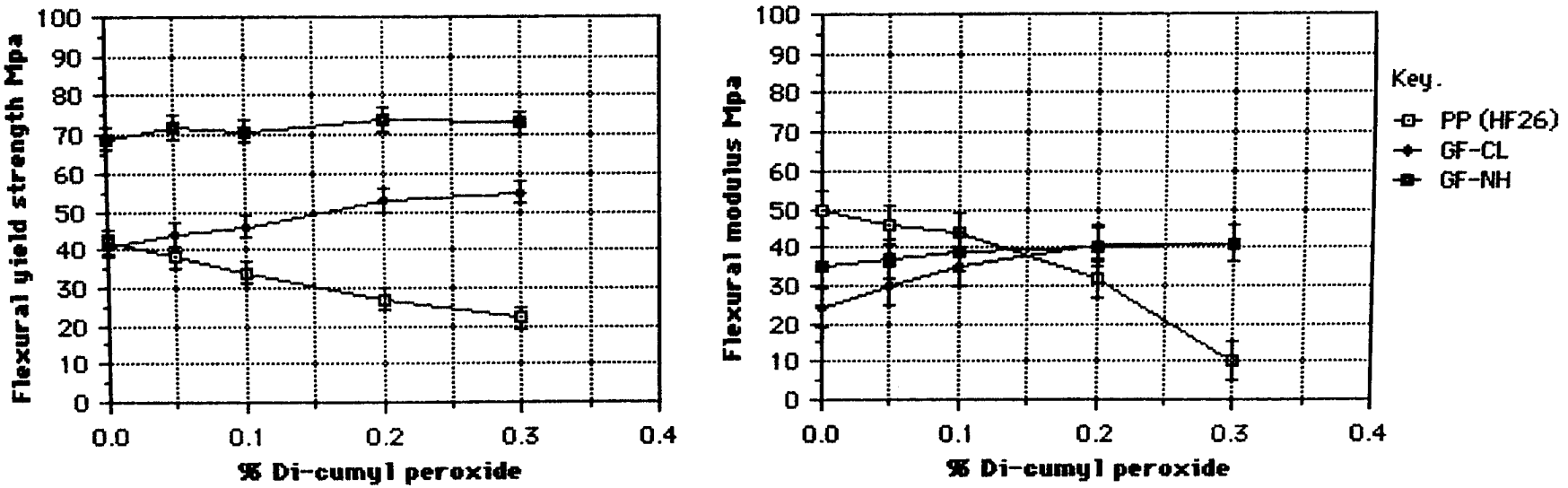


Figure 4.6. Flexural strength and flexural modulus of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with ACCT (1%) and DCP (0-0.3%).

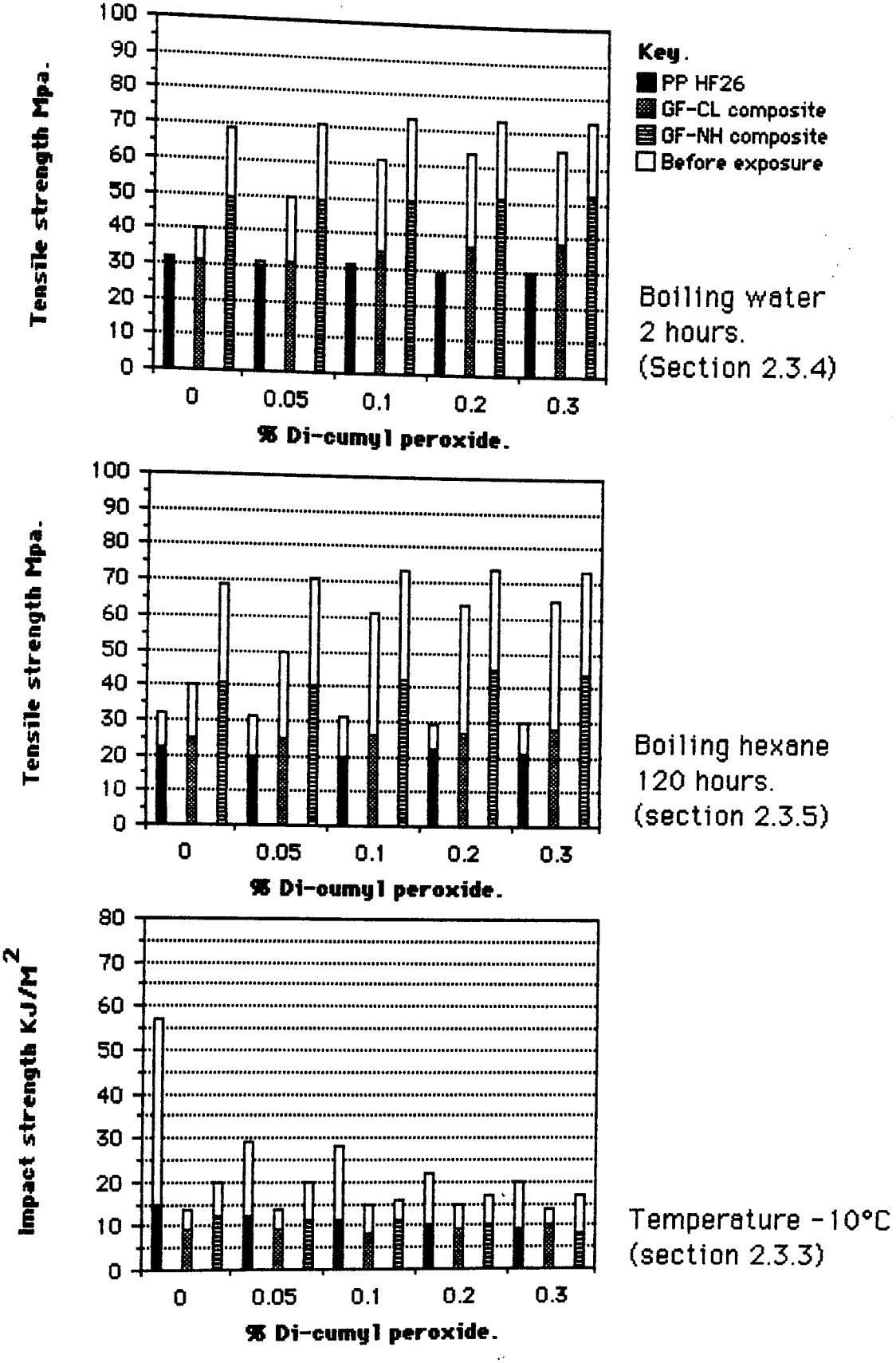


Figure 4.7. Tensile yield strength of PP Hf26, its GF-CL and GF-NH composites modified according to scheme 4.3 with ACCT (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 4.2. The binding of ACCT (1%) to PP (HF26) determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.82	0	0
0.1	1	0.86	0.01	1
0.3	1	0.84	0.01	1
	No of modifier molecules per 10000 PP repeat units.			
0	20.6	16.9	0	-
0.1	20.6	17.7	0.21	-
0.3	20.6	17.3	0.21	-

4.8

Table 4.3. The effect of DCP concentration on the mechanical properties of PP (HF26) modified with ACCT (1%) (see scheme 4.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those that did break.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	32	42	57	42	50
0.05	-	-	31	36	29	38	46
0.1	-	-	31	29	28	34	44
0.2	-	-	29	12	22	27	32
0.3	-	-	30	8	20	22	10
0	30	-	40	7	14	41	24
0.05	30	-	50	7	14	44	30
0.1	30	-	61	7	15	46	35
0.2	30	-	64	7	15	53	41
0.3	30	-	65	7	14	55	41
0	-	30	69	11	20	69	35
0.05	-	30	71	11	20	72	37
0.1	-	30	73	11	16	71	39
0.2	-	30	74	11	17	74	40
0.3	-	30	73	11	17	73	41
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

4.1

Table 4.4. The effect of adverse environments of boiling water for 2 hours, of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with ACCT (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples, table 4.3).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-20°C) KJ/M^2
0	-	-	31 (0%)	22 (-31%)	15 (-73%)
0.05	-	-	30 (0%)	20 (-35%)	12 (-58%)
0.1	-	-	31 (0%)	20 (-35%)	11 (-60%)
0.2	-	-	29 (0%)	22 (-24%)	10 (-54%)
0.3	-	-	30 (0%)	21 (-30%)	9 (-55%)
0	30	-	31 (-22%)	25 (-37%)	9 (-35%)
0.05	30	-	31 (-38%)	25 (-50%)	9 (-35%)
0.1	30	-	35 (-42%)	26 (-57%)	8 (-46%)
0.2	30	-	37 (-42%)	27 (-58%)	9 (-40%)
0.3	30	-	38 (-41%)	28 (-57%)	10 (-28%)
0	-	30	49 (-29%)	41 (-40%)	12 (-40%)
0.05	-	30	49 (-31%)	40 (-43%)	11 (-45%)
0.1	-	30	50 (-31%)	42 (-42%)	11 (-31%)
0.2	-	30	51 (-31%)	45 (-39%)	10 (-41%)
0.3	-	30	52 (-28%)	44 (-39%)	8 (-53%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

4.4

4.3 The Mechanochemical modification of PP with 2-chloro-4,6-diallyamino-1,3,5-triazine (AACT).

The purpose of modifiying PP with AACT was to try to achieve more binding by having two rather than one unsaturated group available for reaction with PP.

The infrared spectrum of PP modified with AACT (1%) in the absence (A) and presence (B) of DCP (0.3%) are shown in figure 4.7. The spectrum of AACT, a nujol mull, is shown in figure 4.7C. The MFI data for the AACT (1%) modified unfilled PP (see scheme 4.1) is shown in figure 4.2, as can be seen the results obtained differed little for those of the analogous unmodified PP (see figure 4.2). The results of the binding studies of AACT modified PP (see scheme 4.1) are shown in table 4.5, it can be seen that only a very small percentage (10%) was unextractable from the PP.

The infrared spectrums of PP modified with AACT (1%) and CLS (1%), to simulate the presence of the chloro silane coupled glass fibres, without (A) and with DCP (0.3%) are shown in figure 4.8. In the absence of DCP (A) the spectrum has peaks at 1633cm^{-1} and 1548cm^{-1} and is broadly similar to that of the analogous sample without CLS (figure 4.7A). In the presence of DCP (0.3%) (B) the spectrum has peaks at 1753cm^{-1}, 1614cm^{-1} and 1556cm^{-1}, the peak at 1695cm^{-1} seen in the analogous sample without CLS (see figure 4.7B) is not present here.

The spectrum of PP modified with AACT (1%) and AMS (1%) to simulate the presence of the amino silane coupled glass fibres (GF-NH) in the absence (A) and presence (B) of DCP (0.3%) are shown in figure 4.9. In the absence of DCP (A) the spectrum has absorptions at 1711cm^{-1}, 1636cm^{-1} and 1558cm^{-1}, whilst in the presence of DCP (B) there are absorptions at 1705cm^{-1}, 1636cm^{-1} and 1560cm^{-1}.

The mechanical properties of the unfilled AACT (1%), modified PP (see scheme 4.3) did not differ significantly from those of the analogous unfilled unmodified PP (cf tables 3.4 and 4.6) (see figures 4.10 to 4.12). There was also no difference in the results obtained in the aggressive environments (cf tables 3.5 and 4.7) (see figure 4.13).

The mechanical properties of the GF-CL and GF-NH filled AACT (1%) modified PP (see scheme 4.3) in both normal and aggressive environments did not differ significantly from those of the analogous filled unmodified PP (cf tables 3.4 and 4.6) (cf tables 3.5 and 4.7) (see figures 4.10 to 4.13).

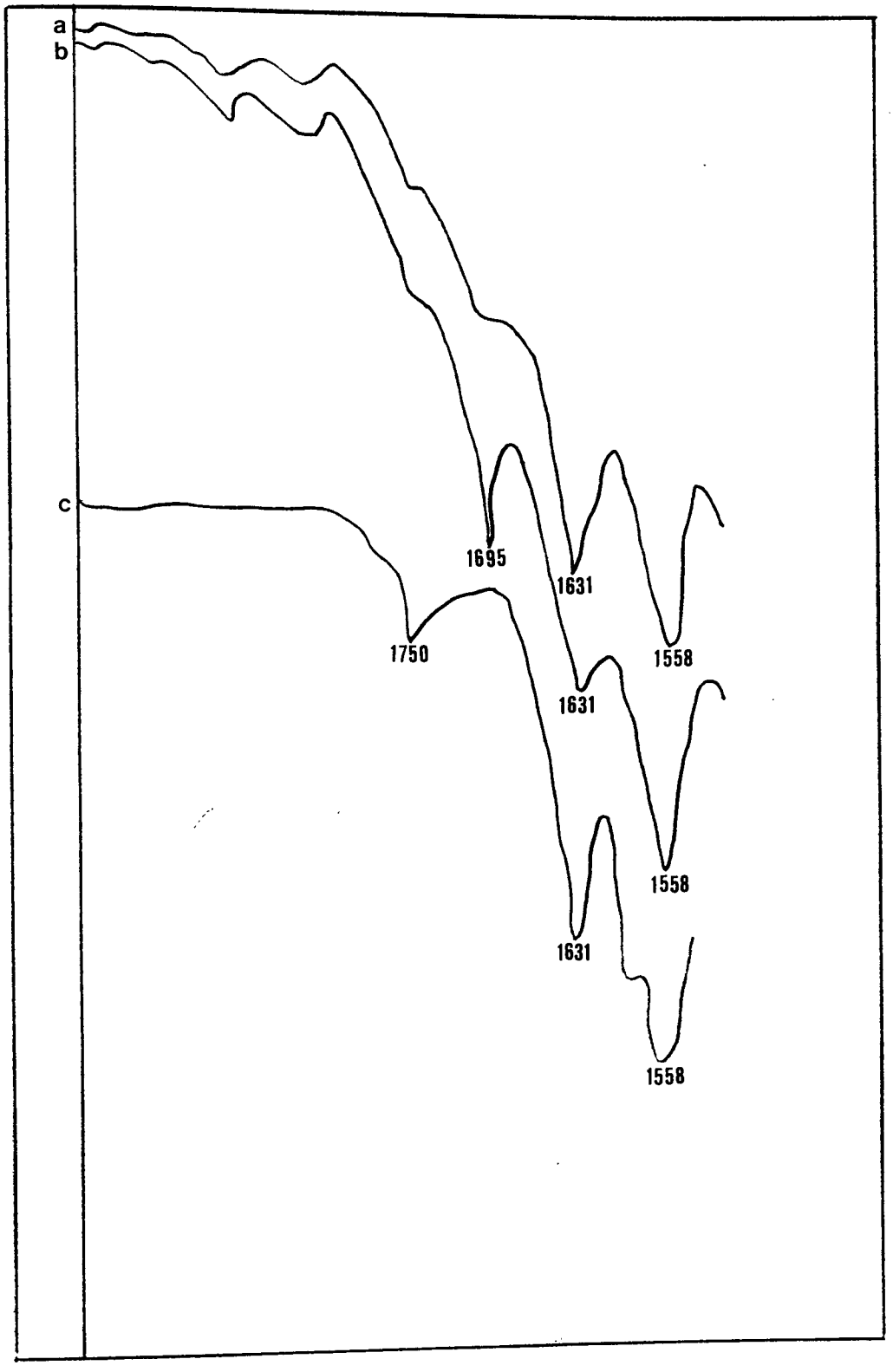


Figure 4.8. a = PP + 1% AACT, b = PP + 1% AACT + 0.3% DCP, c = AACT (nujol mull).

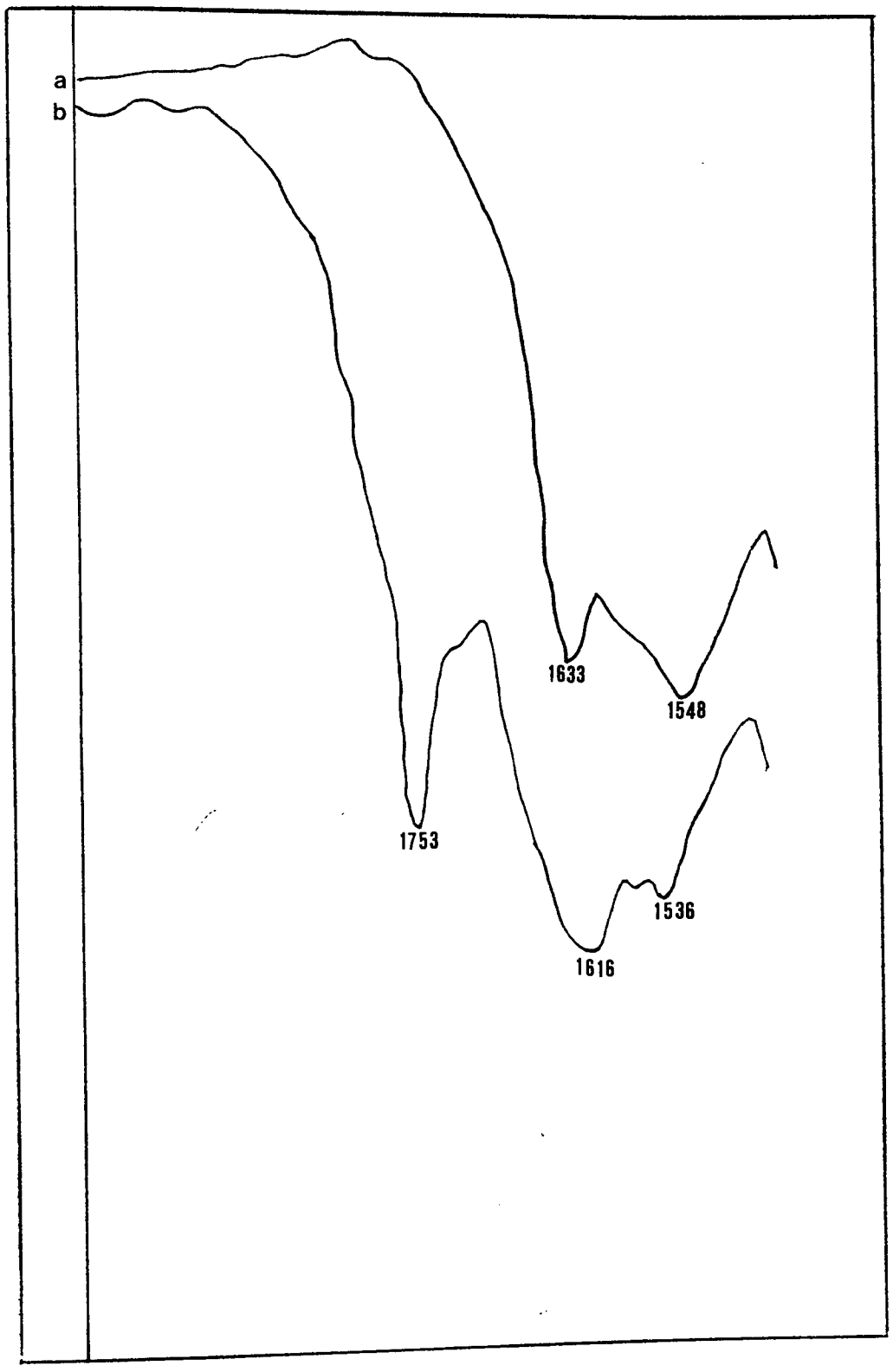


Figure 4.9. a = PP + 1% AACT + 1% CLS, b = PP + 1% AACT + 0.3% DCP + 1% CLS

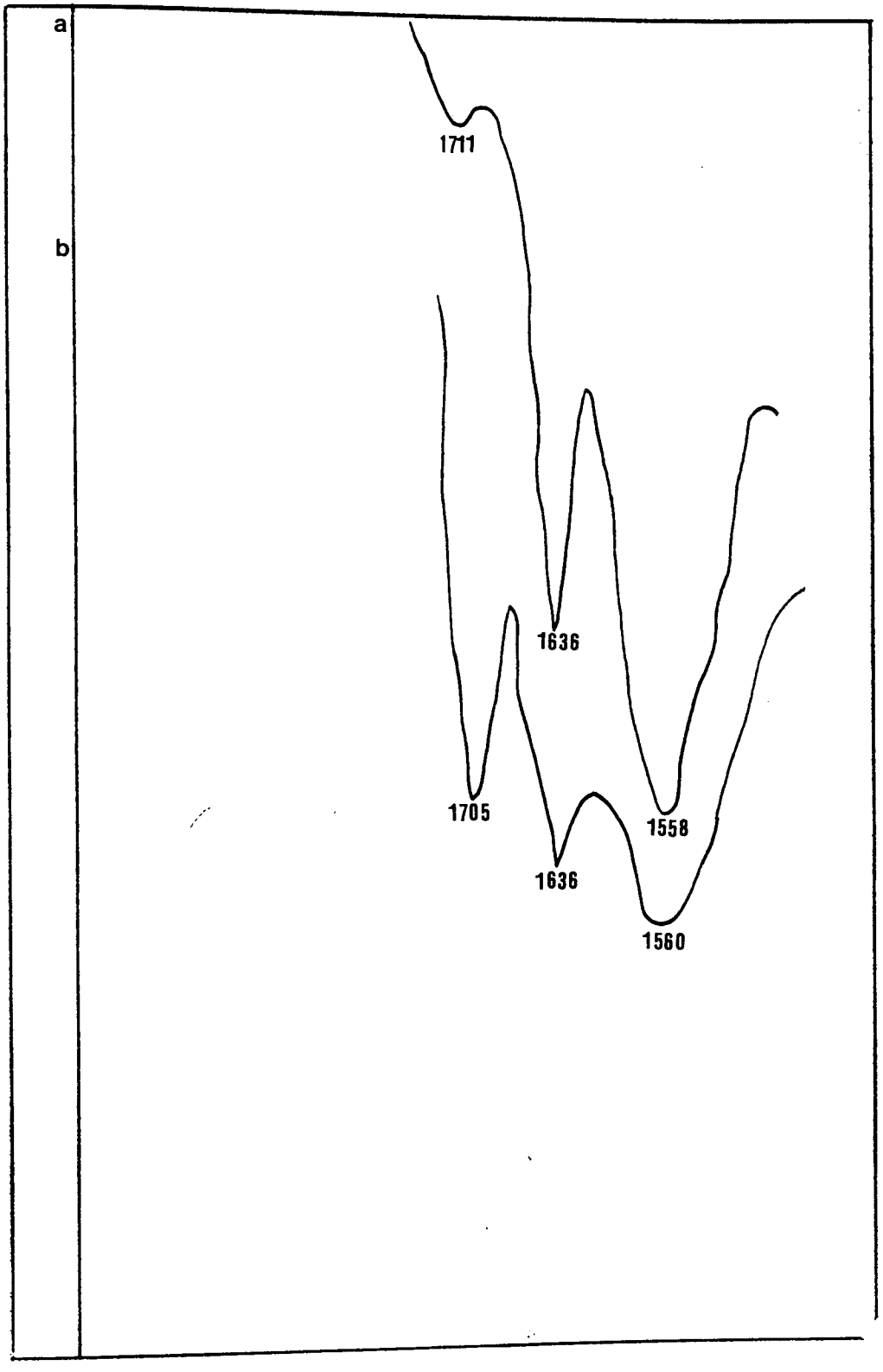


Figure 4.10. a = PP + 1% AACT + 1% AMS, b = PP + 1% AACT + 0.3% DCP + 1% AMS.

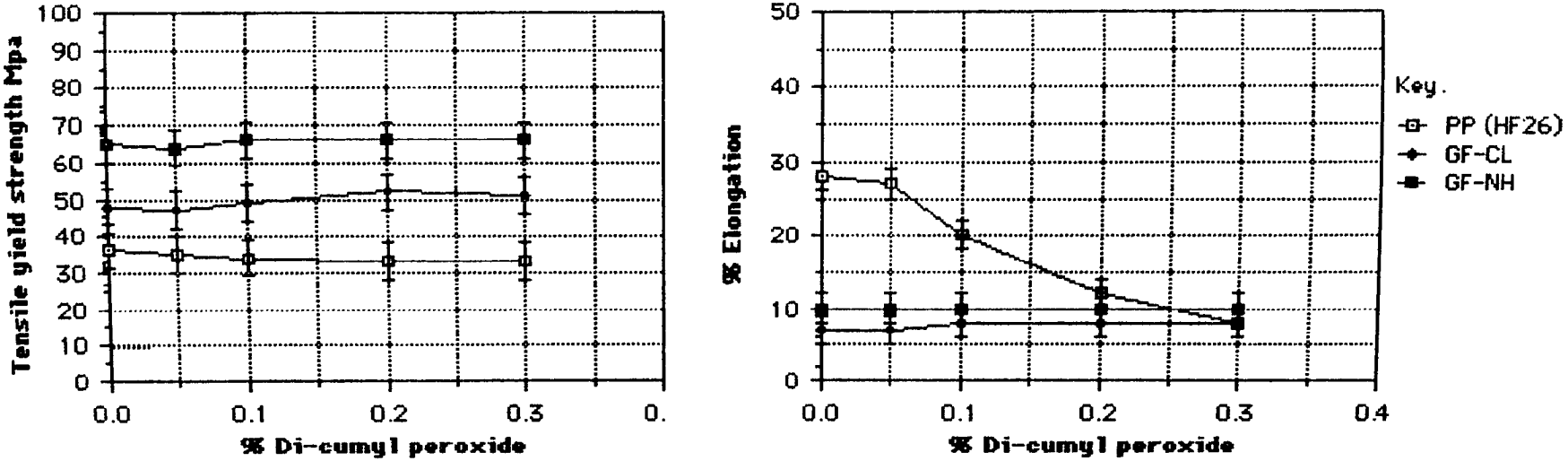


Figure 4.11Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with AACT (1%) and DCP (0-0.3%).

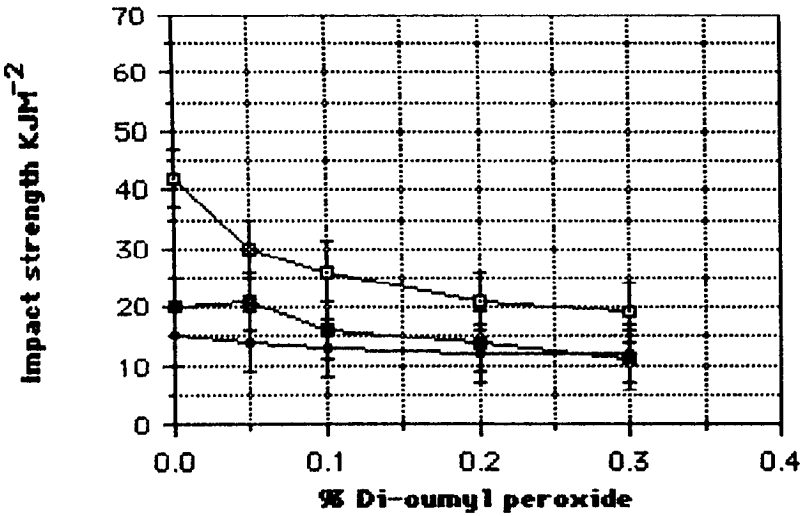


Figure 4.12 Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with AACT (1%) and DCP (0-0.3%).

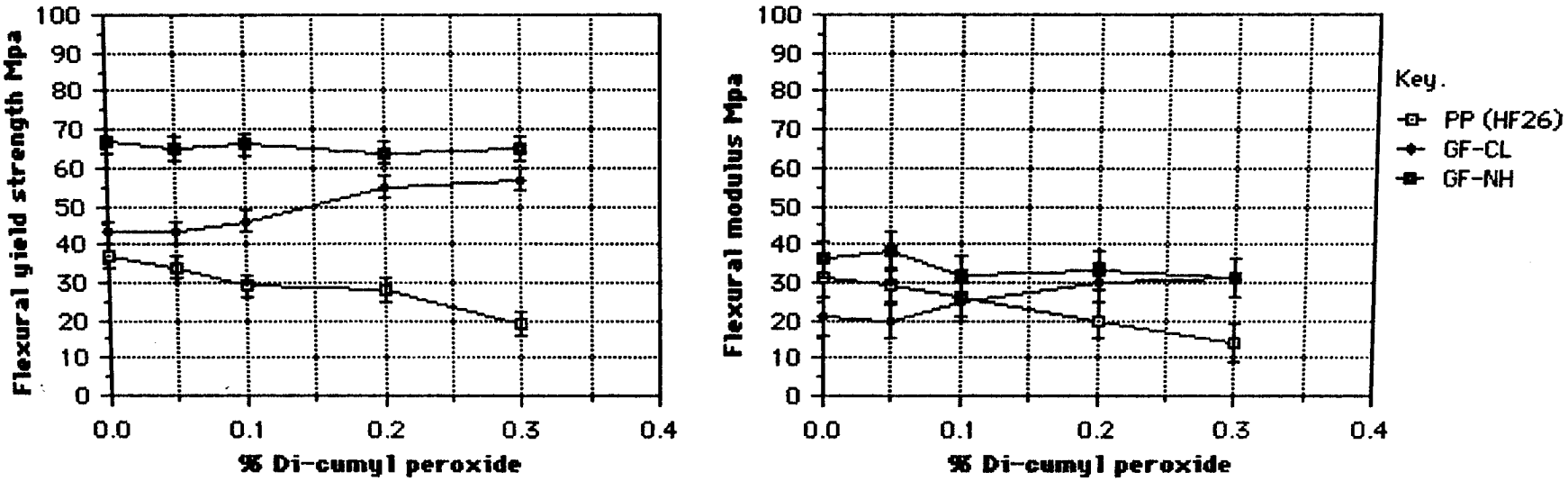


Figure 4.13 Flexural strength and flexural modulus of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with AACT (1%) and DCP (0-0.3%).

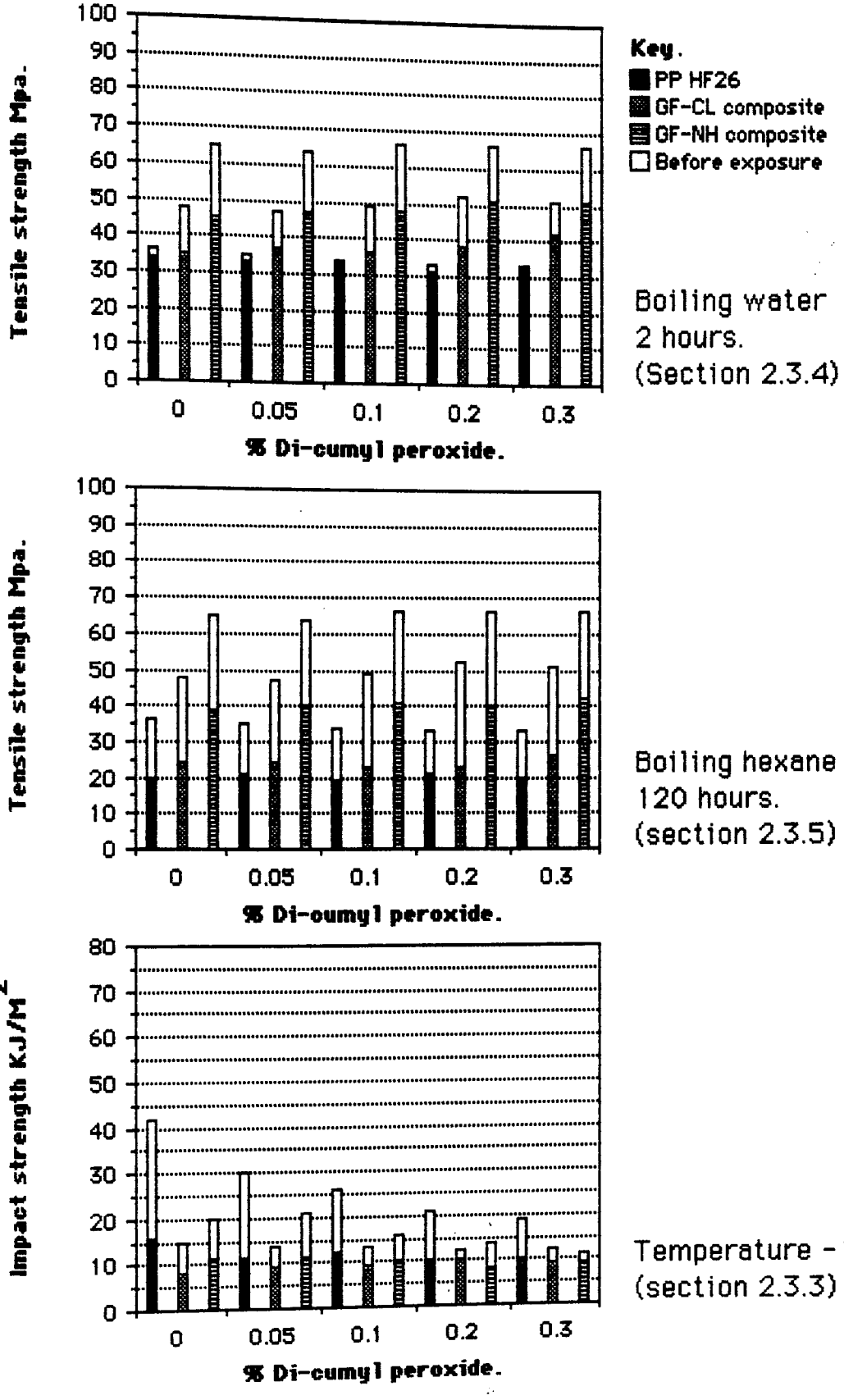


Figure 4.14. Tensile yield strength of PP HF26, its GF-CL and GF-NH composites modified according to scheme 4.3 with AACT (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 4.5. The binding of AACT (1%) to PP (HF26) determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.91	0.00	0
0.1	1	0.96	0.06	6
0.3	1	0.94	0.10	10
	No of modifier molecules per 10000 PP repeat units.			
0	18.6	17.0	0	-
0.1	18.6	17.9	1.1	-
0.3	18.6	17.5	1.9	-

4.9

Table 4.6. The effect of DCP concentration on the mechanical properties of PP (HF26) modified with AACT (1%) (see scheme 4.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those that did break.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	36	28	42	37	31
0.05	-	-	35	27	30	34	29
0.1	-	-	34	20	26	29	26
0.2	-	-	33	12	21	28	20
0.3	-	-	33	8	19	23	14
0	30	-	48	7	15	43	21
0.05	30	-	47	7	14	43	20
0.1	30	-	49	8	13	46	25
0.2	30	-	52	8	12	55	30
0.3	30	-	51	8	12	57	31
0	-	30	65	10	20	67	36
0.05	-	30	64	10	21	65	38
0.1	-	30	66	10	16	66	32
0.2	-	30	66	10	14	64	33
0.3	-	30	66	10	11	65	31
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

4.2

Table 4.7. The effect of adverse environments of boiling water for 2 hours, of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with ACCT (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples, table 4.6).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-20°C) KJ/M^2
0	-	-	34 (0%)	20 (-44%)	16 (-62%)
0.05	-	-	33 (0%)	21 (-40%)	11 (-63%)
0.1	-	-	34 (0%)	19 (-44%)	12 (-54%)
0.2	-	-	31 (0%)	21 (-36%)	10 (-52%)
0.3	-	-	33 (0%)	20 (-40%)	10 (-47%)
0	30	-	35 (-27%)	24 (-50%)	8 (-46%)
0.05	30	-	37 (-21%)	24 (-49%)	9 (-35%)
0.1	30	-	36 (-26%)	23 (-53%)	9 (-30%)
0.2	30	-	38 (-26%)	23 (-56%)	10 (-16%)
0.3	30	-	42 (-17%)	26 (-49%)	9 (-25%)
0	-	30	45 (-30%)	39 (-40%)	11 (-45%)
0.05	-	30	47 (-26%)	40 (-37%)	11 (-47%)
0.1	-	30	48 (-27%)	41 (-37%)	10 (-37%)
0.2	-	30	51 (-22%)	40 (-39%)	8 (-43%)
0.3	-	30	51 (-22%)	42 (-36%)	9 (-18%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

4.5

4.4 Mechanochemical modification of PP with 2-allylamino-4-chloro-6-dibutlyamino-1,3,5-triazine (ABCT) and DCP.

ABCT was evaluated as a modifier to ascertain the effect of blocking one of the chloro groups and thus allowing an assessment of the reactivity of only one chloro group to the amino silane coupled glass fibres (GF-NH).

The infrared spectrum of a nujol mull of ABCT is shown in figure 4.15 **a**, this has absorptions at 1572cm^{-1} and 1554 cm^{-1}. The infrared spectra of PP modified with ABCT (1%) in the absence (**b**) and presence (**c**) of DCP (0.3%) are shown in figure 4.15. Both spectra have absorptions at 1572cm^{-1} and 1554cm^{-1}, as well as one at 1694cm^{-1}. The size of the 1694cm^{-1} appears to increase with the addition of DCP (cf figures 4.15 **b** and **c**). The MFI data for the ABCT (1%) modified PP (see scheme 4.1) is shown in figure 4.2, as can be seen the MFI does not differ from that of the analgous unmodified PP. The binding studies (see table 4.8) show that no ABCT is bound to the PP.

The infrared spectra of PP modified with ABCT (1%) and CLS (1%) to simulate the presence of the glass fibres GF-CL in the absence (**a**) and presence (**b**) of DCP (0.3%) are shown in figure 4.16. Both spectra possess peaks at 1572 cm^{-1} and 1554 cm^{-1}, however, the peak at 1694cm-1 seen in earlier spectra (figure 4.15 **b** and **c**) is not present, instead a peak at 1750cm^{-1} can be observed.

The infrared spectrum of PP modified with ABCT (1%) and AMS (1%) to simulate the presence of the GF-NH glass fibres in the absence (**a**) and presence (**b**) of DCP (0.3%) are shown in figure 4.17. Absorptions at 1710cm^{-1}, 1580cm^{-1} and 1554cm^{-1} can be observed in both these spectra.

The mechanical properties of the unfilled PP, the GF-CL and GF-NH filled PP in both normal and aggressive environments did not differ significantly from those of the analgous unmodified PP.

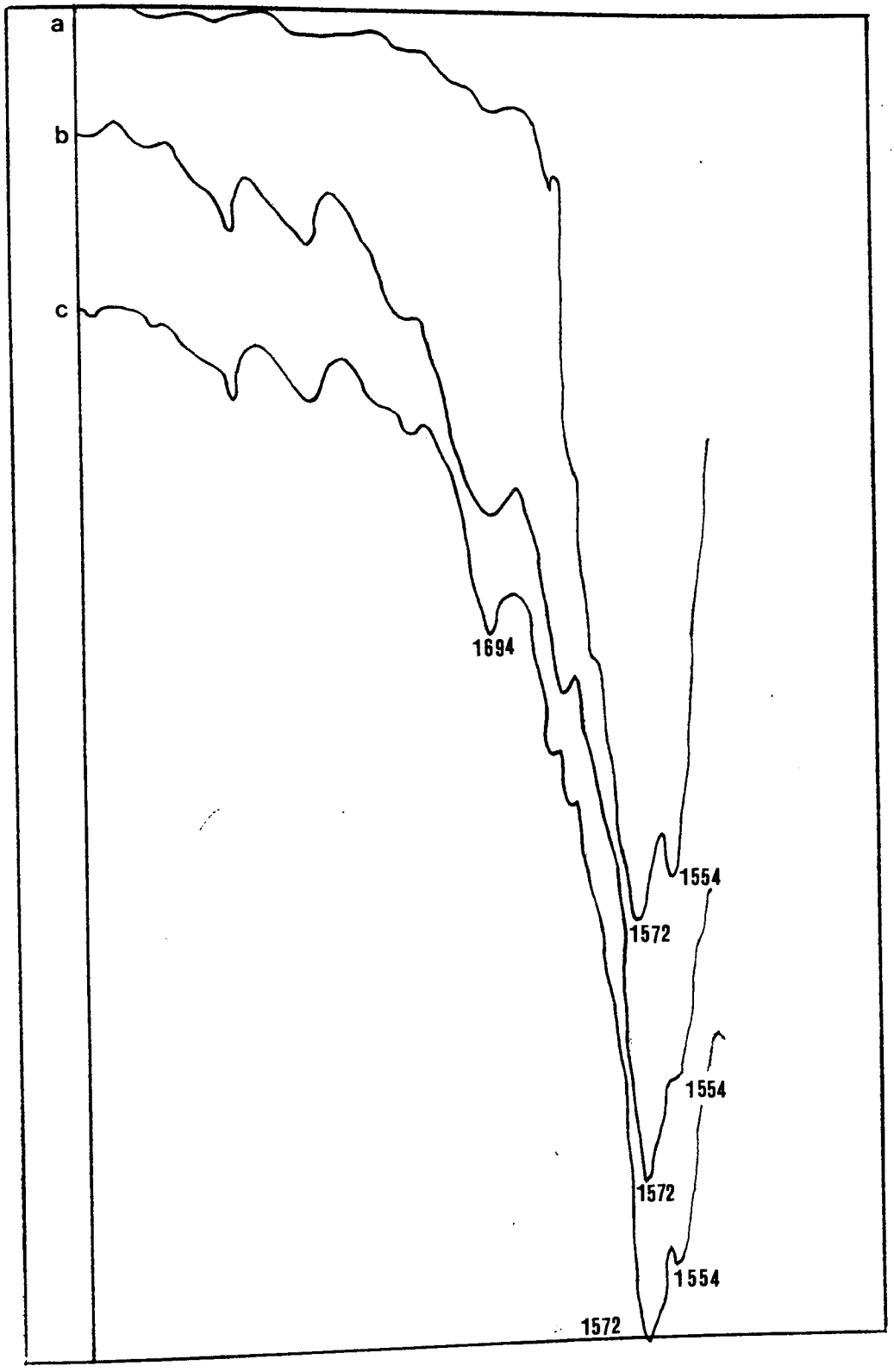


Figure 4.15. a = ABCT (nujol mull), b = PP + 1% ABCT, c = PP + 1% ABCT + 0.3% DCP.

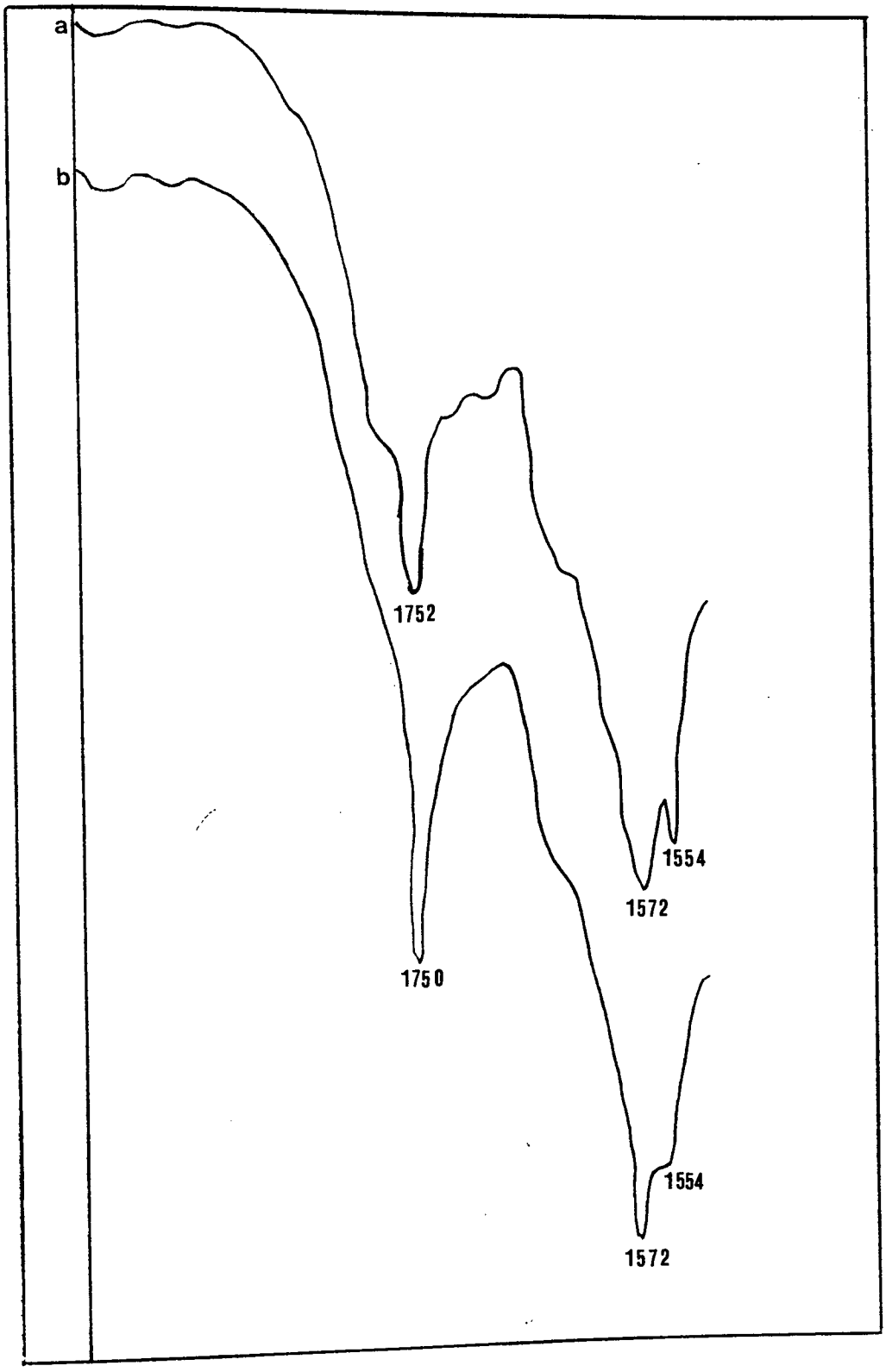


Figure 4.16. a = PP + 1% ABCT + 1% CLS, b = PP + 1% ABCT + 1% CLS + 0.3% DCP.

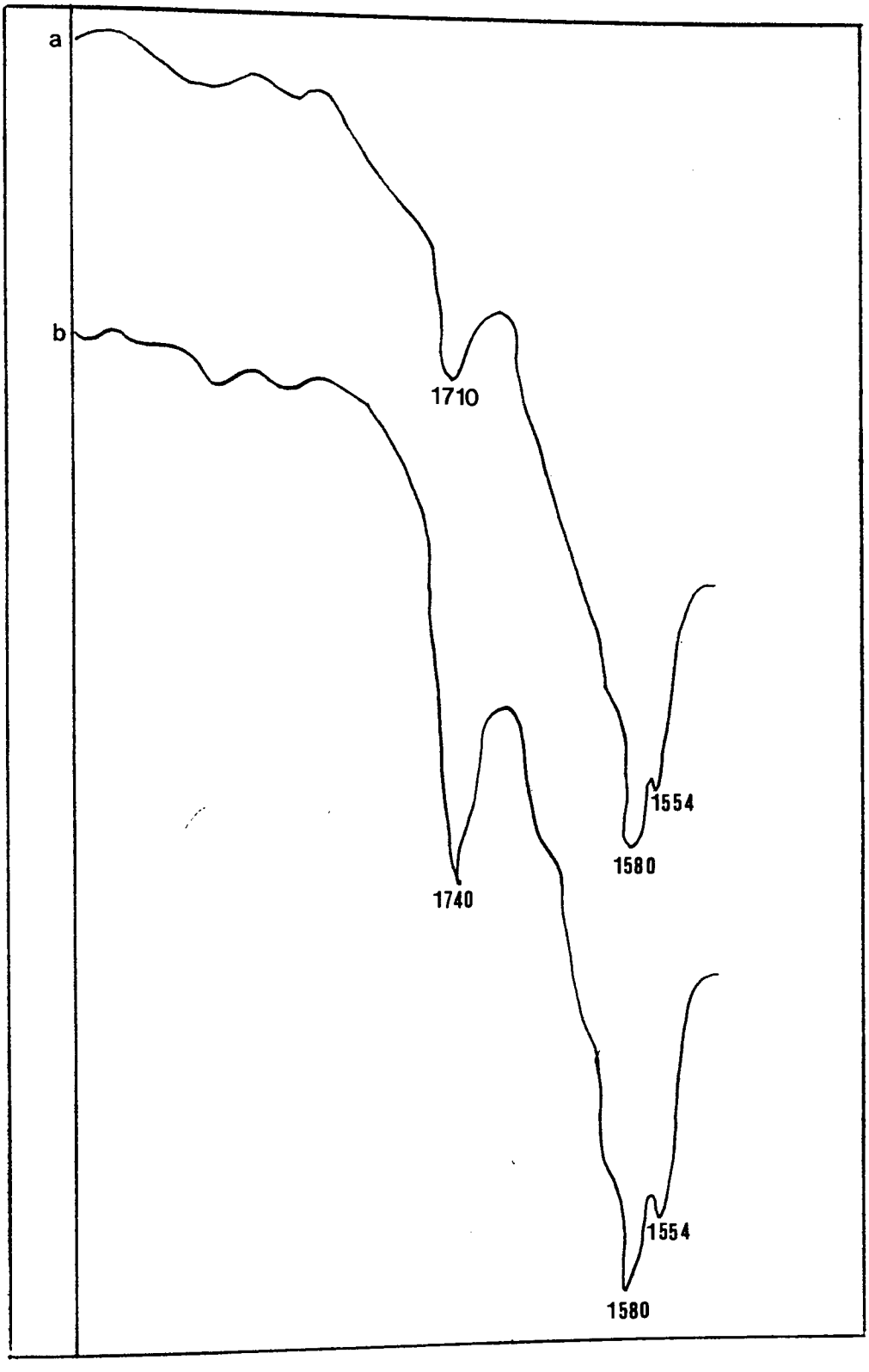


Figure 4.17. a = PP + 1% ABCT + 1% AMS, b = PP + 1% ABCT + 1% AMS + 0.3% DCP.

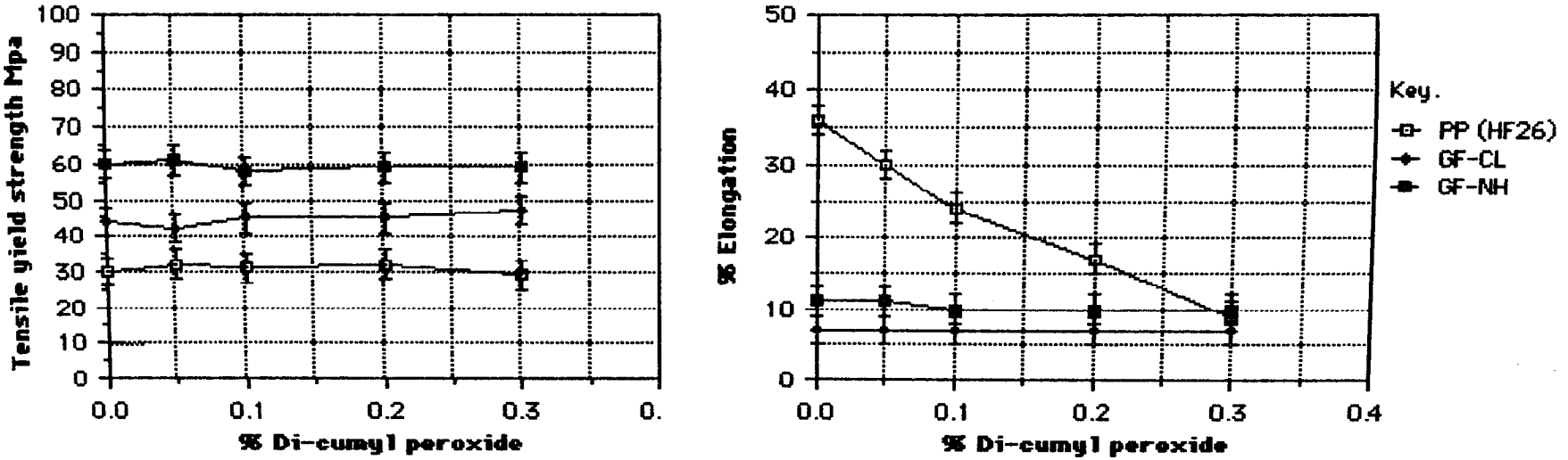


Figure 4.18Tensile strength and elongation of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with ABCT (1%) and DCP (0-0.3%).

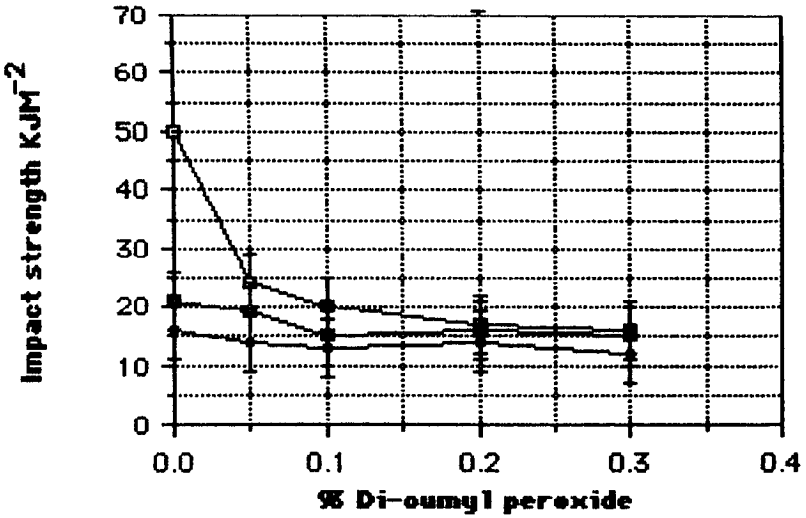


Figure 4.19 Impact strength of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with ABCT (1%) and DCP (0-0.3%).

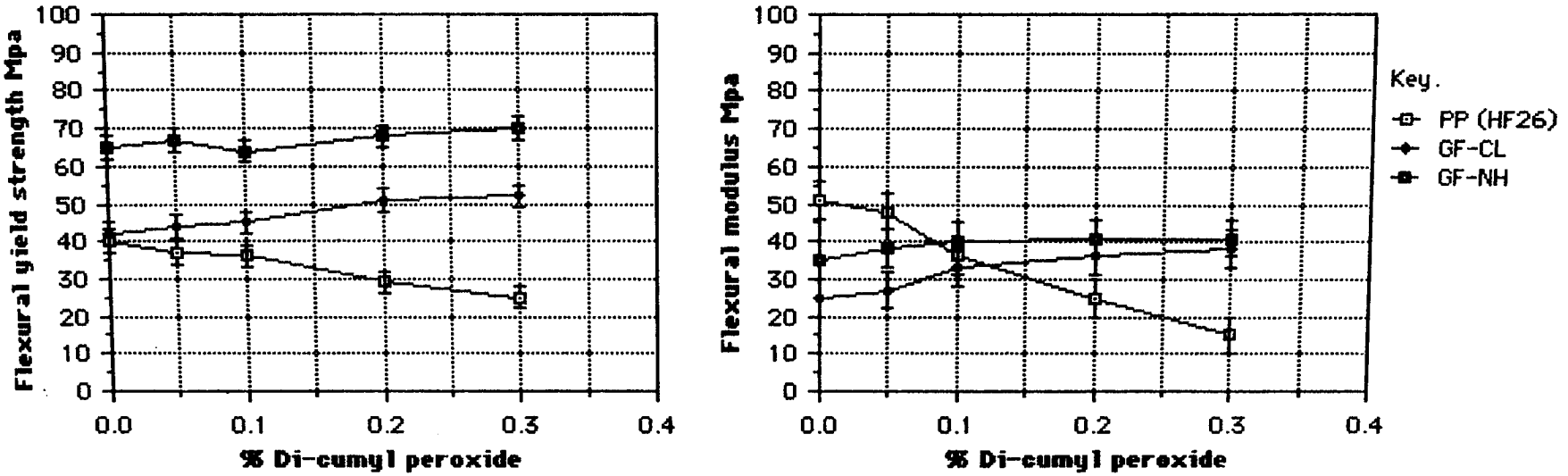


Figure 4.20 Flexural strength and flexural modulus of PP (HF26), its GF-CL and GF-NH composites modified according to scheme 4.3 with ABCT (1%) and DCP (0-0.3%).

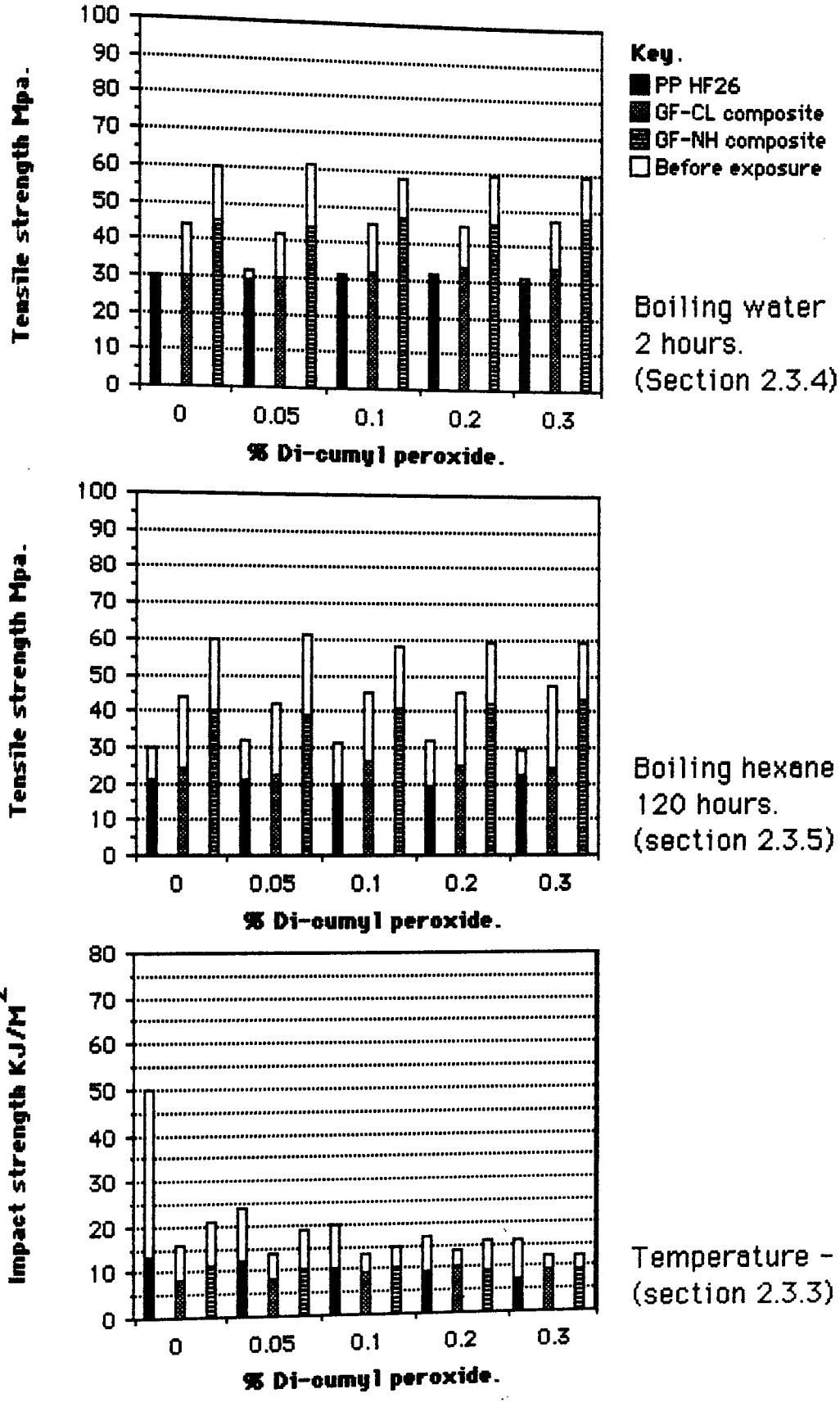


Figure 4.21. Tensile yield strength of PP Hf26, its GF-CL and GF-NH composites modified according to scheme 4.3 with ABCT (1%) and DCP (0-0.3%) before and after exposure to boiling water for 2 hours or boiling hexane for 120 hours and the impact strength at 20°C and -10°C.

Table 4.8. The binding of ABCT (1%) to PP (HF26) determined according to section 2.4.4.4.

% DCP	Modifier theoretical	Modifier pre-extraction	Modifier post extraction	Modifier bound
	(g/100g PP).	(g/100g PP).	(g/100g PP).	(%)
0	1	0.61	0.01	1
0.1	1	0.56	0.00	0
0.3	1	0.52	0.00	0
	No of modifier molecules per 10000 PP repeat units.			
0	14.1	8.6	0.14	-
0.1	14.1	7.9	0	-
0.3	14.1	7.3	0	-

4.10

Table 4.9. The effect of DCP concentration on the mechanical properties of PP (HF26) modified with ACCT (1%) (see scheme 4.3) in the absence and presence of GF-CL and GF-NH. The symbol > by impact results means that some samples did not break when tested and the average quoted is therefore based on those that did break.

%DCP	% GF-CL	% GF-NH	Tensile Yield (MPa).	%Elong	Impact strength (KJ/M^2)	Flexural Yield (MPa).	Flexural modulus (MPa).
0	-	-	30	36	50	40	51
0.05	-	-	32	30	24	37	48
0.1	-	-	31	24	20	36	36
0.2	-	-	32	17	17	29	25
0.3	-	-	29	9	16	25	15
0	30	-	44	7	16	42	25
0.05	30	-	42	7	14	44	27
0.1	30	-	45	7	13	45	33
0.2	30	-	45	7	14	51	36
0.3	30	-	47	7	12	52	38
0	-	30	60	11	21	65	35
0.05	-	30	61	11	19	67	38
0.1	-	30	58	10	15	64	40
0.2	-	30	59	10	16	68	41
0.3	-	30	59	10	15	70	41
HWM 25			33	39	>60	41	56
HW60/GR30			75	11	24	75	38

4.3

Table 4.10. The effect of adverse environments of boiling water for 2 hours, of boiling hexane for 120 hours and impact strength at -10°C on TS retention and IS retention. For unfilled, GF-CL and GF-NH filled PP (HF26) modified with ABCT (1%) and containing variable concentrations of DCP (0-0.3%). (The figures in brackets () are the percentage loss in the property from the unexposed samples, table 4.9).

%DCP	% GF-CL	% GF-NH	Tensile strength. (Water) Mpa.	Tensile strength (Solvent) Mpa.	Impact strength (-20°C) KJ/M^2
0	-	-	30 (0%)	21 (-30%)	13 (-74%)
0.05	-	-	29 (0%)	21 (-34%)	12 (-50%)
0.1	-	-	31 (0%)	20 (-35%)	10 (-50%)
0.2	-	-	31 (0%)	19 (-40%)	9 (-47%)
0.3	-	-	30 (0%)	22 (-24%)	7 (-56%)
0	30	-	30 (-32%)	24 (-45%)	8 (-50%)
0.05	30	-	30 (-28%)	22 (-47%)	8 (-49%)
0.1	30	-	32 (-29%)	26 (-42%)	9 (-30%)
0.2	30	-	34 (-24%)	25 (-44%)	10 (-28%)
0.3	30	-	34 (-27%)	24 (-49%)	9 (-25%)
0	-	30	45 (-25%)	40 (-33%)	11 (-48%)
0.05	-	30	44 (-28%)	39 (-36%)	10 (-47%)
0.1	-	30	47 (-19%)	41 (-29%)	10 (-33%)
0.2	-	30	46 (-22%)	42 (-29%)	9 (-43%)
0.3	-	30	48 (-18%)	43 (-29%)	9 (-40%)
HWM 25			32 (0%)	27 (-18%)	17 (-71%)
HW60/GR30			73 (0%)	40 (-46%)	12 (-50%)

4.6

4.6 Discussion

4.6.1 The properties of unfilled PP HF26 modified with ACCT, AACT and ABCT

All three of the triazine based modifiers (see table 4.1) behaved in a broadly similar fashion when melt processed with PP (see scheme 3.1). There was little or no binding of the modifier to the PP, even in the case of the AACT with two allyl groups (see tables 4.2, 4.5 and 4.8). The MFI studies (see figure 4.2) indicate similar behavior with all three modifiers to the PP processed with DCP only.

The infrared spectra of all three modifiers indicate broadly similar behavior. On addition to the PP a peak at 1697cm^{-1} (attributed to carboxylic acid) (see figure 4.1, 4.7, 4.15) is observed in addition to those otherwise present. In the case of both the AACT and ABCT modified PP the size of this peak increases in the presence of DCP. The other absorptions in the spectrum remain unchanged. For ACCT (see figure 4.1) the peaks observed at 1753cm^{-1} (acid chloride) 1643cm^{-1} (carbon carbon double bond) and 1553cm^{-1} (C=N of triazine) remain unchanged. The triazine based modifiers were supposed to link to PP in an analogous fashion to MA (see figure 4.2.1), however, this does not appear to be the case. The failure of the allyl group to bind to PP may be due to the relative stability of the allylic radical (A1) which delocalises the free radical.

The only reaction which appears to occur with the triazine based modifiers is the formation of carboxylic acid. This could occur in an analgous fashion to that of MA (see figure 3.?) (see figure 4.22). The water for the reaction could come from the atmosphere or could condence out on the cold polymer (polymer is stores at -10^{o}C to prevent degradation) during the mixing of the additions.

The mechanical properties of the PP modified with the triazine derivation (see scheme 4.3) are all unaffected by that modification.

4.6.2 The properties of ACCT, AACT and ABCT modified PP (HF26) filled with GF-CL.

The infrared spectra indicate no reaction of the CLS with the triazine based modifiers. In the case of the ACCT based modifiers there is no eveidience for a reaction between ACCT and CLS. The spectra of the melt reactions in the presence of CLS are identical to those in the absence of CLS (cf figure 4.2a and b with 4.1B and C). The same can be seen for the AACT modified PP (cf figures 4.8 and 4.7) and the ABCT modified PP (cf figure 4.14 and 4.15). The lack of any reaction between modifier and PP or CLS means that the mechanical properties of the GF-CL filled components are not significantly different

from those of the analgous filled unmodified PP.

4.5.3 The properties of ACCT, AACT and ABCT modified PP (HF26) filled with GF-NH.

For all three of the modifiers ACCT, AACT and ABCT there is spectroscopic evidence for a reaction taking place in the melt with the AMS. In the case of all three modifiers the reaction appears to be one between the acid chloride of the modifier and the amino group of the silane, see figure 4.24. The ACCT has a peak at 1714cm^{-1} attributed to the amide formed, whilst in the AACT this peak appears at 1705cm^{-1} and in the ABCT at 1710cm^{-1}, other Absorptions remain unaffected. However, because there is no reaction with the PP, these modifiers do not improve the properties of the AMS coupled glass filled GF-NH.

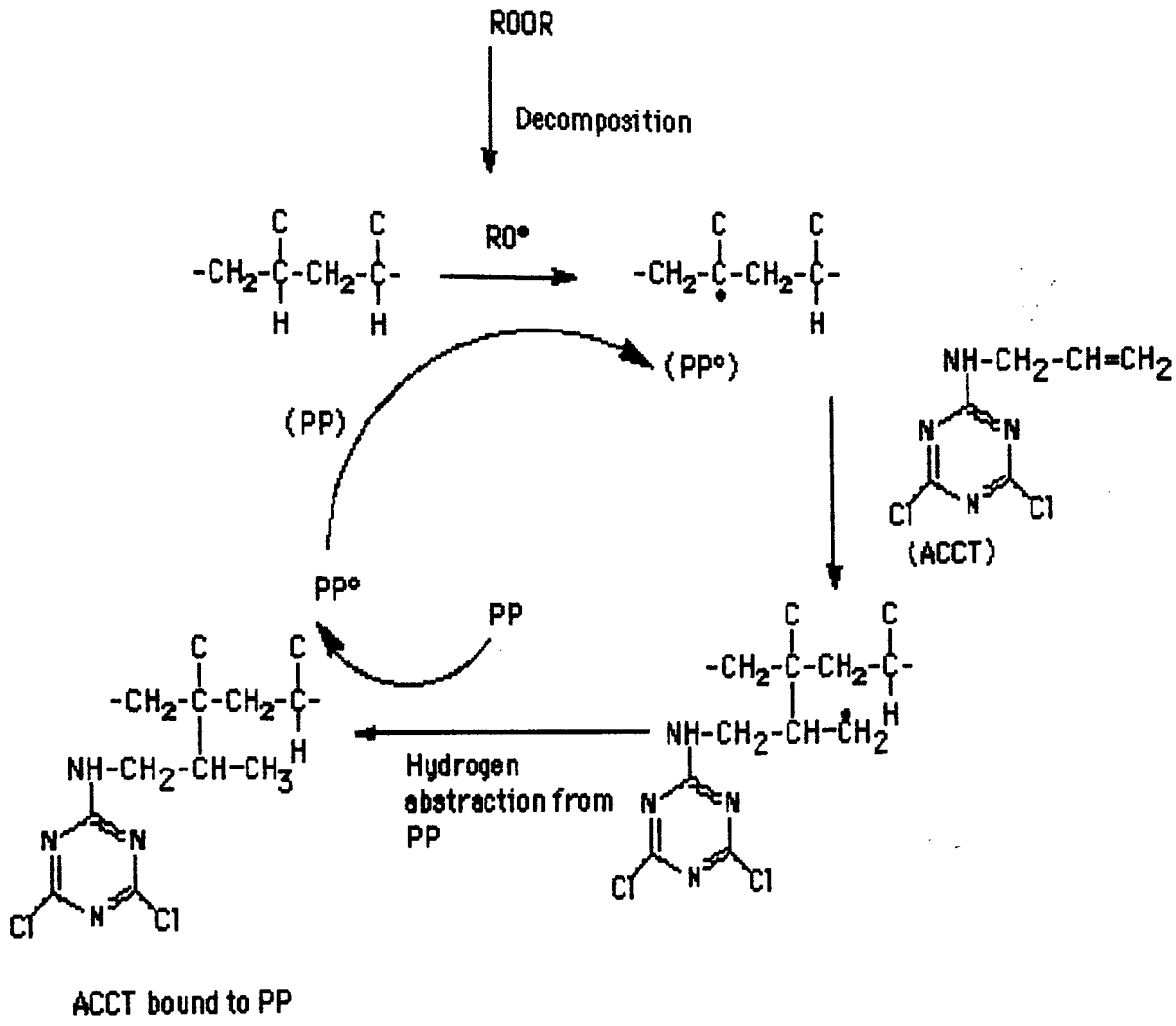


Figure 4.21. Desired reaction between ACCT based modifiers and PP.

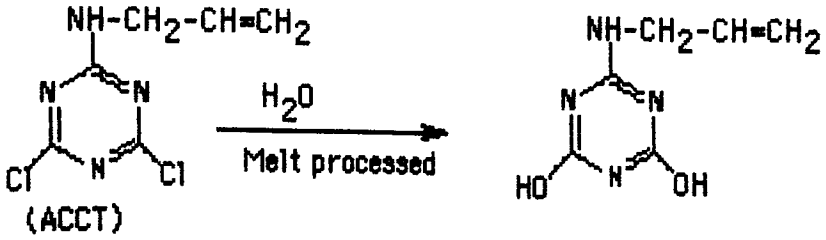


Figure 4.22 Possible reaction between water and ACCT based modifiers during melt processing.

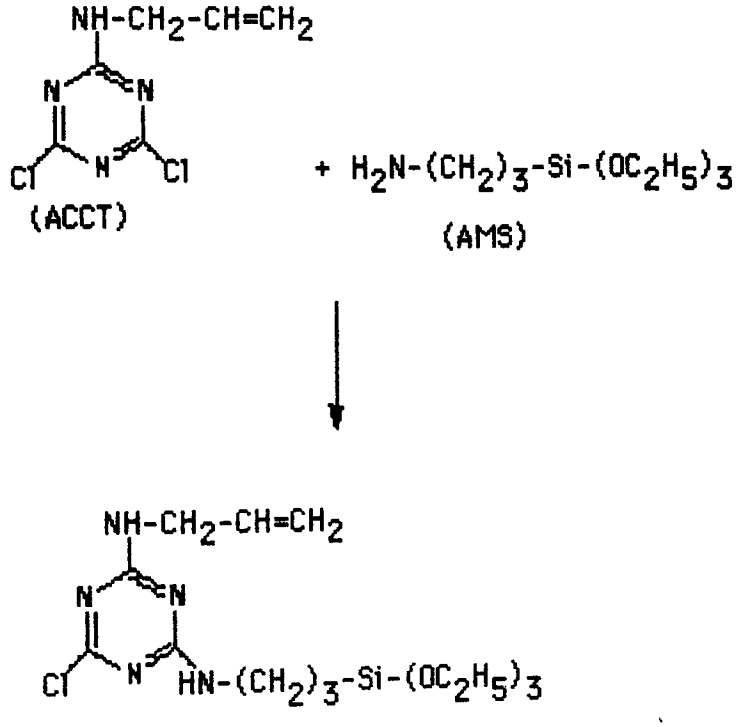


Figure 4.23. Reaction between ACCT based modifiers and AMS during melt processing.

Chapter 5.
Conclusions.

5. Conclusions.

From the experimental results obtained the following conclusions can be drawn:

1. A reaction of MA and chloro silane coupled glass fibres occurred which enhanced the mechanical properties of an MA modified GF-CL filled composite. The reaction occurred via the formation of maleic acid followed by an esterification reaction with the chloro group of the CLS coupled fibres.

2. A reaction between the bound maleic anhydride and amino silane coupled glass fibres occurred to form a maleamic acid. Despite the presence of this chemical bond between the PP and glass fibre, the mechanical properties of the GF-NH filled PP composite were not improved.

3. Simply producing a chemical bond between glass and PP does not necessarily enhance the mechanical properties of the resulting compound as can be seen in the case of the reaction of the bound MA with GF-NH. Further all the modified systems did not produce a TS which significantly exceeded that of the commercial composite (HW60/GR30)

4. The modification of PP with small amounts (1%) of NMM, NEM or MA produces an enhancement of the IS and EL of unfilled PP.

5. Modifiers based on ACCT did not bind to PP due to the relative stability of the allyl group. As a result it was not possible to enhance the properties of the resulting GF-CL and GF-NH filled composites.

6. The addition of a second allyl group (AACT) did not significantly improve the binding of the ACCT based modifiers. This can be seen by comparing the binding of AACT with ACCT and ABCT.

7. Modifiers based on ACCT did not react with react with the CLS, this can be seen from the identical spectra produced when PP was melt processed with the ACCT based modifiers with and without CLS.

8. Modifiers based on ACCT did react with the AMS to produce an amide but did not enhance the mechanical properties of a GF-NH filled composite due to the lack of binding to the PP.

9. None of the modified composite systems examined in this work greatly out performed the commercial composite (HW60/GR30).

Chapter 6.

Further work.

6. Further work.

1. The reactions of MA, SA and the triazine derivatives appear to take place via hydrolysis. The source of the water for these reactions has not been determined, but could possibly be by thoroughly drying the PP prior to melt processing and determining the extent of hydrolysis of the chosen modifier.

2. The triazine based modifiers are unsuccessful because of a lack of binding the the PP, a substitution of the allyl group for another may change this. It should be possible to substitute the NMM or NEM onto a triazine ring, both these modifiers show high degree of binding to PP. This would then leave two acid chloride groups available for further modification or for reaction with the AMS coupled glass fibres.

3. Silane coupling agents based on compound formed in the melt could be synthesised, eg, the reaction between NMM and AMS could be used to synthesise a novel coupling agent. Based on the results obtained with NMM this should have a high degree of reactivity to PP and may only require to be homogenised with the polymer prior to moulding.

4. The use of the imide based modifiers, that is, NMM and NEM as modifiers of unfilled PP could be exploited. These modifiers enhance particularly the IS, the mechanism by which this happens need to be investigated. This ability to improve the mechanical properties could be used to improve the properties of recycled PP.

5. Modification of the glass fibres prior to homogenisation with PP could be carried out. A solution of say MA, could be added to the CLS or AMS coupled glass fibres and the reaction carried out on the surface of the glass. This modified glass could then be processed with the PP to produce a modified composite.

6. The possibility of carrying out the homogenisation of the glass fibres with the PP and modifiers in one step in the moulding machine could be investigated. This would eliminate two processing stages which can only serve to degrade the PP and glass.

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Appendix 1.

Tensile testing programme.

1. Tensile testing programme.

The tensile testing programme has been designed to interface with a testometric 500M tensometer in order to collect and process the data from it. The programme is an extensively modified version of the original software supplied, the only original part remaining is the interfacing routine which performs the actual data collection. The programme collects the data in the form of load versus extension and from this calculates the peak load, strain, % elongation, load stress and modulus for each sample. For each batch of samples the programme calculates the highest and lowest value, the average and standard deviation. All the results are tabulated and can be printed on a line printer. There are also facilities to allow stress strain curves and load extension curves to be plotted on an attached XY plotter. The programme runs on an Apple IIe computer under Applesoft basic using an RS232 interface for communication with the 500M. A simplified flow diagram of the programme is shown in figure A1.1 with a listing of variables in tables A1.1 and A1.2.

2. Tensile testing programme listing.

```
      10    REM TENSILE PROGRAMME
      20    REM BY I.R.SURRY
      30    LET E$="mm" : REM UNITS OF EXTENSION
(A)   40    LET D$=CHR$(13) + CHR$(4) : PRINT D$; "PR#0" : REM
            PRINTER SWITCH
(B)   50    DIM L3(1000) : REM LOAD ARRAY
(C)   60    DIM E3(1000) : REM EXTENSION ARRAY
(D)   70    LET M3=999
(E)   80    LET L1=100 : LET L2=1000
      90    LET E1=20
(F)   100   DIM M(30), N(30), U(30), V(30), P(30), B(30)
      150   REM FIND LOAD CELL
(G)   160   HOME
      170   PRINT : PRINT
      180   PRINT TAB(5); "THE 500M TENSILE TEST ANALYSER."
(H)   190   VTAB(22) : PRINT "CONTINUE WITH ANOTHER TEST?
            (Y/N)."
      200   GET A$
      210   IF A$="Y" THEN GOTO 240
      220   IF A$="N" THEN STOP
      230   GOTO 200
(I)   240   HOME
      250   PRINT : PRINT
      260   PRINT "PRESS KEY FOR LOAD CELL RANGE."
      270   PRINT
```

```
        280   PRINT TAB(4); "(1)-2500KG CELL."
        290   PRINT
        300   PRINT TAB(4); "(2)-100N CELL."
        310   GET A$
(J)     320   IF A$="1" THEN LET L$="KN" : LET U$="KN/mm^2" :
              LET C2=20; GOTO 350
        330   IF A$="2" THEN LET L$="N" : LET U$="N/mm^2" : LET
              C2=100 : GOTO 350
        340   GOTO 310
(K)     350   PRINT : PRINT "LOAD RANGE IN"; L$
        360   PRINT
        370   PRINT "HIGH="; C2; " "; L$,"LOW="; C2/10; " "; L$
        380   PRINT : PRINT "EXTENSION RANGE 850.0"; E$
        390   PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
        400   GET A$
(L)     410   HOME
        420   PRINT : PRINT
(M)     430   PRINT : INPUT "ENTER SAMPLE WIDTH (mm)-"; W
(N)     440   PRINT : INPUT "ENTER SAMPLE LENGTH (mm)-"; L7
(O)     450   PRINT : INPUT "ENTER SAMPLE THICKNESS (mm)-"; G
(P)     460   PRINT : INPUT "ENTER ANY TEST REFERENCE-"; A$
(Q)     470   PRINT : INPUT "ENTER TEST SPEED-"; A1$
(R)     480   PRINT : INPUT "HARD COPY OF RESULTS (Y/N)-"; A$
        490   IF A$="Y" THEN PR=1 ELSE PR=0
(S)     500   LET T=1
(T)     510   IF PR=1 AND T=1 THEN GOSUB 2140 : GOSUB 3000
(U)     520   FOR N=1 TO 40 : PRINT "*"; : NEXT N
        530   PRINT : PRINT "    WIDTH    LENGTH    THICKNESS" :
              PRINT
        540   HTAB(7) : PRINT W;
        550   HTAB (17)  : PRINT L7;
        560   HTAB (30)  : PRINT G
        570   PRINT : PRINT "   TEST REFERENCE = "; A$; "mm/min."
        580   PRINT : PRINT "   TEST SPEED = "; A1$
        590   PRINT : PRINT "   TEST NUMBER = "; T
        600   PRINT : PRINT



(U)     650   LET F=0 : LET J=0
        651   LET D$= CHR$(13) + CHR$(4) : PRINT D$; "PR#0"
        655   LET F$="" : REM CTRL-A
        660   PRINT D$; "PR#2" : PRINT F$; "F4" : FOR N=1 TO 20 :
              PRINT " "; : NEXT N : PRINT
        670   PRINT D$; "IN#2"
        680   UTAB(22) : PRINT "D" : PRINT F$; "00" : UTAB(22) :
```

```
        INPUT LD$, EH$, A$ : PRINT F$; "01"
    690 IF F=1 THEN GOTO 770
    700 IF A$="F" THEN GOTO 680
    710 IF A$="1" THEN LET R=L1 : GOTO 750
    720 IF A$="H" THEN LET R=L2 : GOTO 750
    730 GOTO 680
    740 PRINT CHR$(7) : PRINT "=> DATA TIMEOUT <=" : GOTO
    750 LET F=1
    760 GOTO 680
    770 IF A$="F" THEN GOTO 810
    780 IF J>M3 THEN GOTO 680
    785 IF VAL (LD$) =0 THEN GOTO 680
    786 IF VAL (EH$) =0 THEN GOTO 680
    790 LET L3(J)=VAL (LD$) : LET E3(J)=VAL (EH$) : LET J=J+1
    800 GOTO 680
    810 LET F=0
    820 PRINT D$; "PR#2"
    830 VTAB(23)
    850 PRINT D$; "IN#0" : PRINT D$"PR#0"
    860 POKE 34,15 : HOME : POKE 34,0


    870 PRINT "============>> RESULTS <<============"
    880 LET J=J-1 : LET L=0
    890 FOR N=0 TO J : IF N > M3 THEN GOTO 920
    900 LET L3(N)=L3(N)/R : LET E3(N)=E3(N) * 100 / (E1*L7)
    910 IF L3(N) >L THEN LET L= L3(N)
    920 NEXT N
(W) 930 LET U=INT ((L/(G*W))*1000)/1000
(H) 940 LET E=E3(J)
    950 LET E=(INT(E*10))/10
(Y) 960 HTAB (5) : PRINT "PEAK LOAD = "; L; L$
    970 PRINT : HTAB (5) : PRINT "EXTENSION = "; E; E$
    980 PRINT "STRESS = "; U; U$
    990 PRINT CHR$(7)
(Z) 1000 PRINT "ACCEPT (Y/N) -"; : GET A$ : PRINT A$
    1010 IF A$="Y" THEN GOTO 1020 ELSE GOTO 510
(AA) 1020 LET L(T)=L : LET E(T)=E : LET M(T)=G : LET N(T)=W : LET
          U(T)=U
(AB) 1030 LET S=E/100
    1040 LET M0=U/S
    1050 LET M0=(INT(M0*10000))/10000
    1060 LET U(T)=M0
(AC) 1070 IF PR=1 THEN GOSUB 2140 : GOSUB 3200
    1080 HOME
(AD) 1085 GOSUB 4000 : REM PLOT RESULTS
```

```
      1090  PRINT "ANOTHER TEST (Y/N)-"; GET A$; PRINT A
(AE)  1100  IF A$="N" THEN GOTO 1170 : REM STATISTICS
      1110  IF A$<>"Y" THEN GOTO 1090
      1120  LET T=T+1 : IF T>M THEN GOTO 1170 : REM STATISTICS
      1130  PRINT : PRINT
(AF)  1140  PRINT : INPUT "INPUT SAMPLE WIDTH (mm)-"; W
      1150  PRINT : INPUT "INPUT SAMPLE THICKNESS (mm)-"; G
      1160  GOTO 510
(AG)  1170  IF PR=1 THEN GOSUB 2140 : GOSUB 3400 : REM
            STATISTICS
      1180  IF PR=0 THEN GOSUB 3400 : REM STATISTICS


(AH)  2140  REM PRINTER SWITCH ON
      2150  PRINT D$; "PR#1"
      2160  RETURN
(AI)  2170  REM PRINTER SWITCH OFF
      2180  PRINT D$; "PR#0"
      2190  RETURN


(AJ)  3000  REM PRINTER HEADER
      3010  FOR N=1 TO 80 : PRINT "*"; : NEXT N
      3020  PRINT : PRINT : INVERSE : HTAB(27) : PRINT
            "TESTOMETRIC 500M ANALYSIS."
      3030  NORMAL
      3040  PRINT : FOR N=1 TO 80 : PRINT "*"; : NEXT N
      3050  PRINT : PRINT TAB(20); "SAMPLE LENGTH = "; L7; E$
      3060  PRINT : PRINT TAB(20); "TEST SPEED = "; R1$;
            "mm/min"
      3070  PRINT : PRINT "TEST REFERENCE = "; R$
      3080  FOR N=1 TO 80 : PRINT "-"; : NEXT N : PRINT
      3090  PRINT "Test  Width  Thickness  Peak  Strain
            Elongation  Stress  Modulus"
      3100  PRINT "Number"; PRINT TAB(27); "Load"
      3110  IF C2=100 THEN GOTO 3150
      3120  PRINT TAB(9); "(mm)"; TAB(18); "(mm)"; TAB(27);
            "KN";
      3130  POKE 36,43 : PRINT "(%)  (KN/mm^2)  (KN/mm^2)"
      3140  GOTO 3170
      3150  PRINT TAB(9); "(mm)"; TAB(18); "(mm)"; TAB(27); "N";
      3160  POKE 36,43 : PRINT "(%)  (N/mm^2)  (N/mm^2)"
      3170  GOSUB 2170 : REM PRINTER SWITCH OFF
      3180  HOME
      3190  RETURN
```

```
(AK)  3200  REM TABULATE RESULTS
      3210  PRINT TAB (2); T; : REM TEST NUMBER
      3220  PRINT TAB (8); W; : REM WIDTH
      3230  PRINT TAB (15); G; : REM THICKNESS
      3240  PRINT TAB (26); L; : REM PEAK LOAD
      3250  PRINT TAB (33); S; : REM STRAIN
      3260  POKE 36,40 : PRINT E; : REM ELONGATION
      3270  POKE 36,53 : PRINT U; : REM STRESS
      3280  POKE 36,63 : PRINT MO : REM MODULUS
      3290  GOSUB 2170 : REM PRINTER OFF
      3300  RETURN


(AL)  3400  REM STATISTICS
      3410  PRINT : FOR N=1 TO 80 : PRINT "-"; : NEHT N
      3420  PRINT : PRINT "          500M TEST SERIES SUMMARY."
(AM)  3430  REM LOAD
      3440  FOR N=1 TO T : LET B(N)=L(N) : NEHT N
      3450  PRINT "LOAD ANALYSIS IN "; L$
      3450  GOSUB 3700 : REM ANALYSIS
      3460  REM EHTENSION
      3470  PRINT "EHTENSION ANALYSIS IN %."
      3480  FOR N=1 TO T : LET B(N)=E(N) : NEHT N
      3490  GOSUB 3700 : REM ANALYSIS
      3500  REM MODULUS
      3510  PRINT "MODULUS ANALYSIS IN "; U$
      3520  FOR N=1 TO T : LET B(N)=U(N) : NEHT N
      3530  GOSUB 3700 : REM ANALYSIS
      3540  REM STRESS
      3550  PRINT "STRESS ANALYSIS IN "; U$
      3560  FOR N=1 TO T : LET B(N)=U(N) : NEHT N
      3570  GOSUB 3700 : REM ANALYSIS
      3580  GOTO 10


(AN)  3700  REM STATISTICAL ANALYSIS OF RESULTS
(AO)  3710  LET HIGH=0 : LET LOW=1E+7 : LET AVE=0
      3720  FOR I=1 TO T
      3730  IF E(I)>HIGH THEN HIGH=E(I)
      3740  IF E(I)<LOW THEN LOW=E(I)
      3750  LET AVE=AVE+E(I)
      3760  NEHT I
      3770  LET AVE=FIH((AVE/T)*10000)/10000
      3780  LET DVE=0
      3790  IF T <=1 THEN RETURN
```

```
      3800  FOR I=1 TO T
      3810  LET DVE=DVE + (E(I)-AVE)^2
      3820  NEXT I
      3830  LET DVE=SQR(DVE/(T-1))
      3840  LET DVE=FIX(DVE*1000)/1000
      3850  PRINT "HIGHEST="; HIGH
      3860  PRINT "LOWEST ="; LOW
      3870  PRINT "AVERAGE="; AVE
      3880  PRINT "STD DVE="; DVE
      3890  RETURN


(AP)  4000  REM PLOT RESULTS
      4010  LET X1=0 : LET Y1=0
      4020  LET X2=0 : LET Y2=0
      4030  TEXT
      4040  PR#0
(AQ)  4050  HOME
      4060  PRINT : PRINT
      4070  PRINT TAB(4); "(1)-PLOT LOAD EXTENSION CURVE."
      4080  PRINT
      4090  PRINT TAB(4); "(2)-PLOT STRESS STRAIN CURVE."
      4100  PRINT
      4110  PRINT TAB(4); "(3)-PLOT BOTH."
      4120  PRINT
      4130  PRINT TAB(4); "(4)-CONTINUE."
      4140  GET A$
(AR)  4150  IF A$="1" THEN GOSUB 8000 : GOSUB 8400 : GOTO 4700
(AS)  4160  IF A$="2" THEN GOSUB 8000 : GOSUB 8400 : GOTO 4800
(AT)  4170  IF A$="3" THEN GOTO 4500
(AU)  4180  IF A$="4" THEN RETURN
      4190  GOTO 4050


(AV)  4500  REM PLOT BOTH
      4510  LET PL=1 : REM SETS SMALL SCALE PLOT
      4520  GOSUB 8000
      4530  PR#4
      4540  PRINT "IN"
(AW)  4550  PRINT "RP; 200,200,0"
      4560  GOSUB 8700 : REM PLOT SMALL SCALE AXIS
      4565  PRINT "RP; 0,-1000,0"
(AX)  4070  GOSUB 4700 REM PLOT
      4080  PRINT "TE"
      4090  PRINT "IN"
      4100  PRINT "RP; 200,1400,0"
```

```
(AY)  4110  GOSUB 8700
      4120  PRINT "RP; 0,-100,0"
(AZ)  4130  GOSUB 4800
(BA)  4140  LET A$="EXTENSION (mm)" : LET B$="LOAD ("+L$+")"
      4150  LET C$=STR$(EMAX) : LET D$=STR$(LMAX)
      4160  LET P(1)=EMAX : LET P(2)=LMAX
(BB)  4170  GOSUB 8900 : REM LABEL SUBROUTINE
      4180  LET PL=0
(BC)  4190  LET A$="STRAIN" : LET B$="STRESS ("+U$+")" : LET
            C$=STR$(STMAX) : LET D$=STR$(UMAX)
      4200  LET P(1)=STMAX : LET P(2)=UMAX : LET P(3)=STMAX :
            LET P(4)=UMAX
      4210  GOSUB 8900 : REM LABEL SUBROUTINE
      4220  PR#0
(BD)  4230  GOTO 4000


(BE)  4700  REM PLOT LOAD EXTENSION CURVE
(BF)  4710  IF PL=0 THEN XSC=2250/EMAX ELSE XSC=1500/EMAX
      4720  IF PL=1 THEN YSC=1500/EMAX ELSE YSC=100/LMAX
(BG)  4730  GOSUB 7200 : REM CALCULATE LOAD EXTENSION VALUES
(BH)  4740  IF PL=1 THEN RETURN
(BI)  4750  GOSUB 4900 : REM LABEL AXIS
(BJ)  4760  GOTO 4000


(BK)  4800  REM PLOT STRESS STRAIN CURVE
(BL)  4810  IF PL=0 THEN XSC=2250/STMAX ELSE XSC=1500/STMAX
      4820  IF PL=0 THEN YSC=1500/UMAX ELSE YSC=1000/STMAX
      4830  GOSUB 7400 : REM CALCULATE STRESS STRAIN VALUES
(BM)  4840  IF PL=1 THEN RETURN
(BN)  4850  GOSUB 5100 : REM LABEL AXIS
(BO)  4860  GOTO 4000


(BP)  4900  REM LABEL AXIS, LOAD EXTENSION
      4910  LET A$="EXTENSION (mm)."
      4920  LET B$="LOAD ("+L$+")"
      4930  LET C$=STR$(EMAX)
      4940  LET D$=STR$(LMAX)
      4950  LET P(1)=EMAX
      4960  LET P(2)=LMAX
      4970  LET P(3)=P(1)
      4980  LET P(4)=P(2)
      4990  IF PL=1 THEN RETURN
      5000  GOSUB 5500 : REM LABEL AXIS LARGE SCALE
```

```
      5010  RETURN


(BQ)  5100  REM LABEL AXIS, STRESS STRAIN
      5110  LET A$="STRAIN"
      5120  LET B$="STRESS ("+U$+")"
      5130  LET C$=STR$(STMAX)
      5140  LET D$=STR$(UMAX)
      5150  LET P(1)=STMAX
      5160  LET P(2)=UMAX
      5170  LET P(3)=P(1)
      5180  LET P(4)=P(2)
      5190  IF PL=1 THEN RETURN
      5200  GOSUB 5500 : REM LABEL AXIS LARGE SCALE
      5210  RETURN


(BR)  5500  REM LABEL AXIS LARGE SCALE
      5510  GOSUB 7000
      5520  PRINT "AS; 1500,10,16,0,"+A$+"&AK"
      5530  GOSUB 7000
      5540  PRINT "AS; 100,1250,16,90,"+B$+"&AK"
      5550  GOSUB 7000
      5560  PRINT "AS; 4800,200,16,0,"+C$+"&AK"
      5570  LET P=4800
      5580  FOR N=0 TO 4
      5590  LET P=P-880 : LET P$=STR$(P)
      5600  LET P(1)=P(1)-(P(3)/5)
      5610  IF P(1)<.000001 THEN P(1)=0
      5620  PRINT "AS; "+P$+",150,16,0,"; P(1); "&AK"
      5630  NEXT N
      5640  GOSUB 7000
      5650  PRINT "AS; 150,3300,16,0,"+D$+"&AK"
      5660  LET P=3300
      5670  FOR N=0 TO 4
      5680  LET P=P-600 : LET P$=STR$(P)
      5690  LET P(2)=P(2)-(P(4)/5)
      5700  IF P(2)<0.000001 THEN P(2)=0
      5700  PRINT "AS; "+P$+",150,16,0,"; P(2); "&AK"
      5710  NEXT N
      5720  PR#0
      5730  RETURN


(BS)  7000  REM CHARACTERS SUBROUTINE
      7010  PRINT "TE"
```

```
        7020  PRINT "EH;"
        7030  PRINT "EB;&"
        7040  PRINT "IN&SP; 1$DF; 1,2&AP; 300,0,0,-3"
        7050  RETURN

(BT)    7100  REM CALCULATE LOAD EXTENSION VALUES
        7110  LET X1=0 : LET Y1=0
        7120  LET SP=1
        7130  IF J>100 THEN SP=2
        7140  IF J>500 THEN SP=5
        7150  FOR N=0 TO J STEP SP
        7160  IF E3(N)=0 THEN GOTO 7310
        7170  LET X=((E3(N)/100)*L7)*XSC
        7180  LET Y=L3(N)*YSC
        7190  LET X=X-X1 : LET Y=Y-Y1
        7200  GOSUB 7250 : REM PLOT VALUES
        7210  NEXT N
        7220  RETURN


(BU)    7250  REM PLOT SUBROUTINE
        7260  LET X=X+X2 : LET Y=Y+Y2
        7270  LET X$=STR$(X) : LET Y$=STR$(Y)
        7280  LET A$="RP; "+X$+","+Y$+",2"
        7290  PRINT A$
        7300  LET Y1=Y1+Y : LET X1=X1+X
        7310  LET X2=X-INT(X) : LET Y2-Y-INT(Y)
        7320  RETURN


(BU)    7400  REM CALCULATE STRESS STRAIN VALUES
        7410  LET X1=0 : LET Y1=0
        7420  LET SP=1
        7430  IFJ>100 THEN LET SP=2
        7440  IF J>500 THEN LET SP=5
        7450  FOR N=0 TO J STEP SP
        7460  IF E3(N)=0 THEN GOTO 7520
        7470  LET X=(E3(N)/100)*XSC
        7480  LET Y=L3(N)/(W*G)
        7490  LET Y=Y*YSX
        7500  LET X=X-X1 : LET Y=Y-Y1
        7510  GOSUB 7250
        7520  NEXT N
        7530  RETURN
```

```
(BW)  8000  REM SCALE AXIS
      8010  IF L<5 THEN LMAX=5 : GOTO 8100
      8020  IF L<10 THEN LMAX=10 : GOTO 8100
      8030  IF L<15 THEN LMAX=15 : GOTO 8100
      8040  IF L<20 THEN LMAX=20 : GOTO 8100
      8050  IF L<25 THEN LMAX=25 : GOTO 8100
      8060  IF L<50 THEN LMAX=50 : GOTO 8100
      8070  IF L<100 THEN LMAX=100 : GOTO 8100
      8080  IF L<150 THEN LMAX=150 : GOTO 8100
      8090  LMAX=200
      8110  LET LNT=(E/100)*L7
      8105  IF LNT <8 THEN LET EMAX=8 : GOTO 8220
      8110  IF LNT <20 THEN LET EMAX=20 : GOTO 8220
      8120  IF LNT <50 THEN LET EMAX=50 : GOTO 8220
      8130  IF LNT <100 THEN LET EMAX=100 : GOTO 8220
      8140  IF LNT <200 THEN LET EMAX=200 : GOTO 8220
      8150  IF LNT <300 THEN LET EMAX=300 : GOTO 8220
      8160  IF LNT <400 THEN LET EMAX=400 : GOTO 8220
      8170  IF LNT <500 THEN LET EMAX=500 : GOTO 8220
      8180  IF LNT <600 THEN LET EMAX=600 : GOTO 8220
      8190  IF LNT <700 THEN LET EMAX=700 : GOTO 8220
      8200  IF LNT <800 THEN LET EMAX=800 : GOTO 8220
      8210  LET EMAX =850
      8220  LET ST=E/100
      8230  IF ST<0.25 THEN STMAX=0.25 GOTO 8300
      8240  IF ST<0.5 THEN STMAX=0.5 GOTO 8300
      8250  IF ST<1 THEN STMAX=1 GOTO 8300
      8260  IF ST<6 THEN STMAX=6 GOTO 8300
      8270  IF ST<10 THEN STMAX=10 GOTO 8300
      8280  IF ST<20 THEN STMAX=20 GOTO 8300
      8290  LET STMAX=100
      8310  IF U<0.01 THEN UMAX=0.01 : GOTO 8395
      8320  IF U<0.05 THEN UMAX=0.05 : GOTO 8395
      8330  IF U<0.1 THEN UMAX=0.1 : GOTO 8395
      8340  IF U<0.5 THEN UMAX=0.5 : GOTO 8395
      8350  IF U<1 THEN UMAX=1 : GOTO 8395
      8360  IF U<5 THEN UMAX=5 : GOTO 8395
      8370  IF U<10 THEN UMAX=10 : GOTO 8395
      8380  IF U<15 THEN UMAX=15 : GOTO 8395
      8390  UMAX=100
      8395  RETURN


(BX)  8400  REM PLOT AXIS LARGE SCALE
      8410  PR#4
      8420  PRINT "IN"
```

```
8430  PRINT "RP;200,200,0"
8440  PRINT "RP;0,1500,0"
8450  PRINT "RP;0,-1500,2"
8460  PRINT "RP;2250,0,0"
8470  PRINT "RP;0,-25,0"
8480  PRINT "RP;0,25,3"
8490  FOR N=0 TO 4
8500  PRINT "RP;-450,0,0"
8510  PRINT "RP;0,-25,2"
8520  PRINT "RP;0,25,3"
8530  NEXT N
8540  PRINT "RP;-25,0,2"
8550  PRINT "RP;25,0,3"
8560  FOR N=0 TO 4
8570  PRINT "RP;0,300,0"
8580  PRINT "RP;-25,0,2"
8590  PRINT "RP;25,0,3"
8600  NEXT N
8610  PRINT "RP;0,-1500,0"
8620  RETURN


(BY)  8700  REM PLOT SMALL AXIS
      8710  PRINT "RP;0,100,0"
      8720  PRINT "RP;0,-100,2"
      8730  PRINT "RP;1500,0,0"
      8740  PRINT "RP;0,-20,2"
      8750  PRINT "RP;0,20,3"
      8760  FOR N=0 TO 4
      8770  PRINT "RP;-300,0,0"
      8780  PRINT "RP;0,-20,2"
      8790  PRINT "RP;0,20,3"
      8800  NEXT N
      8810  PRINT "RP;-20,0,2"
      8820  PRINT "RP;20,0,3"
      8830  FOR N=0 TO 4
      8840  PRINT "RP;0,200,0"
      8850  PRINT "RP;-20,0,2"
      8860  PRINT "RP;20,0,3"
      8870  NEXT N
      8880  RETURN


(BZ)  8900  REM LABEL SMALL AXIS
      8910  IF PL=0 THEN PRINT "AS;1000,2500,8,0,"+A$++&AK"
            ELSE PRINT "AS;1000,10,8,0,"+A$+"&AK"
```

```
8920  GOSUB 7000
8930  IF PL=0 THEN PRINT "A$;100,3000,8,90,"+B$+"&AK"
      ELSE PRINT "A$;100,500,8,90,"+B$+"&AK"
8940  GOSUB 7000
8950  IF PL=0 THEN PRINT "A$;3400,2600,8,0,"+C$+"&AK"
      ELSE PRINT "A$;3400,200,8,0,"+C$+"&AK"
8960  LET P=3400
8970  FOR N=0 TO 4
8980  LET P=P-600
8990  LET P$=STR$(P)
9000  LET P(1)=P(1)-(P(3)/5)
9010  IF P(1)<0.00001 THEN P(1)=0
9020  IF PL=0 THEN PRINT "A$;";P$;",2600,8,0,";P(1);"&AK"
      ELSE PRINT "A$;"+P$+",200,8,0,"+P(1)+"&AK"
9030  NEXT N
9040  GOSUB 7000
9045  IF PL=0 THEN PRINT "A$;150,4800,8,0,"+D$+"&AK"
      ELSE PRINT "A$;150,2300,8,0"+D$+"&AK"
9050  LET P=2300
9060  IF PL=0 THEN P=4700
9070  FOR N=0 TO 4
9080  LET P=P-400
9090  LET P$=STR$(P)
9100  LET P(2)=P(2)-(P(4)/5)
9110  IF P(2)<0.00001 THEN P(2)=0
9120  PRINT "A$;150,"+P$+",8,0,"+P(2)+"&AK"
9130  NEXT N
9140  RETURN
```

2.1 Key to the tensile testing programme.

(A) This line defines the switch to turn the printer on and off.

(B) This line dimensions the array, (**L3()**) for the storage of load data from the 500M.

(C) This line dimensions the array, (**E3()**) for the storage of extension data from the 500M.

(D) This line sets the maximum number of data points collected from the 500M, (**M3**) to 999.

(E) This line sets the 500M scaling values (**L1**, **L2**).

(F) This line dimensions the arrays (**M()**, **N()**, **U()**, **V()**, **P()**, **B()**) for results storage and analysis.

(G) These lines print the initial display screen, figure A1.2.

(H) These lines prompt for another test, figure A1. 2.

(I) These lines print the load cell selection screen, figure A1.3.

(J) These lines define the variables (**L$**), the units of load, N or KN, (**U$**), the units of stress Nmm^{-2} or $KNmm^{-2}$ and (**C2**) the load cell variable, 100 or 20 dependent on the selected load cell.

(K) These lines print the load range dependent on the selected load cell, figure A1.3.

(L) These lines print the initial input values screen, figure A1.4.

(M) This line allows the sample width, (**W**) to be input.

(N) This line allows the sample length, (**L7**) to be input.

(O) This line allows the sample thickness, (**G**) to be input.

(P) This line allows the test reference, (**R$**) to be input.

(Q) This line allows the test speed, (**R1$**) to be input.

(R) This line switches the line printer on or off by defining the variable (**PR**). If **PR=1** then the printer is on, if **PR=0** then the printer is off.

(S) This line sets the test count variable (**T**) to 1.

(T) If the printer has been switched on (**PR=1**) and the test is the first (**T=1**) then this line first calls the subroutine to switch on the printer followed by the header printing subroutine, figure A1.5.

(U) These lines print the results screen, figure A1.6.

(V) These lines collect the data from the 500M. They are an unchanged part of the original software. The routine assumes that the RS232C interface is in slot 2 of the computer. The load data is stored in the array (**L3(**)) and the extension data in the array (**E3()**).

(W) These lines calculate and round off the value for the stress (**U**).

(X) These line calculate and round off the value for the extension (**E**) mm.

(Y) These line print the calculated results for the peak load (**L**), the extension (**E**) and the stress (**U**), figure A1.7.

(Z) These lines prompt to accept the calculation results, figure A1.7.

(AA) These lines store the results in the storage arrays (**L()**, **E()**, **M()**, **N()**, **U()**).

(AB) These lines calculate the modulus (**MO**) and store it in its storage array (**U()**).

(AC) If the printer has been selected then this line calls the printer on subroutine and then calls the subroutine to print the results under the correct heading.

(AD) This line calls the plotting menu subroutine, figure A1.8.

(AE) These lines prompt for another test.

(AF) If another test is selected then this line allows a new sample width (**W**) and thickness (**G**) to be input.

(AG) If another test is not selected then these lines call the statistics calculation subroutine.

(AH) This is the printer on subroutine.

(AI) This is the printer off subroutine.

(AJ) This is the header printing subroutine, figure A1.5.

(AK) This is the results tabulation subroutine which prints the test results under the correct headings, figure A1.5.

(AL) This is the statistics printing subroutine

(AM) These lines print the header for the statistics subroutine.

(AN) These lines calculate the statistics for the load data. The header is printed, the stored data in the array (**L()**), is transfered to the calculation array (**B()**) and the calculation subroutine accessed. The statistics for the extension, modulus and stress are all calculated in the same way.

(AM) This subroutine calculates the statistics. The maximum, (**HIGH**), minimum, (**LOW**), average (**AVE**), and standard deviation (**DVE**) are all calculated and printed by this subroutine.

(AN) This is the results plotting subroutine.

(AO) These line print the plotting menu, figure A1.8.

(AP) This line calls the subroutines to plot the load extension graph.

(AQ) This line calls the subroutines to plot the stress strain graph.

(AR) This line selects the subroutine to plot both graphs, figure A1.9.

(AS) This line returns to the main programme.

(AT) This subroutine controls the plotting of the twin curves.

(AU) This line calls the subroutine to plot the small axis.

(AV) This line calls the subroutine to calculate and plot the load extension curve.

(AW) This line calls the plot small axis subroutine to plot the second set of axis.

(AX) This line calls the subroutine to calculate and plot the stress strain curve.

(AY) These lines define the axis lables, (**A$**, **B$**, **C$**, **D$**,) for the load extension plot.

(AZ) This line calls the label axis subroutine.

(BA) These lines define the axis lables, (**A$**, **B$**, **C$**, **D$**,) for the stress strain plot.

(BB) This line calls the label axis subroutine.

(BC) This line returns to the plotting menu, figure A1.8.

(BD) This subroutine calculates and plots the load extension curve.

(BE) These lines calculate the scaling values for the X and Y axis, (**HSC**, **VSC**) depending on the scale of the plot selected (**PL**).

(BF) This line calls the plotting subroutine.

(BG) If small scale axis were selected then the programme returns to the required subroutine.

(BH) For large scale axis the label axis subroutine is called.

(BI) This line returns the programme to the main menu, figure A1.8.

(BJ) This subroutine calculates and plots the stress strain curve.

(BK) These lines calculate the scaling values for the X and Y axis, (**HSC**, **VSC**)

depending on the scale of the plot selected (**PL**).

(BL) This line calls the plotting subroutine.

(BM) If small scale axis were selected then the programme returns to the required subroutine.

(BN) For large scale axis the label axis subroutine is called.

(BO) This line returns the programme to the main menu, figure A1.8.

(BP) This subroutine lables the large scale load extension curve. It defines the axis lables, (**A$**, **B$**, **C$**, **D$**) and the maximum X and Y values (**EMAX**, **LMAX**).

(BQ) This subroutine lables the large scale stress strain axis. It defines the axis lables, (**A$**, **B$**, **C$**, **D$**) and the maximum X and Y values (**STMAX**, **UMAX**).

(BR) This subroutine lables the large scale axis.

(BS) This subroutine switches the plotter into the mode to plot characters.

(BT) This subroutine calculates the load extension values.

(BU) This subroutine plots the curve on the axis.

(BV) This subroutine calculates the stress strain values.

(BW) This subroutine scales the maxima for the stress strain and load extension curves.

(BX) This subroutine plots the large scale axis.

(BY) This subroutine plots the small scale axis.

(BZ) This subroutine plots the lables on the small scale axis.

3. Use of the tensile testing programme.

On first running the programme, the initial screen is printed, figure A1.2, along with the prompt for another test, pressing the 'Y' key continues the programme and pressing 'N' terminates it. The programme then prompts for which strain gauge is in use, 2500Kg or 100N. Pressing the '1' key selects the 2500Kg cell and pressing the '2' key selects the 100N cell, figure A1.3. The limits of the selected strain gauge are then printed on the monitor along with a prompt for any key to be pressed, figure A1.3. The programme then executes the initial input routine, figure 4, where the initial setup conditions of the 500M are recorded. At this stage the programme requires 7 inputs, the sample length (mm), sample width (mm), sample thickness (mm), test reference (60 characters), test speed (mm/Min) and hard copy (Y/N), the return key must be pressed after entering all these values. The header information is then printed on the line printer, figure A1.5. The data from the 500M is then collected and displayed on the monitor, figure A1.6, pressing the strain key of the 500M starts the data collection and pressing the zero key terminates it. When the data has been collected the results are then calculated and a prompt to accept the data given, figure A1.7, at this point the data can be rejected from the statistical analysis for any reason. If the data is accepted then

the results are printed on the printer, figure A1.5, if the data is rejected then the programme goes to a point where a new test can be started. The programme now prompts for a plot of the load deflection curve, stress strain curve or both curves on the X Y plotter, figure A1.8, if selected a plot is produced, figure A1.9. If not selected then the programme then prompts for another test. If another test is selected then the new sample width and thickness can be input, the programme then proceeds as before. If another test is not required then the programme calculates the maximum, minimum, average and standard deviation of the collected results and prints this on the line printer, figure A1.5. The programme then returns to the begining for another batch of results. figure A1.10 illustrates the use of this programme in a simplified form.

Table 1. Main programme variables.

Variable	Function
Arrays	
L3()	Load data storage.
E3()	Deflection data storage.
L()	Peak load data storage.
E()	Extension data storage.
M()	Thickness data storage.
N()	Width data storage.
U()	Array for modulus storage.
V()	Array for stress storage.
B()	Array for statistical analysis.
Strings	
E$	Units of extension (mm).
L$	Units of load (KN or N).
U$	Units of stress (KN/mm^2 or N/mm^2)
R$	Sample reference.
R1$	Test speed.
LD$	Load value from 500M.
EH$	Extension value from 500M
F$	Control A character.
Decimals	
M3	Sets maximum number of data points
L1	Scale value for 500M
L2	Scale value for 500M
C2	Load cell variable (20 or 100).
L7	Sample length.
W	Sample width.
G	Sample thickness.
PR	Sets printer status 1=on, 0=off.
T	Test number.
F	500M status control variable.
J	Data collected variable 1-1000
L	Peak load.
U	Stress.
S	Strain.
MO	Modulus.
E	Elongation.
HIGH	Maximum value.
LOW	Minimum value.
AVE	Average value.
DVE	Standard deviation.

Table 2. Plotting subroutine variables.

Variable	Function
Strings	
A$	X axis label
B$	Y axis label
C$	X axis maximum value label
D$	Y axis maximum value label
P$	General axis division label
H$	Character for X axis position
V$	Character for Y axis position.
Decimals.	
PL	Plot scale value, 0=large, 1=small.
P1	Maximum deflection or stress
P2	Maximum load or strain
LMAX	Adjusted maximum load
LNT	Peak deflection
EMAX	Adjusted peak deflection.
ST	Strain.
STMAX	Adjusted strain value.
UMAX	Adjusted stress value.
HSC	X axis scaling value.
VSC	Y axis scaling value.
SP	Plotting step.
H	Numerical X axis position.
V	Numerical Y axis position.

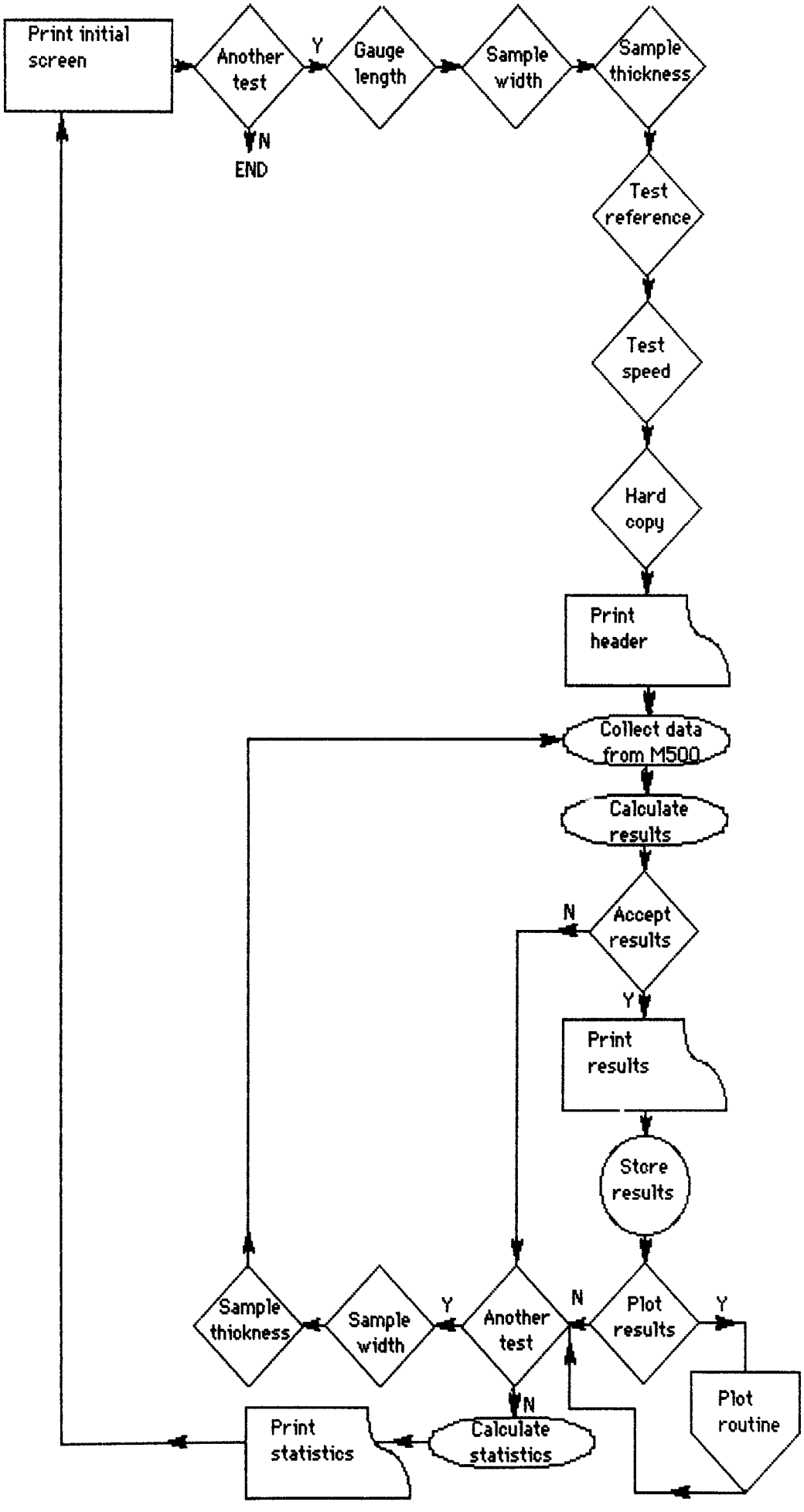


Figure A1.1. Simplified flow diagram of tensile programme.

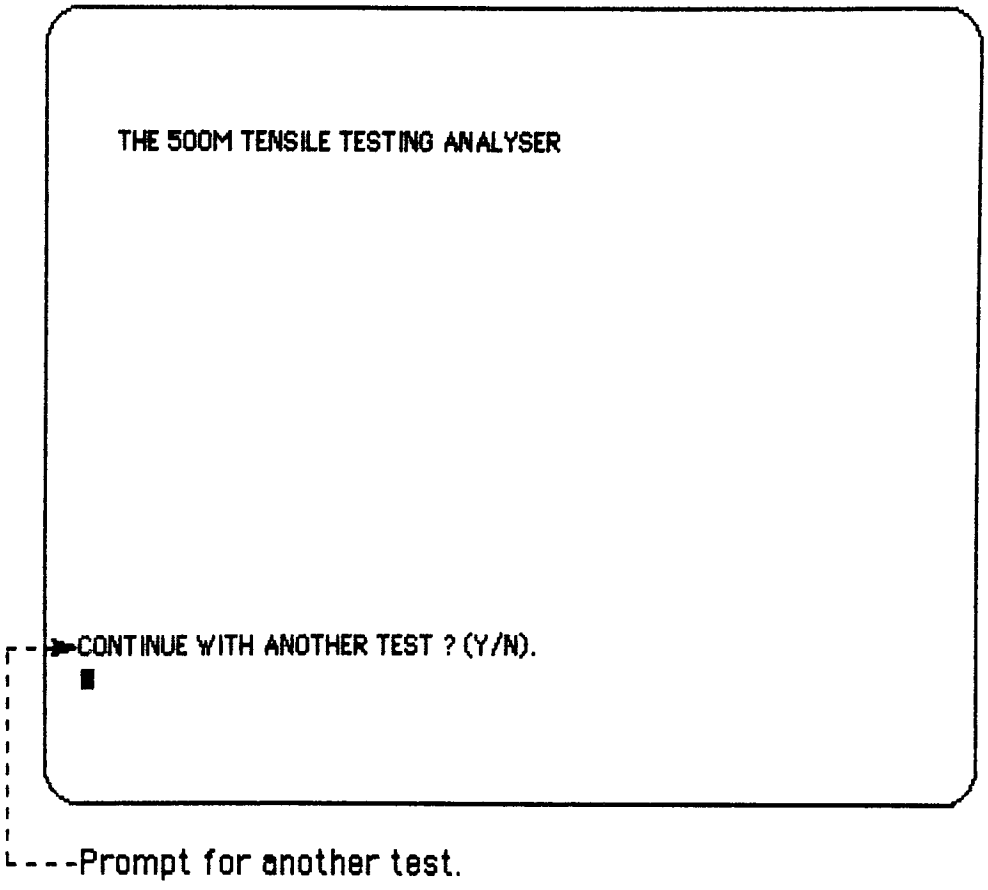


Figure A1.2. Initial display screen of the tensile testing programme.

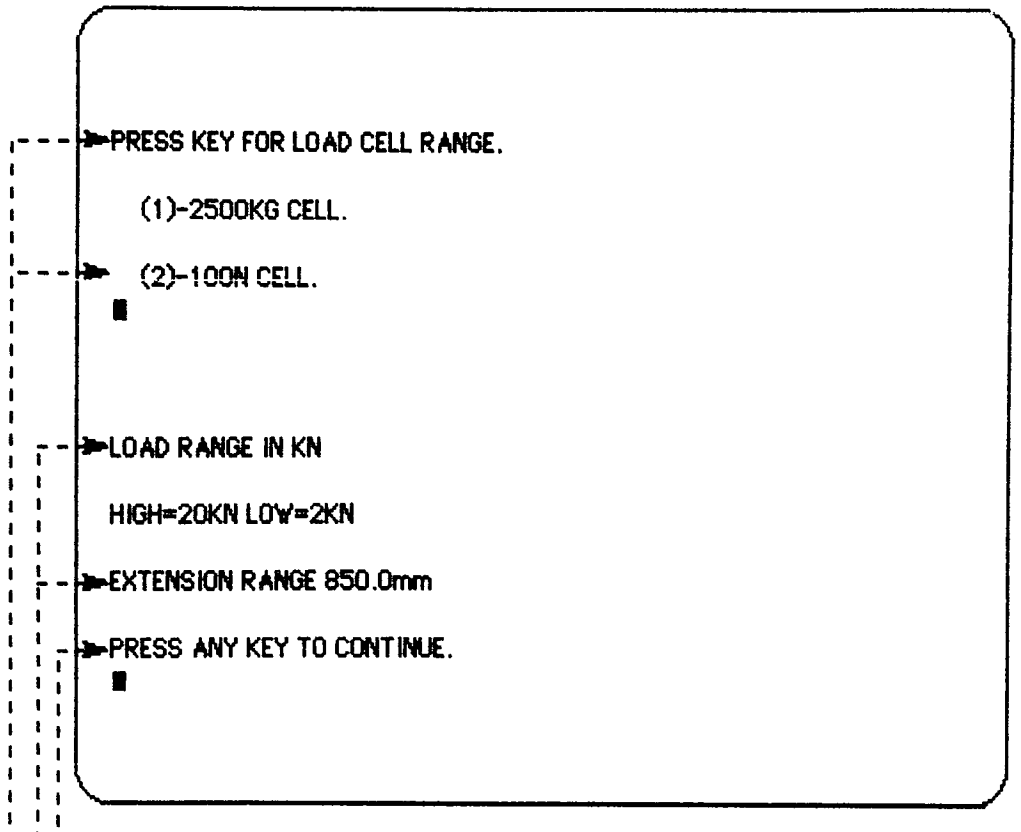


Figure A1.3. Load cell selection screen of the tensile testing programme.

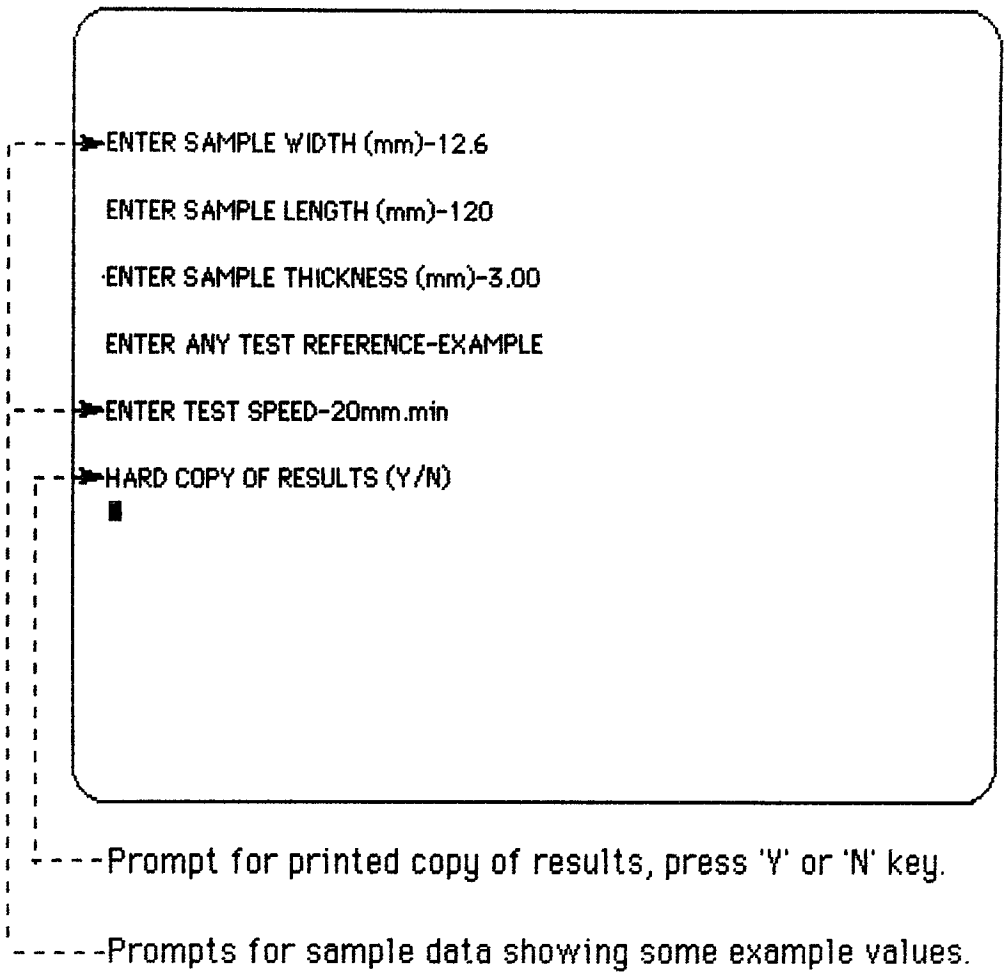


Figure A1.4. Screen for initial input values from the tensile testing programme.

****

TESTOMETRIC 500M ANALYSIS

****

SAMPLE LENGTH =120mm
TEST SPEED = 20mm/min

TEST REFERENCE = EXAMPLE

Test Number	Width (mm)	Thickness (mm)	Peak load (KN)	Strain	Elongation (%)	Stress (KN/mm^2)
1	12.6	3.00	1.57	0.79	79	0.41
2	12.61	2.57	1.59	0.85	85	0.42
3	12.59	2.58	1.58	0.82	82	0.48

500M TEST SERIES SUMMARY.

NUMBER OF TESTS = 3

LOAD ANALYSIS IN KN
HIGHEST =1.59
LOWEST = 1.57
AVERAGE=1.58
STD DVE =0.01

EXTENSION ANALYSIS %
HIGHEST =85
LOWEST =79
AVERAGE=82
STD DVE =3

MODULUS ANALYSIS IN KN/mm^2
HIGHEST =0.42
LOWEST =0.41
AVERAGE=0.415
STD DVE =0.17

STRESS ANALYSIS IN KN/mm^2
HIGHEST =0.48
LOWEST =0.41
AVERAGE=0.43
STD DVE =0.04

Figure A1.5. Printed output from the tensile testing programme.

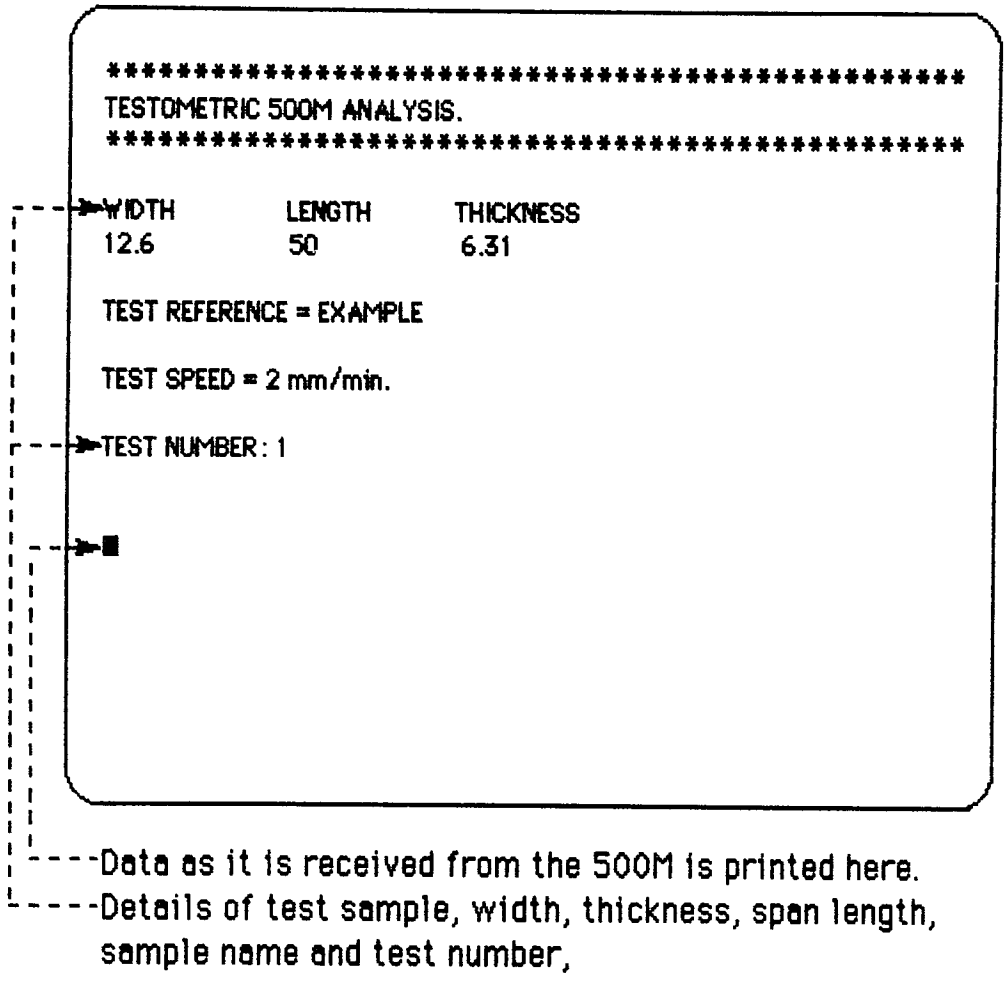


Figure A1.6. Data collection screen from the tensile testing programme.

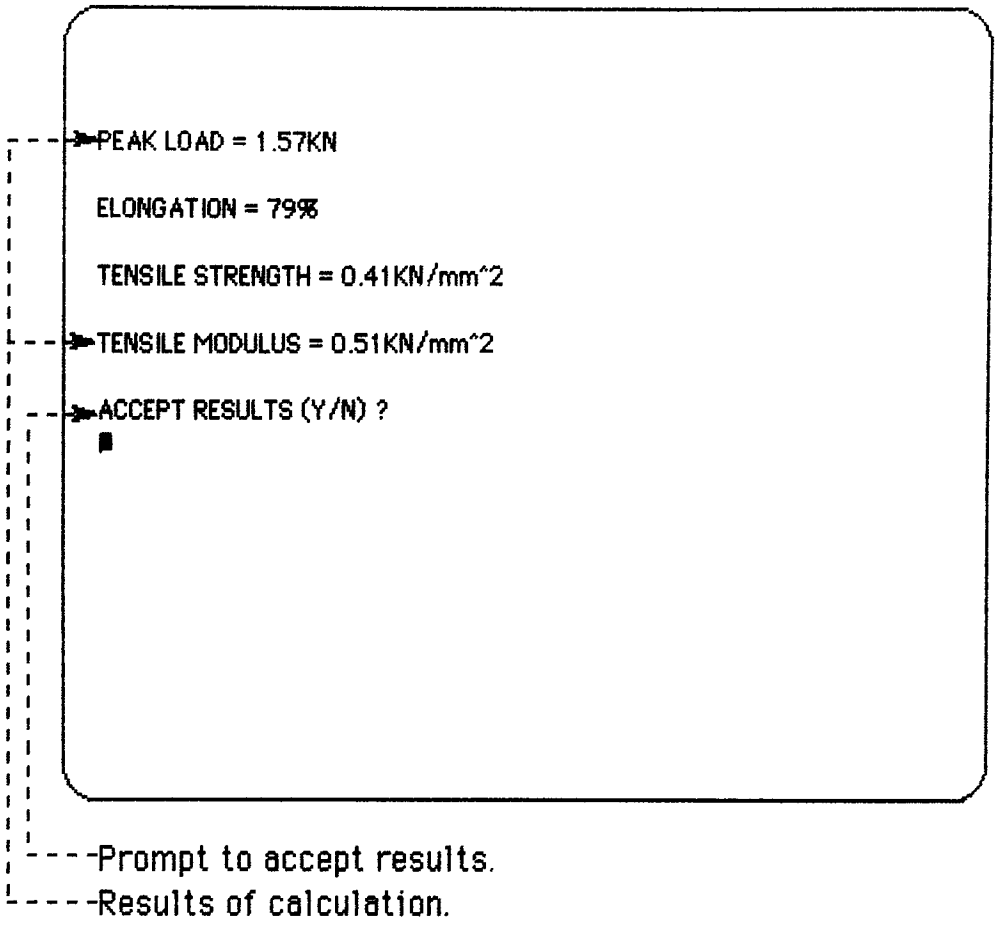


Figure A1.7. Results screen of the tensile testing programme.

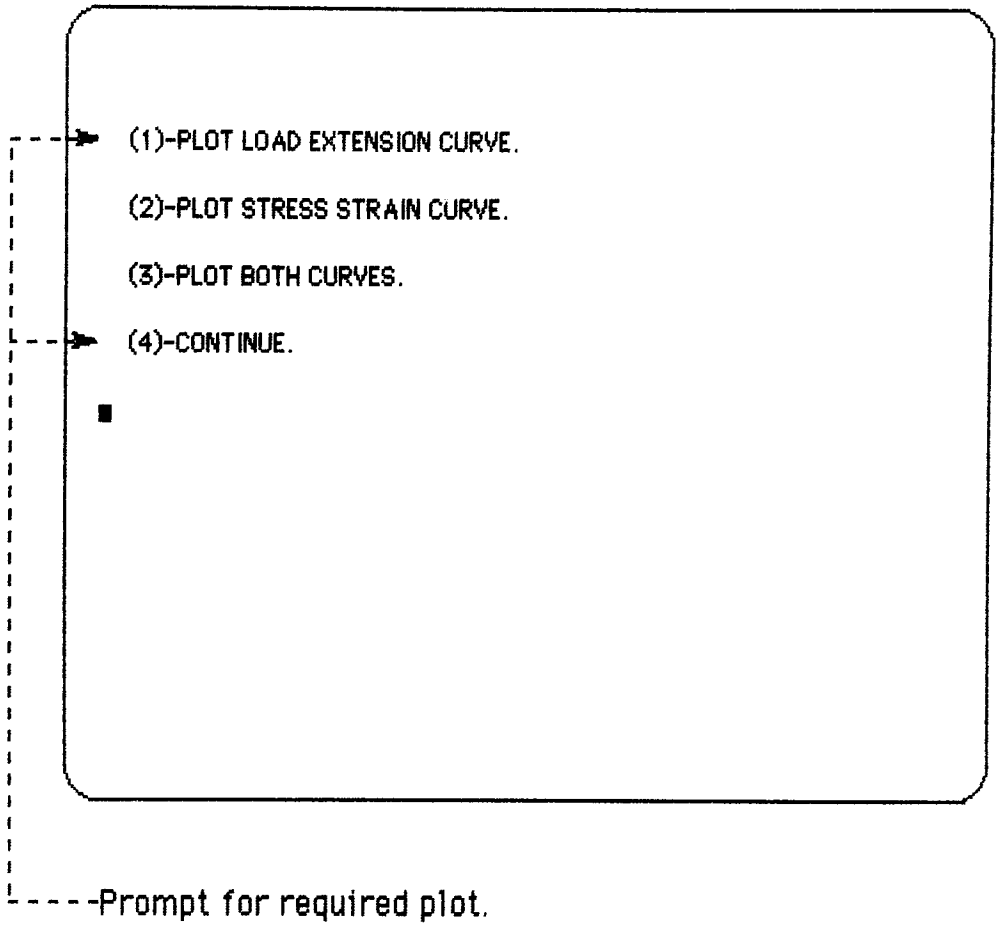


Figure A1.8. The plotting menu from the tensile testing programme.

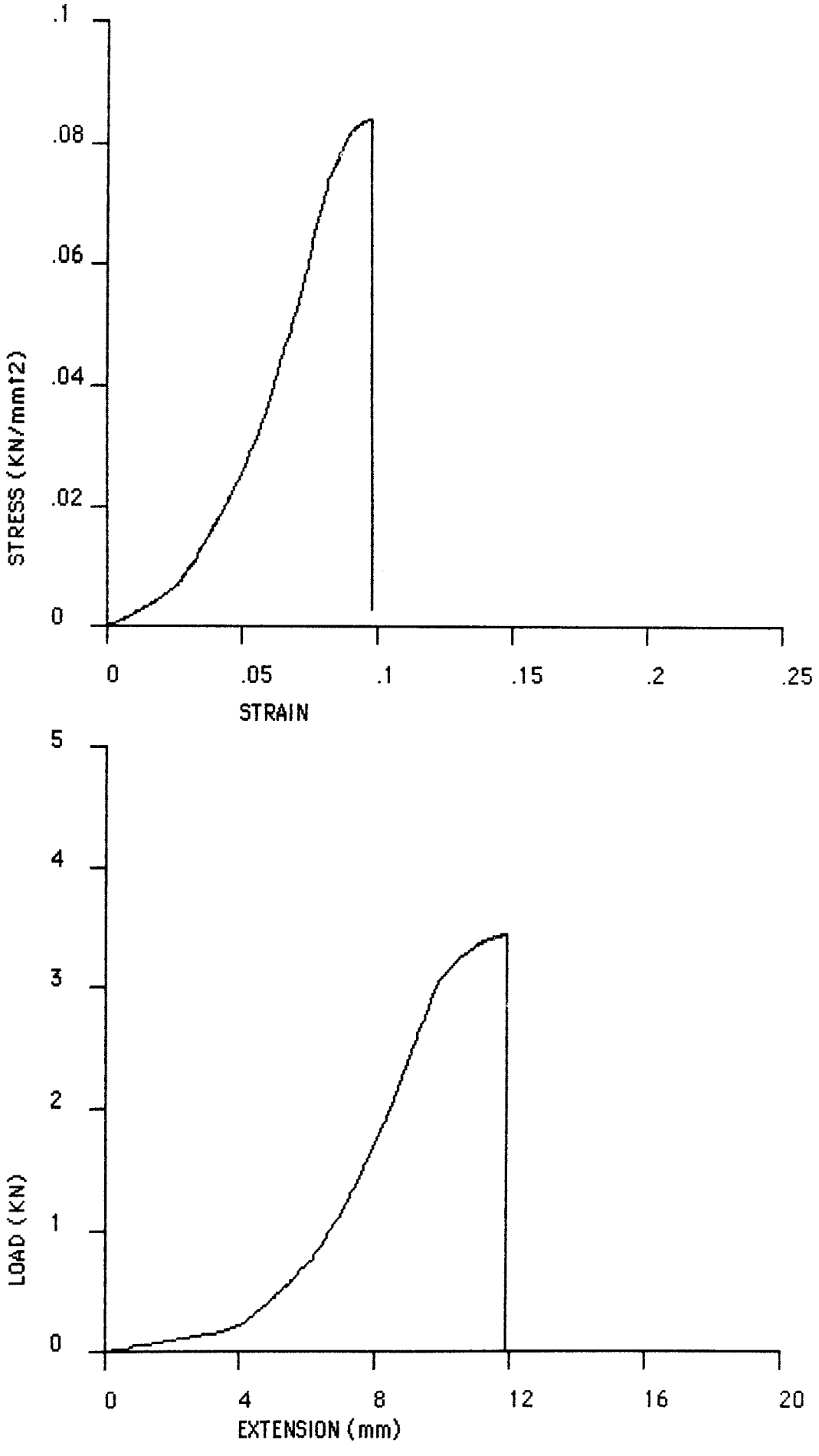


Figure A1.9. Plotted output from the tensile testing programme.

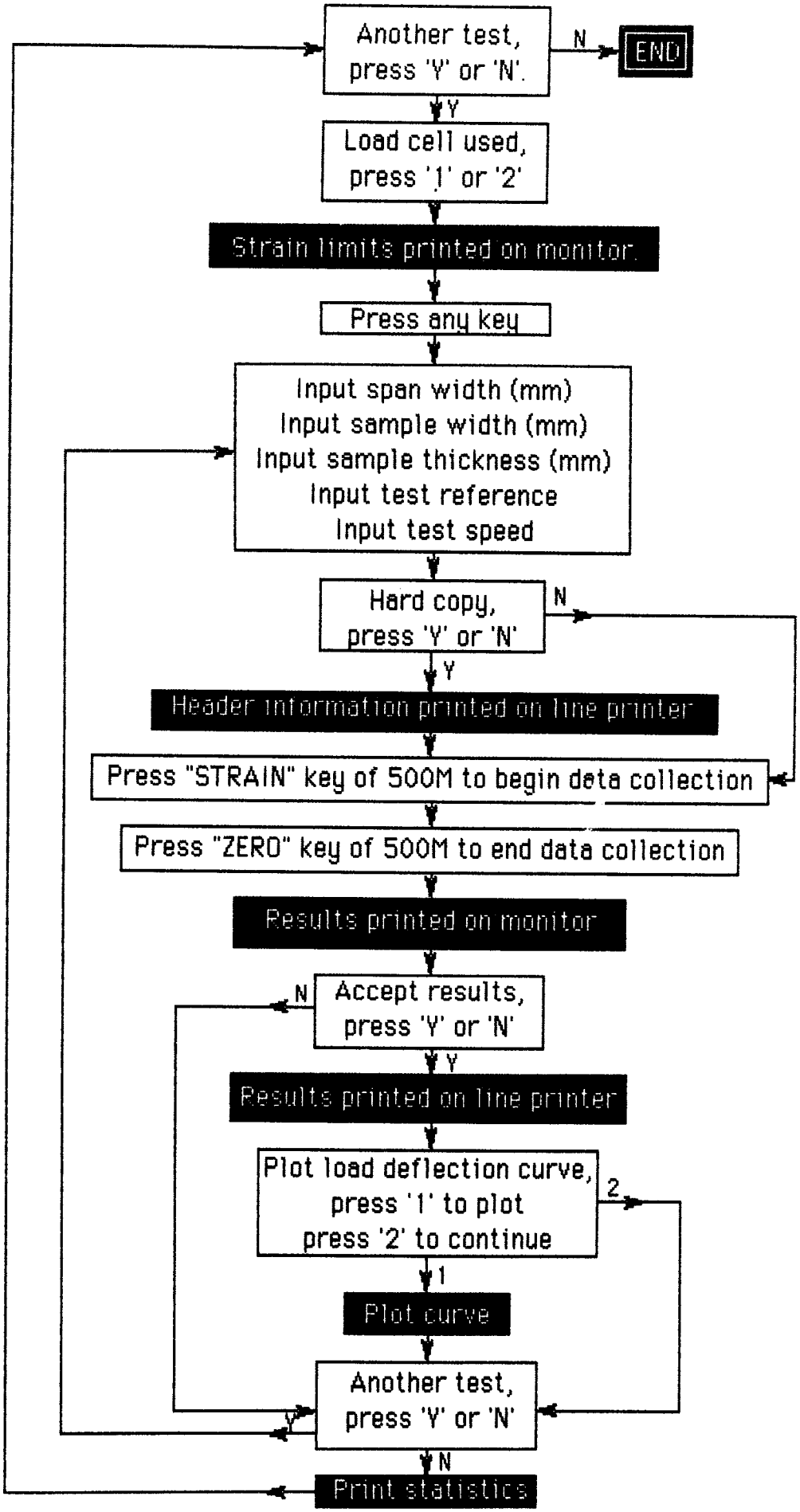


Figure A1.10. Flow diagram showing the use of the tensile testing programme.

Appendix 2

Flexural testing

Programme.

1. Flexural testing programme.

The flexural testing programme has been designed to interface with the Testometric 500M tensometer. The programme is a modified version of the tensile testing programme (Appendix 1). The programme collects the raw data of load verses deflection and from this calculates the peak load, deflection, flexural strength and flexural modulus for each sample. For each batch of samples the programme calculates the highest, lowest, average and standard deviation of the load, deflection, flexural strength and flexural modulus. The programme tabulates and prints the results on a dot matrix printer as well as plotting the load deflection curve on an X Y plotter. The programme runs on an Apple IIe computer under Applesoft basic using an RS232C interface for communication to the 500M. A simplified flow diagram for the programme is shown in figure A2.1. The variables used in the main programme are listed in table A2.1, the variables used in the plotting subroutine in table A2.2.

2. Programme listing.

```
      10    REM FLEXURAL PROGRAMME
      20    REM BY I.R.SURRY
      30    LET E$="mm" : REM UNITS OF EXTENSION
      40    LET D$=CHR$(13) + CHR$(4) : PRINT D$;"PR#0" : REM
            PRINTER SWITCH
(A)   50    DIM L3(1000) : REM LOAD ARRAY
(B)   60    DIM E3(1000) : REM EXTENSION ARRAY
(C)   70    LET M3=999
(D)   80    LET L1=100 : LET L2=1000
      90    LET E1=20
(E)   100   DIM L(30), E(30), M(30), N(30), FS(30), FM(30), B(30)
(F)   150   REM FIND LOAD CELL
      160   HOME
      170   PRINT : PRINT
      180   PRINT TAB(5);"THE 500M FLEXURAL TEST ANALYSER."
(G)   190   VTAB(22) : PRINT "CONTINUE WITH ANOTHER TEST?
            (Y/N)."
      200   GET A$
      210   IF A$="Y" THEN GOTO 240
      220   IF A$="N" THEN STOP
      230   GOTO 200
      240   HOME
(H)   250   PRINT : PRINT
      260   PRINT "PRESS KEY FOR LOAD CELL RANGE."
      270   PRINT
      280   PRINT TAB(4);"(1)-2500KG CELL."
      290   PRINT
```

```
      300   PRINT TAB(4);"(2)-100N CELL."
      310   GET A$
(I)   320   IF A$="1" THEN LET L$="KN" : LET U$="KN/mm^2" :
            LET C2=20; GOTO 350
      330   IF A$="2" THEN LET L$="N" : LET U$="N/mm^2" : LET
            C2=100 : GOTO 350
      340   GOTO 310


(J)   350   PRINT : PRINT "LOAD RANGE IN ";L$
      360   PRINT
      370   PRINT "HIGH=";C2;" ";L$,"LOW=";C2/10;" ";L$
      380   PRINT : PRINT "EXTENSION RANGE 850.0";E$
      390   PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
      400   GET A$
      410   HOME
(K)   420   PRINT : PRINT
(L)   430   PRINT : INPUT "ENTER SPAN LENGTH (mm)-";L7
(M)   440   PRINT : INPUT "ENTER SAMPLE WIDTH (mm)-";W
(N)   450   PRINT : INPUT "ENTER SAMPLE THICKNESS (mm)-";G
(O)   460   PRINT : INPUT "ENTER SAMPLE REFERENCE-";R$
(P)   470   PRINT : INPUT "ENTER TEST SPEED-";R1$
(Q)   472   PRINT : INPUT "HARD COPY OF RESULTS (Y/N)-";A$
      474   IF A$="Y" THEN PR=1
      480   LET T=1
(R)   490   IF PR=1 AND T=1 THEN GOSUB 3500 : REM PRINTER
            SWITCH
(S)   500   IF PR=1 AND T=1 THEN GOSUB 3600 : REM PRINT
            HEADER
(T)   510   FOR N=1 TO 40 : PRINT "*"; : NEXT N
      520   PRINT : INVERSE
      530   HTAB(7) : PRINT "  TESTOMETRIC 500M ANALYSIS " :
            NORMAL
      540   FOR N=1 TO 40 : PRINT "*"; : NEXT N : PRINT
      550   PRINT "  WIDTH  LENGTH   THICKNESS" : PRINT
      560   HTAB(7) : PRINT W; : HTAB(17) : PRINT L7; : HTAB(30) :
            PRINT G
      570   PRINT : PRINT "  TEST REFERENCE = ";R$
      580   PRINT : PRINT "  TEST SPEED = ";R1$;"mm/min"
      590   PRINT
      600   PRINT "TEST NUMBER : ";T
      610   PRINT : PRINT


(U)   650   LET F=0 : LET J=0
      651   LET D$= CHR$(13) + CHR$(4) : PRINT D$;"PR#0"
```

```
      655   LET F$="" : REM CTRL-A
      660   PRINT D$;"PR#2" : PRINT F$;"F4" : FOR N=1 TO 20 :
            PRINT " "; : NEHT N : PRINT
      670   PRINT D$;"IN#2"
      680   UTAB(22) : PRINT "D" : PRINT F$;"00" : UTAB(22) :
      INPUT LD$, EH$, A$ : PRINT F$;"01"
      690   IF F=1 THEN GOTO 770
      700   IF A$="F" THEN GOTO 680
      710   IF A$="1" THEN LET A=L1 : GOTO 750
      720   IF A$="H" THEN LET A=L2 : GOTO 750
      730   GOTO 680
      740   PRINT CHR$(7) : PRINT "=> DATA TIMEOUT <=" : GOTO
      750   LET F=1
      760   GOTO 680
      770   IF A$="F" THEN GOTO 810
      780   IF J>M3 THEN GOTO 680
      785   IF UAL (LD$) =0 THEN GOTO 680
      786   IF UAL (EH$) =0 THEN GOTO 680
      790   LET L3(J)=UAL (LD$) : LET E3(J)=UAL (EH$) : LET J=J+1
      800   GOTO 680
      810   LET F=0
      820   PRINT D$;"PR#2"
      830   UTAB(23)


850   PRINT D$;"IN#0" : PRINT D$"PR#0"
      860   POKE 34,15 : HOME : POKE 34,0

(U)   870   PRINT "============>> RESULTS <<============"
      880   LET J=J-1 : LET L=0
      890   FOR N=0 TO J : IF N > M3 THEN GOTO 920
      900   LET L3(N)=L3(N)/A : LET E3(N)=E3(N) * 100 / (E1*L7)
      910   IF L3(N) > L THEN LET L= L3(N)
      920   NEHT N
(W)   930   REM FLEHURAL STRENGTH
      940   LET FS=(3*L*L7)/(2*W*(G*G))
(H)   950   REM FLEHURAL MODULUS
      960   LET E=E3(J) : LET E=(INT(E*10))/20
      970   LET FM=(L7*L7*L7)/4*W*(G*G))
      975   LET FM=(L*E)/FM
(Y)   976   LET FS=(FS*10000)/10000
      977   LET FM=(FM*10000)/10000
(Z)   980   PRINT : PRINT "PEAK LOAD = ";L;L$
      990   PRINT : PRINT "DEFLECTION = ";E;"mm."
      1000  PRINT : PRINT "FLEHURAL STRENGTH = ";FS;U$
      1010  PRINT : PRINT "FLEHURAL MODULUS = ";FM
```

```
(AA)  1020  PRINT : PRINT "ACCEPT RESULTS (Y/N)?"
      1030  GET A$
      1040  IF A$="N" THEN GOTO 490
      1042  IF A$="Y" THEN GOTO 1050
      1045  GOTO 1030


(AB)  1050  LET L(T)=L : LET E(T)=E
      1060  LET M(T)=G : LET N(T)=W
      1070  LET FS(T)=FS : LET FM(T)=FM
(AC)  1080  IF PR=1 THEN GOSUB 3500 : REM PRINTER SWITCH
      1090  PRINT T; : REM TEST NUMBER
      1100  PRINT TAB(9);W; : REM WIDTH
      1110  PRINT TAB(17);G; : REM THICKNESS
      1120  PRINT TAB(27);L; : REM LOAD
      1130  PRINT TAB(34);E; : REM DEFLECTION
      1140  POKE 36,42 : PRINT FS;"  ";FM : REM FLEXURAL
            STRENGTH, FLEXURAL MODULUS
(AD)  1160  PRINT D$;"PR#0"
      1170  REM PLOTTER
      1180  LET X1=0 : LET Y1=0
      1190  LET X2=0 : LET Y2=0
      1200  TEXT
      1210  HOME
(AE)  1220  PRINT : PRINT
      1230  PRINT TAB(5);"(1)-PLOT LOAD DEFLECTION CURVE."
      1240  PRINT
      1250  PRINT TAB(5);"(2)-CONTINUE."
      1260  GET A$
      1270  IF A$="1" THEN GOTO 4000
      1280  IF A$="2" THEN GOTO 1300
      1290  GOTO 1260
      1300  HOME
      1310  PRINT : PRINT
(AF)  1320  PRINT TAB(5);"ANOTHER TEST (Y/N) ?"
      1330  GET A$
      1340  IF A$="N" THEN GOTO 1420 : REM STATISTICS
      1350  IF A$="Y" THEN GOTO 1370 : REM ANOTHER TEST
      1360  GOTO 1330
(AG)  1370  REM ANOTHER TEST
      1380  PRINT : PRINT
      1390  PRINT : INPUT "ENTER SAMPLE WIDTH (mm)-";W
      1400  PRINT : INPUT "ENTER SAMPLE THICKNESS (mm)-";G
      1410  GOTO 540
(AH)  1420  REM STATISTICS
      1430  LET D$=CHR$(13) + CHR$(4) : PRINT D$;"PR#0"
```

```
      1440  IF PR=1 THEN GOSUB 3500 : REM PRINTER SWITCH
      1450  FOR N=1 TO 80 : PRINT "-"; : NEXT N
      1460  PRINT : PRINT TAB(25);"500M TEST SERIES SUMMARY:"
      1470  PRINT : PRINT "NUMBER OF TESTS = ";T : PRINT
(AI)  1480  REM LOAD
      1490  FOR N=1 TO T : LET B(N)=L(N) : NEXT N
      1500  PRINT "LOAD ANALYSIS IN ";L$
      1510  GOSUB 3800 : STATISTICAL ANALYSIS AND PRINT
      1520  REM DEFLECTION
      1530  FOR N=1 TO T : LET B(N)=E(N) : NEXT N
      1540  PRINT "DEFLECTION ANALYSIS IN mm"
      1550  GOSUB 3800 : STATISTICAL ANALYSIS AND PRINT
      1560  REM FLEXURAL STRENGTH
      1570  FOR N=1 TO T : LET B(N)=FS(N) : NEXT N
      1580  PRINT "FLEXURAL STRENGTH ANALYSIS IN ";U$
      1590  GOSUB 3800 : STATISTICAL ANALYSIS AND PRINT
      1600  REM FLEXURAL MODULUS
      1610  FOR N=1 TO T : LET B(N)=FM(N) : NEXT N
      1615  PRINT "FLEXURAL MODULUS ANALYSIS IN ";L$
      1620  GOSUB 3800 : STATISTICAL ANALYSIS AND PRINT
      1630  PRINT D$;"PR#0"
      1640  PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
      1650  GET A$
      1660  HOME
(AJ)  1670  RUN


(AK)  3500  REM PRINTER SWITCH
      3510  PRINT D$;"PR#1"
      3520  RETURN


(AL)  3600  REM PRINT HEADER
      3610  FOR N=1 TO 80 : PRINT "*"; : NEXT N
      3620  PRINT : PRINT : INVERSE : HTAB(27) : PRINT "
            TESTOMETRIC 500M ANALYSIS  "
      3630  NORMAL
      3640  FOR N=1 TO 80 : PRINT "*"; : NEXT N
      3650  PRINT : PRINT TAB(20);"SPAN LENGTH = ";L;E$
      3660  PRINT : PRINT TAB (20); "TEST SPEED =
            ";R1$;"mm/min"
      3670  PRINT : PRINT "TEST REFERENCE = ";R$
      3680  FOR N=1 TO 80 : PRINT "-"; : NEXT N
      3690  PRINT "Test   Width Thickness  Peak  Deflection
            Flexural  Flexural"
      3700  PRINT "Number                      Load
```

```
        Strength Modulus"
 3710   PRINT TAB(9);"(mm)"; TAB(17);"(mm)";
 3720   IF C2=20 THEN PRINT TAB(27);"KN";
 3730   IF C2=100 THEN PRINT TAB(27);"N";
 3740   IF C2=20 THEN POKE 36,34 : PRINT "(mm)
        (KN/mm^2)"
 3750   IF C2=100 THEN POKE 36,34 : PRINT "(mm)
        (N/mm^2)"
 3760   PRINT D$;"PR#0"
 3770   HOME
 3780   RETURN


(AM) 3800   REM STATISTICAL ANALYSIS OF RESULTS
 3810   LET HIGH=0 : LET LOW=1E+7 : LET AVE=0
 3820   FOR I=1 TO T
 3830   IF E(I)>HIGH THEN HIGH=E(I)
 3840   IF E(I)<LOW THEN LOW=E(I)
 3850   LET AVE=AVE+E(I)
 3860   NEXT I
 3870   LET AVE=FIX((AVE/T)*10000)/10000
 3880   LET DVE=0
 3890   IF T<=1 THEN RETURN
 3900   FOR I=1 TO T
 3910   LET DVE=DVE + (E(I)-AVE)^2
 3920   NEXT I
 3930   LET DVE=SQR(DVE/(T-1))
 3940   LET DVE=FIX(DVE*1000)/1000
(AN) 3950   PRINT "HIGHEST=";HIGH
 3960   PRINT "LOWEST =";LOW
 3970   PRINT "AVERAGE=";AVE
 3980   PRINT "STD DVE=";DVE
 3990   RETURN


(AO) 4000   REM PLOTTER SUBROUTINE
(AP) 4010   GOSUB 5000 : REM SCALE AXIS
(AQ) 4020   PR#4
 4030   PRINT "IN"
 4040   PRINT "RP;200,200,0"
(AR) 4050   GOSUB 5300 : REM PLOT SMALL AXIS
 4060   PRINT "RP;0,-1000,0"
(AS) 4070   GOSUB 5500 : REM PLOT GRAPH
 4080   PRINT "TE"
 4090   PRINT "IN"
(AT) 4100   LET A$="DEFLECTION (mm)" : LET B$="LOAD ("+U$+")"
```

```
      4110  LET C$=STR$(EMAX) : LET D$=STR$(LMAX)
      4120  LET P(1)=EMAX : LET P(2)=LMAX
(AU)  4130  GOSUB 5700 : REM LABEL SUBROUTINE
(AU)  4140  PRINT "AS;1000,10,8,0,"+A$+"&AK"
      4150  GOSUB 5700
      4160  PRINT "AS;100,500,8,90,"+B$+"&AK"
      4170  GOSUB 5700
      4180  PRINT "AS;3400,200,8,0,"+C$+"&AK"
      4190  LET P=3400
      4200  FOR N=0 TO 4
      4210  LET P=P-600
      4220  LET P$=STR$(P)
      4230  LET P(1)=P(1)-(P(3)/5)
      4240  IF P(1)<0.00001 THEN P(1)=0
      4250  PRINT "AS;"+P$+",200,8,0,"+P(1)+"&AK"
      4260  NEXT N
      4270  GOSUB 5700
      4280  PRINT "AS;150,2300,8,0"+D$+"&AK"
      4290  LET P=2300
      4300  FOR N=0 TO 4
      4310  LET P=P-400
      4320  LET P$=STR$(P)
      4330  LET P(2)=P(2)-(P(4)/5)
      4340  IF P(2)<0.00001 THEN P(2)=0
      4350  PRINT "AS;150,"+P$+",8,0,"+P(2)+"&AK"
      4360  NEXT N
      4370  GOTO 1300


(AW)  5000  REM SCALE AXIS
      5010  IF L<5 THEN LMAX=5 : GOTO 5100
      5020  IF L<10 THEN LMAX=10 : GOTO 5100
      5030  IF L<15 THEN LMAX=15 : GOTO 5100
      5040  IF L<20 THEN LMAX=20 : GOTO 5100
      5050  IF L<25 THEN LMAX=25 : GOTO 5100
      5060  IF L<50 THEN LMAX=50 : GOTO 5100
      5070  IF L<100 THEN LMAX=100 : GOTO 5100
      5080  IF L<150 THEN LMAX=150 : GOTO 5100
      5090  LMAX=200
      5110  LET LNT=(E/100)*L7
      5105  IF LNT <8 THEN LET EMAX=8 : GOTO 5220
      5110  IF LNT <20 THEN LET EMAX=20 : GOTO 5220
      5120  IF LNT <50 THEN LET EMAX=50 : GOTO 5220
      5130  IF LNT <100 THEN LET EMAX=100 : GOTO 5220
      5140  IF LNT <200 THEN LET EMAX=200 : GOTO 5220
      5150  IF LNT <300 THEN LET EMAX=300 : GOTO 5220
```

```
5160  IF LNT<400 THEN LET EMAX=400 : GOTO 5220
5170  IF LNT<500 THEN LET EMAX=500 : GOTO 5220
5180  IF LNT<600 THEN LET EMAX=600 : GOTO 5220
5190  IF LNT<700 THEN LET EMAX=700 : GOTO 5220
5200  IF LNT<800 THEN LET EMAX=800 : GOTO 5220
5210  LET EMAX =850
5220  RETURN


(AX)  5300  REM PLOT SMALL AXIS
      5310  PRINT "RP;0,100,0"
      5320  PRINT "RP;0,-100,2"
      5330  PRINT "RP;1500,0,0"
      5340  PRINT "RP;0,-20,2"
      5350  PRINT "RP;0,20,3"
      5360  FOR N=0 TO 4
      5370  PRINT "RP;-300,0,0"
      5380  PRINT "RP;0,-20,2"
      5390  PRINT "RP;0,20,3"
      5400  NEXT N
      5410  PRINT "RP;-20,0,2"
      5420  PRINT "RP;20,0,3"
      5430  FOR N=0 TO 4
      5440  PRINT "RP;0,200,0"
      5450  PRINT "RP;-20,0,2"
      5460  PRINT "RP;20,0,3"
      5470  NEXT N
      5480  RETURN


(AY)  5500  REM PLOT GRAPH
(AZ)  5510  LET XSC=1500/EMAX
(BA)  5520  LET YSC=1000/LMAX
(BB)  5530  REM CALCULATE LOAD DEFLECTION VALUES
      5540  LET X1=0 : LET Y1=0
(BC)  5550  LET SP=1
      5560  IF J>100 THEN SP=2
      5570  IF J>500 THEN SP=5
      5580  FOR N=0 TO J STEP SP
      5590  IF E3(N)=0 THEN GOTO
      5600  LET X=((E3(N)/100)*L7)*XSC
      5570  LET Y=L3(N)*YSC
      5580  LET X=X-X1 : LET Y=Y-Y1
      5590  LET X=X+X2 : LET Y=Y+Y2
      5600  LET X$=STR$(X) : LET Y$=STR$(Y)
      5610  LET A$="RP;"+X$+","+Y$+",2"
```

```
5620  PRINT A$
5630  LET Y1=Y1+Y : LET H1=H1+H
5640  LET H2=H-INT(H) : LET Y2=Y-INT(Y)
5650  NEXT N
5660  RETURN

(BD) 5700  REM LABEL SUBROUTINE
     5710  PRINT "TE"
     5720  PRINT "EH;"
     5730  PRINT "EB;@"
     5740  PRINT "IN@SP;1@DF;1,2@AP;300,0,0,-3"
     5750  RETURN
```

A2.1 Key to the flexural testing programme.

(A) This line dimensions the array (**L3()**) for storage of the load data from the 500M.

(B) This line dimensions the array (**E3()**) for storage of the extension data from the 500M.

(C) This line sets the maximum number of data points (**M3**) to 999.

(D) This line sets the 500M data scaling values (**L1**, **L2**).

(E) This line dimensions the arrays(**L()**, **E()**, **M()**, **N()**, **FS()**, **FM()**, **B()**) for results storage and analysis.

(F) These lines print the initial display screen, figure A2.2.

(G) These lines prompt for another test, figure A2.2.

(H) These lines print the load cell selection screen, figure A2.3.

(I) These lines define the variables (**L$**), the units of load, N or KN, (**U$**), the units of stress Nmm^{-2} or $KNmm^{-2}$ and (**C2**) the load cell variable, 100 or 20.

(J) This line prints the load range depending on the load cell selected, figure A2.3.

(K) These lines print the initial input values screen, figure A2.4.

(L) This line allows the span length (**L7**) to be entered.

(M) This line allows the sample width (**W**) to be entered.

(N) This line allows the sample thickness (**G**) to be entered.

(O) This line allows the test reference (**R$**) to be entered.

(P) This line allows the test speed (**R1$**) to be entered.

(Q) This line allows the printer to be selected by defining the value of (**PR**), if PR=1 then the printer is on, if PR=0 then the printer is off.

(R) This line accesses the printer switch subroutine if required.

(S) This line accesses the header printer subroutine, figure A2.5.

(T) These lines print the test details on the monitor, figure A2.6.

(U) These lines collect the data from the 500M, this is part of the original programme. The collected load data is stored in (**L3()**) and the extension data in (**E3()**).

(V) These lines calculate the elongation (**L**).

(W) These lines calculate the flexural strength (**FS**).

(X) These lines calculate the flexural modulus (**FM**).

(Y) These lines round off the values of flexural strength (**FS**) and flexural modulus (**FM**).

(Z) These lines print the calculation results on the monitor screen, figure A2.7.

(AA) These lines allow the results to be accepted or rejected from the tabulation and statistical analysis.

(AB) These lines store the calculation results in the arrays (**L()**, **E()**, **M()**, **N()**, **FS()**, and **FM()**).

(AC) These lines print the results under the correct headings on the line printer, figure A2.5.

(AD) This line switches the line printer off.

(AE) These lines print the plot menu screen , figure A2.8.

(AF) This line prompts for another test.

(AG) These lines allow new sample width (**W**) and sample thickness values (**G**) to be entered.

(AH) These lines print the statistical analysis header on the line printer, figure A2.5.

(AI) These lines access the statistical analysis for the calculated results, the data is transfered fron the storage array into the array (**B()**) and the analysis peformed on this array.

(AJ) This line returns to the begining of the programme so another batch of samples may be tested.

(AK) This subroutine switches the printer on.

(AL) This subroutine prints the tabulated results heading on the line printer.

(AM) This subroutine carries out the statistical analysis, it calculates the maximum (**HIGH**), minimum (**LOW**), average (**AVE**) and standard deviation (**DVE**) for the data stored in the array (**B()**).

(AN) These lines print out the results of the statistical analysis.

(AO) This subroutine controls the plotting of data on the X Y plotter.

(AP) This line calls the subroutine to scale the X and Y axis for the plotter.

(AQ) This line switches the X Y plotter on.

(AR) This line calls the routine to draw the X and Y axis on the plotter, figure A2.9

(AS) This line calls the subroutine to plot the graph on the plotter, figure A2.9.

(AT) These lines define the lables (**A$**, **B$**, **C$**, **D$**) to be printed on the graph, figure A2.9.

(AU) This line calls the subroutine which switches the plotter into the correct mode to label the graph.

(AV) These lines label the axis, figure A2.9.

(AW) This subroutine scales the data to fit the X and Y axis of the graph.

(AX) This subroutine plots the X and Y axis of the graph, figure A2.9.

(AZ) This line sets the scaling factor (**HSC**) for the X axis.

(BA) This line sets the scaling factor (**YSC**) for the Y axis.

(BB) These lines calculate the load and deflection values.

(BC) These lines set the plotting step (**SP**).

(BD) This subroutine sets the plotter into the correct mode to label the axis.

A2.3. Using the flexural testing programme.

On first running the programme, the initial screen is printed, figure A2.2, along with the prompt for another test, pressing the 'Y' key continues the programme, pressing 'N' terminates it. The programme then prompts for which strain gauge is in use, 2500Kg or 100N. Pressing the '1' key selects the 2500Kg cell and pressing the '2' key selects the 100N cell, figure A2.3. The programme then prints the limits of the selected strain gauge on the monitor and waits for any key to be pressed, figure A2.3. The programme then executes the initial input routine, figure A2.4, where the initial setup conditions of the 500M are recorded. At this stage the programme requires 7 inputs, the span width (mm), sample width (mm), sample thickness (mm), test reference (60 characters), test speed (mm/Min) and hard copy (Y/N), the return key must be pressed after entering all these values. The header information is then printed on the line printer, figure A2.5. The data from the 500M is then collected and displayed on the monitor, figure A2.6, pressing the strain key of the 500M starts the data collection and pressing the zero key terminates it. When the data has been collected the results are then calculated and a prompt to accept the data given, figure A2.7, at this point the data can be rejected from the statistical analysis for any reason. If the data is accepted then the results are printed on the printer, figure A2.5, if the data is rejected then the programme goes to a point where a new test can be started. The programme now prompts for a plot of the load deflection curve on the X Y plotter figure A2.8, if selected a plot is produced, figure A2.9. If not selected then the programme then prompts for another test. If another test is selected then the new sample width and thickness can be input, the programme then proceeds as before. If another test is not required then the programme calculates the maximum, minimum, average and standard deviation of the

collected results, prints this on the line printer, figure A2.5, then returns to the begining of the programme for another batch of results. figure A2.10 illustrates the use of this programme in a simplified form.

Table A2.1. Main programme variables.

Variable	Function
Arrays	
L3()	Load data storage.
E3()	Deflection data storage.
L()	Peak load data storage.
E()	Deflection data storage
M()	Thickness data storage.
N()	Width data storage.
FS()	Flexural strength data storage.
FM()	Flexural modulus data storage.
B()	Array for statistical analysis.
Strings	
E$	Units of extension (mm).
L$	Units of load (KN or N).
U$	Units of stress (KN/mm^2 or N/mm^2)
R$	Sample reference.
R1$	Test speed.
LD$	Load value from 500M.
EH$	Extension value from 500M
F$	Control A character.
Decimals	
M3	Sets maximum number of data points
L1	Scale value for 500M
L2	Scale value for 500M
C2	Load cell variable (20 or 100).
L7	Span length.
W	Sample width.
G	Sample thickness.
PR	Sets printer status 1=on, 0=off.
T	Test number.
F	500M status control variable.
J	Data collected variable 1-1000
L	Peak load.
FS	Flexural strength
FM	Flexural modulus.
E	Deflection.
HIGH	Maximum value.
LOW	Minimum value.
AVE	Average value.
DVE	Standard deviation.

Table A2.2. Plotting subroutine variables.

Variable	Function
Strings	
A$	X axis label
B$	Y axis label
C$	X axis maximum value label
D$	Y axis maximum value label
P$	General axis division label
H$	Character for X axis position
Y$	Character for Y axis position.
Decimals.	
P1	Maximum deflection.
P2	Maximum load.
LMAX	Adjusted maximum load
LNT	Peak deflection
EMAX	Adjusted peak deflection.
XSC	X axis scaling value.
YSC	Y axis scaling value.
SP	Plotting step.
X	Numerical X axis position.
Y	Numerical Y axis position.

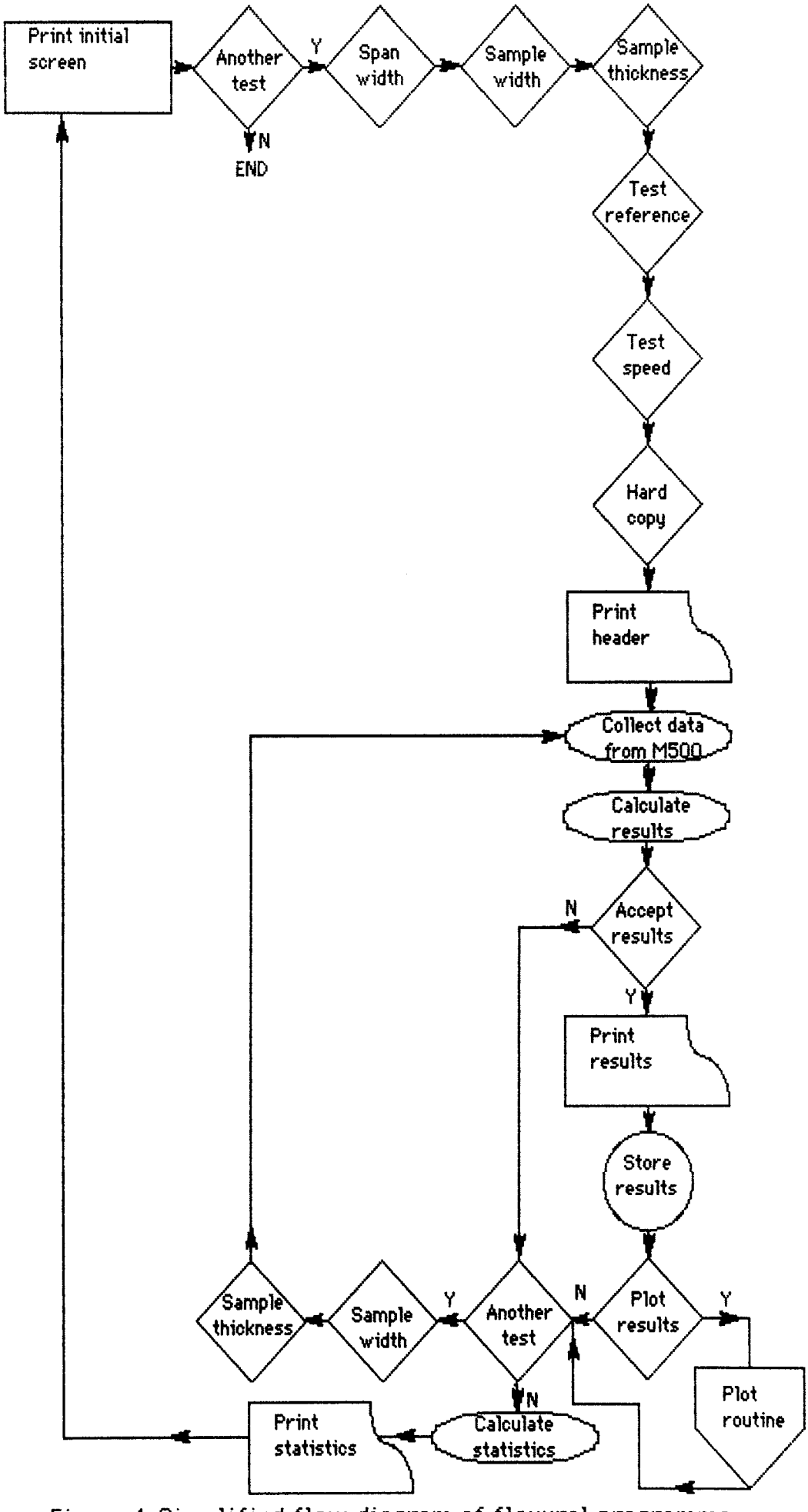


Figure 1. Simplified flow diagram of flexural programme.

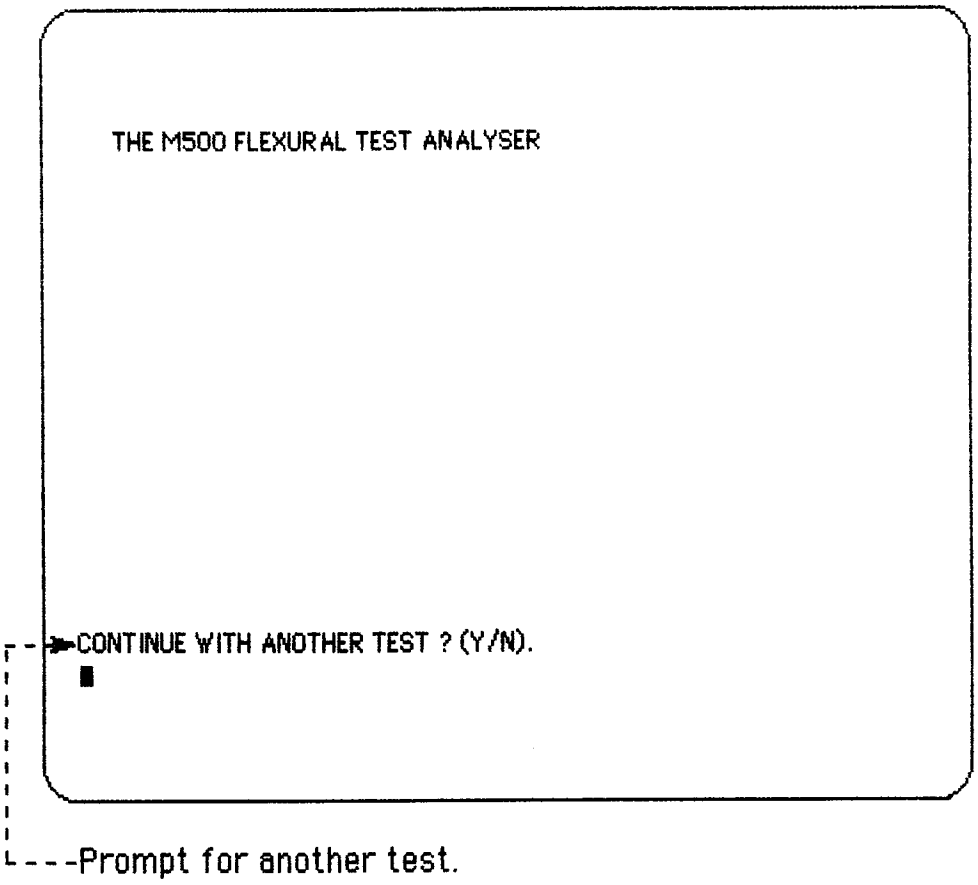


Figure A2.2. Initial display screen of flexural programme.

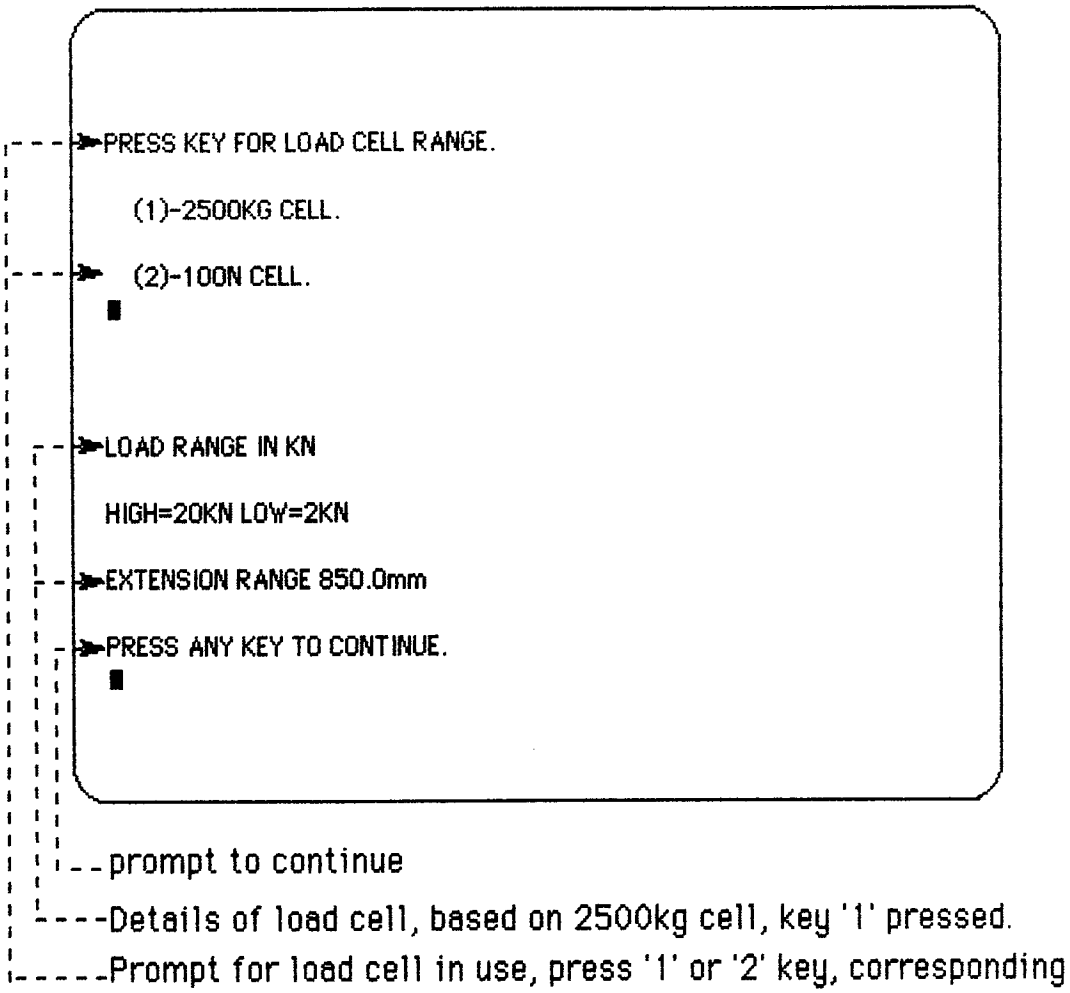


Figure A2.3. Load cell selection screen of flexural programme.

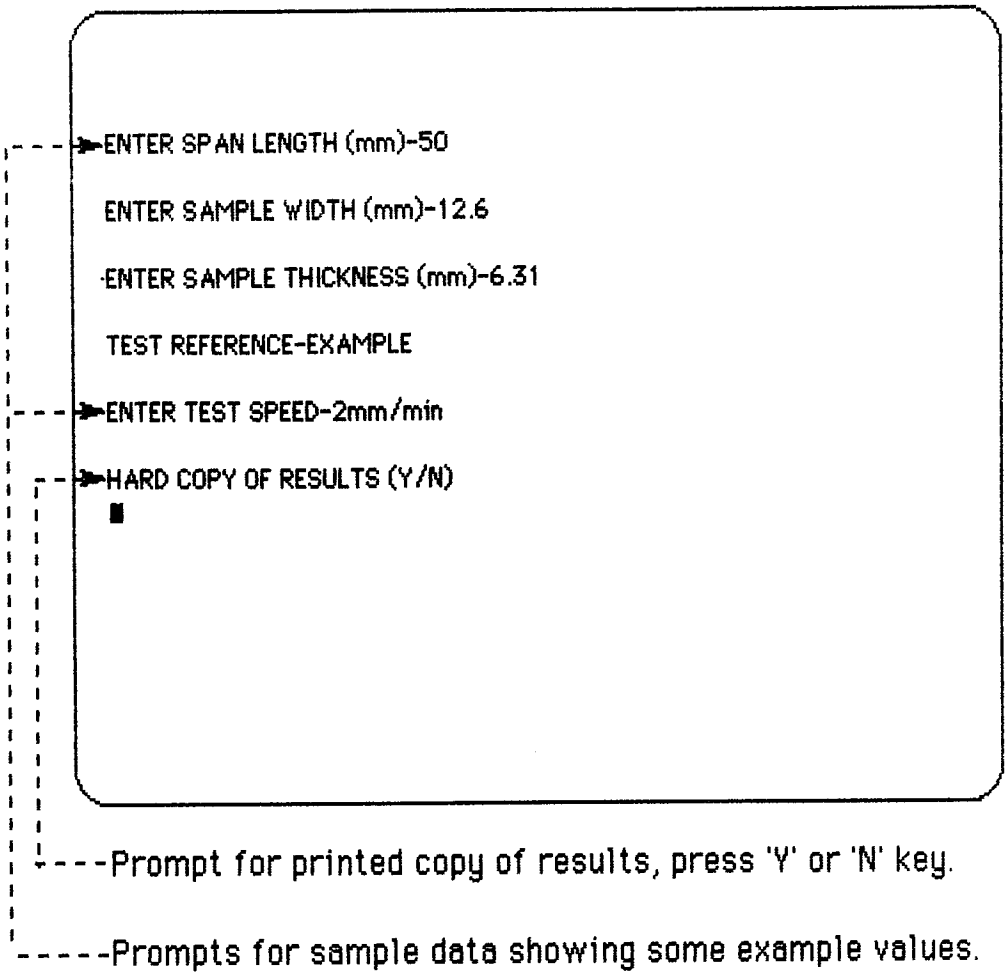


Figure A2.4. Screen for initial input values of flexural programme.

****

TESTOMETRIC 500M ANALYSIS

****

SPAN LENGTH = 50mm
TEST SPEED = 2mm/min

TEST REFERENCE = EXAMPLE

Test Number	Width (mm)	Thickness (mm)	Peak Load (KN)	Deflection (mm)	Flexural Strength (KN/mm^2)	Flexural Modulus (KN/mm^2)
1	12.6	6.31	0.28	7.3	0.0418	0.0211
2	12.61	6.2	0.29	5.3	0.0448	0.0328
3	12.59	6.2	0.27	5.05	0.0418	0.0259

500M TEST SERIES SUMMARY.

NUMBER OF TESTS = 3

LOAD ANALYSIS IN KN
HIGHEST =0.29
LOWEST =0.27
AVERAGE=0.28
STD DVE =0.01

DEFLECTION ANALYSIS IN mm
HIGHEST =7.3
LOWEST =5.05
AVERAGE=5.8833
STD DVE =1.233

FLEXURAL STRENGTH ANALYSIS IN KN/mm^2
HIGHEST =0.0448
LOWEST =0.0418
AVERAGE=0.0428
STD DVE = 0.001

FLEXURAL MODULUS ANALYSIS IN KN/mm^2
HIGHEST =0.0328
LOWEST = 0.0211
AVERAGE=0.0259
STD DVE =0.006

Figure A2.5. Printed output from flexural testing programme.

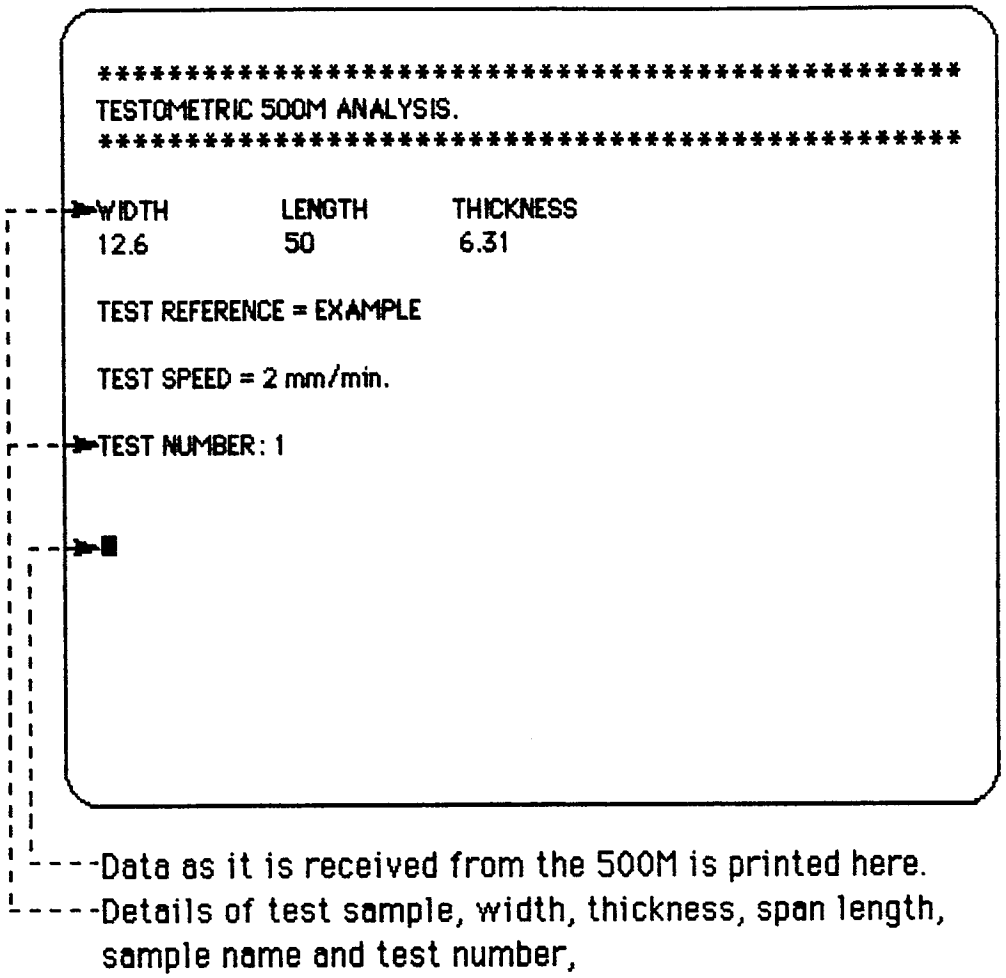


Figure A2.6. Data output screen from 500M.

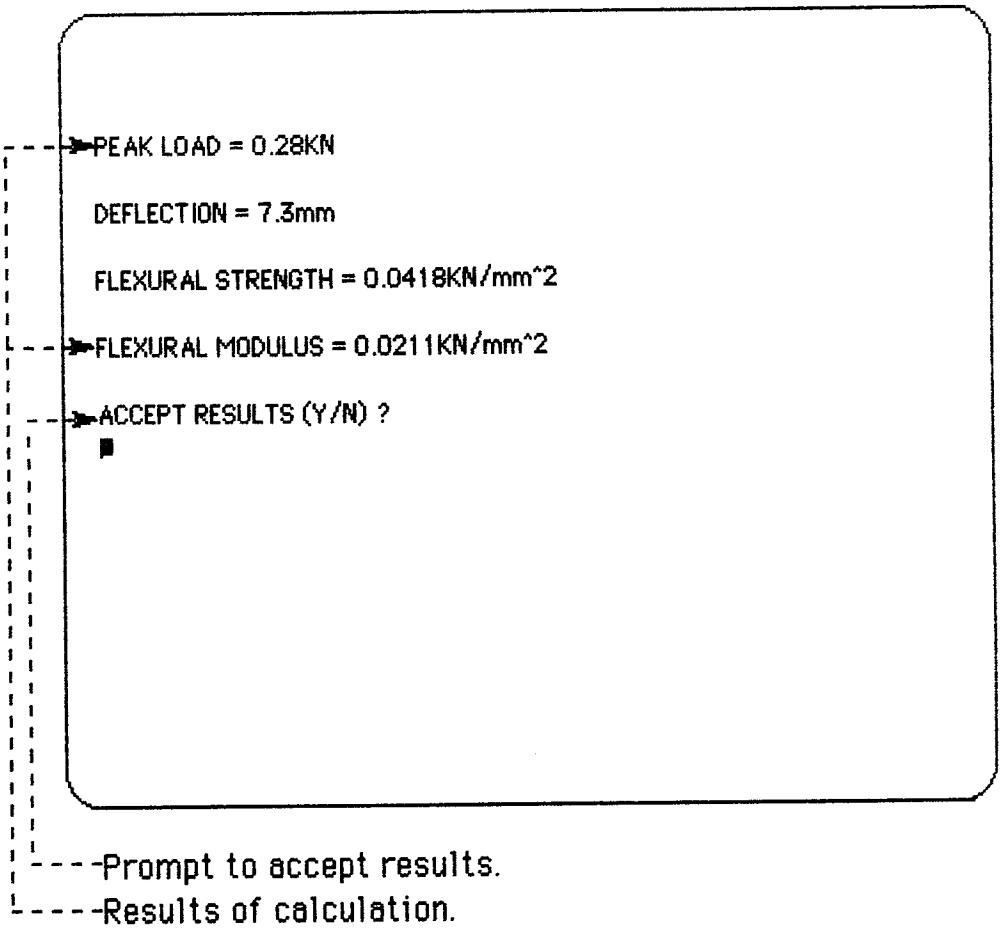


Figure A2.7. Results screen of flexural programme.

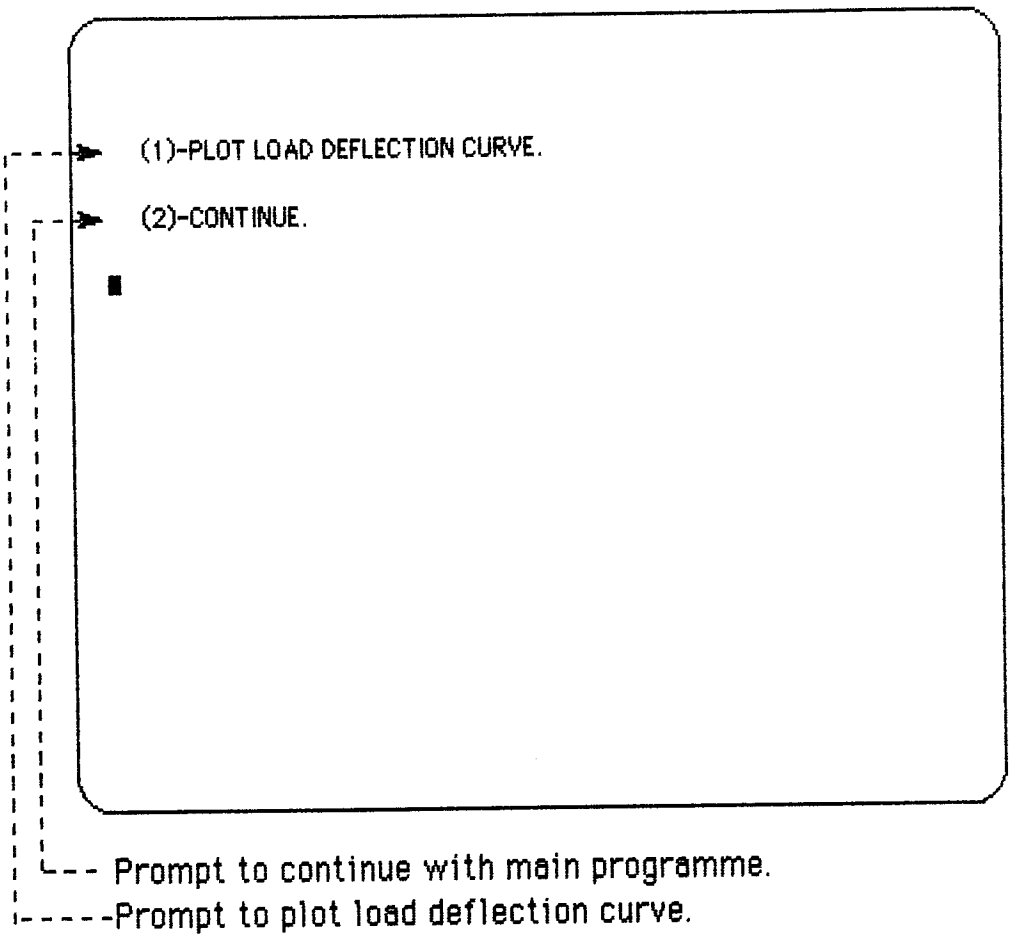


Figure A2.8. The plotting menu from the flexural testing programme.

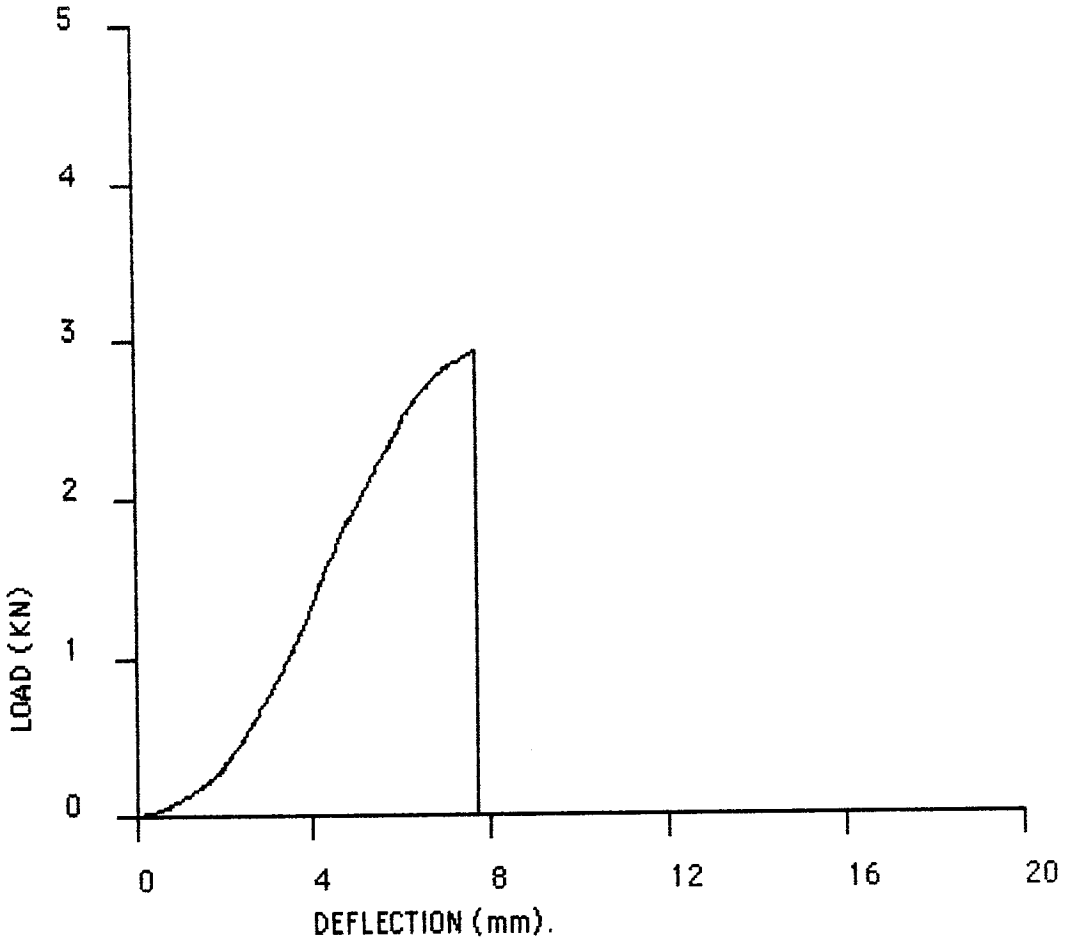


Figure A2.9. Load deflection plot from flexural testing programme.

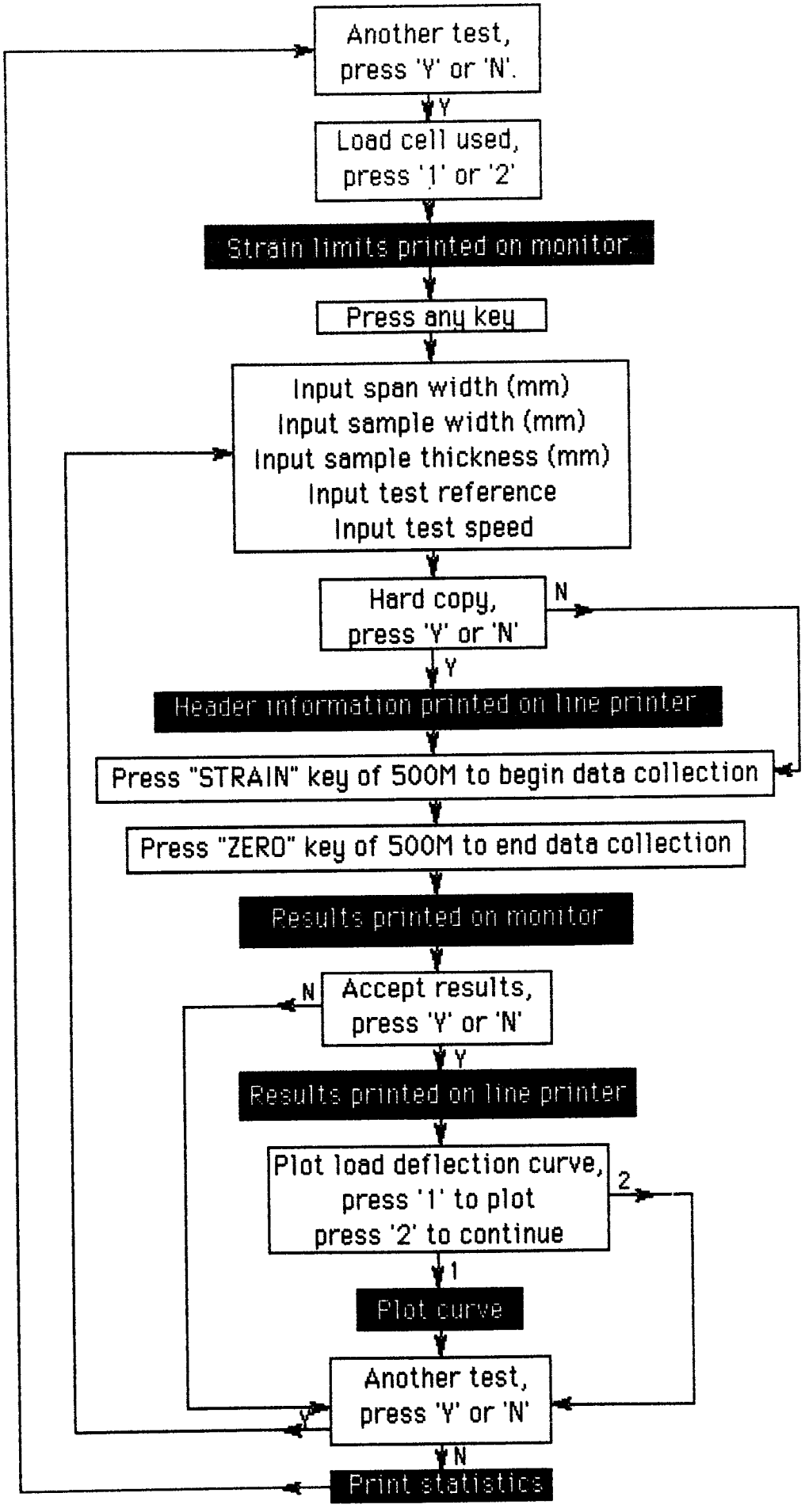


Figure A2.10. Flow diagram showing use of flexural testing programme.

Appendix 3

Impact testing programme.

1. The impact testing programme.

The impact testing programme has been designed to calculate from the raw data of sample width (mm), sample thickness (mm) and dial reading the impact strengths of polymer bars in KJ M^{-2} from Ft Lb in^{-2} in which the instrument was originally calibrated. The programme presents the results in a tabulated form calculating the maximum, minimum, average and standard deviation of the impact strength and impact energy. The programme is written in Microsoft basic and runs on an Apple IIe computer under CP/M 80. A simplified flow diagram of the programme is shown in figure A3.1 and a description of the variables used in table A3.1 .

2. Programme listing.

```
     10   REM IMPACT TESTING PROGRAMME
     20   REM INPUT INITIAL CONSTANTS, SAMPLE NAME AND
          MASS OF TUP
     30   HOME
(A)  40   PRINT "_____"
     50   PRINT TAB(10);"IMPACT TESTING, RESULTS
          CALCULATION AND CONVERSION PROGRAMME."
     60   PRINT "_____"
     70   PRINT : PRINT
(B)  80   PRINT "INPUT SAMPLE NAME ( MAX OF 60
          CHARACTERS )."
     90   INPUT N$
(C)  100  IF LEN(N$)>60 THEN GOTO 10
     110  PRINT
(D)  120  PRINT "INPUT MASS OF IMPACTING TUP IN lb."
     130  INPUT M
(E)  140  IF M=2 OR M=1 OR M=0.5 OR M=0.25 OR M=0.125 OR
          M=0.06128 THEN GOTO 150 ELSE GOTO 120
     150  HOME
(F)  160  LPRINT "**********************************"
     170  LPRINT TAB(25);"IMPACT TESTING SAMPLE RESULTS."
     180  LPRINT "**********************************"
     190  LPRINT
     200  LPRINT "SAMPLE NAME =";N$
     210  LPRINT "MASS OF IMPACTING TUP= ";M;" lb."
     220  LPRINT
     230  LPRINT "**********************************"
     240  LPRINT "SAMPLE SAMPLE DIAL IMPACT IMPACT
          IMPACT"
     250  LPRINT "WIDTH THICKNESS READING ENERGY
          STRENGTH STRENGTH"
```

```
        260   LPRINT "(mm)  (mm)   (J)  (J/mm^2)  (KJ/M^2)"
        270   LPRINT
        280   REM A MAXIMUM OF 30 SAMPLES IN EACH RUN
(G)     290   DIM D(30,2)
        300   DIM E(30)
(H)     310   FOR I=1 TO 30
        320   HOME
(I)     330   PRINT "_____"
        340   PRINT TAB(31);"DATA FOR SAMPLE ";I
        350   PRINT "_____"
        360   PRINT
(J)     370   PRINT "INPUT SAMPLE WIDTH (mm)."
        380   INPUT W
(K)     390   PRINT "INPUT SAMPLE THICKNESS (mm)."
        400   INPUT T
(L)     410   PRINT "INPUT DIAL READING."
        420   INPUT D
        430   PRINT
(M)     440   PRINT "PRESS E TO EDIT THESE RESULTS C TO
              CONTINUE."
        450   GET A$
        460   IF A$="" THEN GOTO 450
        470   IF A$="E" THEN GOTO 320
        480   IF A$<>"C"" THEN GOTO 450
        490   REM 1Ft Lb = 4.214011 E-2 J
        500   REM CONVERT DIAL READING TO Ft Lb BY
              MULTIPLYING READING BY TUP MASS."
(N)     510   LET FT=D*M
        520   REM CONVERT Ft Lb TO J MULTIPLY BY 1.35582
(O)     530   LET J=FT*1.35582
        540   REM IMPACT STRENGTH DIVIDE J BY C.S.A.
(P)     550   LET S=J/(W*T)
        560   REM OUTPUT RESULTS TO SCREEN
(Q)     570   PRINT
        580   PRINT "IMPACT ENERGY=";J
        590   PRINT
        600   PRINT "IMPACT STRENGTH=";S;"J/MM^2
              ";S*1000;"KJ/M^2"
        610   PRINT
(R)     620   PRINT "DO YOU ACCEPT THESE RESULTS Y/N ?"
        630   GET A$
        640   IF A$="" THEN GOTO 630
        650   IF A$="N" THEN GOTO 320
        660   IF A$<>"Y" THEN GOTO 630
        670   REM OUTPUT RESULTS TO PRINTER
(S)     680   LET W=(FIX (W*100))/100
```

```
        1120  FOR I=1 TO COUNT
        1130  IF E(I)>HIGH THEN HIGH=E(I)
        1140  IF E(I)<LOW THEN LOW=E(I)
        1150  LET AVE=AVE+E(I)
        1160  NEXT I
        1170  LET AVE=FIX((AVE/COUNT)*10000)/10000
        1180  LET DVE=0
        1190  IF COUNT <=1 THEN RETURN
        1200  FOR I=1 TO COUNT
        1210  LET DVE=DVE + (E(I)-AVE)^2
        1220  NEXT I
        1230  LET DVE=SQR(DVE/(COUNT-1))
        1240  LET DVE=FIX(DVE*1000)/1000
(CA)    1250  LPRINT "HIGHEST=";HIGH
        1260  LPRINT "LOWEST =";LOW
        1270  LPRINT "AVERAGE=";AVE
        1280  LPRINT "STD DVE=";DVE
(DA)    1290  RETURN
```

2.1 Key to impact testing programme.

(A) These lines print the header to the initial screen, figure A3.2 .

(B) These lines allow the input of the sample name (**N$**), figure A3.2 .

(C) This line checks that the sample name (**N$**) does not exceed the maximum length of 60 characters.

(D) These lines allow the tup mass (**M**) to be input, figure A3.2 .

(E) This line checks that the tup mass (**M**) has one of the permitted values of 2, 1, 0.5, 0.25, 0.125 or 0.06128.

(F) These lines print out the initial header on the line printer, figure A3.3 .

(G) These lines dimension the arrays (**D()** and **E()**) for results storage and statistical analysis.

(H) This line starts the main programme loop and counts the number of samples to a maximum of 30.

(I) These lines print the header for the data input screen, figure A3.4 .

(J) These lines allow the sample width (**W**) in mm to be input, figure A3.4 .

(K) These lines allow the sample thickness (**T**) in mm to be input, figure A3.4 .

(L) These lines allow the dial reading (**D**) to be input, figure A3.4 .

(M) These lines allow the input data to be edited, if the data requires editing then the programme returns to the begining of the data input routine (I).

(N) This line converts the dial reading to impact energy (**FT**) in ft lb, this is achieved by multiplying the dial (**D**) reading by the tup mass (**M**).

(O) This line converts the impact energy in ft lb (**FT**) to J (**J**), this is achieved by

multiplying the energy in ft lb by a conversion factor of 1.35582.

(P) This line calculates the impact strength (**S**) in Jmm^{-2}, this is achieved by dividing the impact energy in J (**S**) by the cross-sectional area (**W**) x (**T**).

(Q) These lines print the results of the calculation on the monitor screen, figure A3.5 .

(R) These lines allow the results to be rejected from printing and statistical analysis.

(S) These lines round off the calculation results.

(T) This line prints the calculation results on the line printer, figure A3.3 .

(U) This line prompts for another sample or statistical analysis of the results.

(V) This line returns the main calculation loop, see (H).

(W) This line prints the statistical analysis header on the line printer, figure A3.3 .

(X) This line sets the number of samples variable (**COUNT**), by making it equal to the main programme loop variable (**I**).

(Y) These lines calculate the statistics for the impact energy by transfering the data from the storage array (**D()**) to the calculation array (**E()**), then accessing the statistical analysis subroutine.

(Z) These lines calculate the statistics for the impact strength, see (Y).

(AA) These lines prompt for more tests.

(BA) These lines carry out the statistical analysis, calculating the maximum (**HIGH**), minimum (**LOW**), average (**AVE**) and standard deviation (**DVE**) of the impact energy and impact strength.

(CA) These lines print the statistical analysis results on the line printer, figure A3.3 .

(DA) This line returns the programme from the subroutine.

3. Using the impact testing programme.

On first running the programme the computer requires two inputs, the sample name and mass of the impacting tup, figure A3.2 . The sample name can only be a maximum of 60 characters long. The mass of impacting tup can only have values of 2, 1, 0.5, 0.25, 0.125 and 0.06128. After the initial inputs the programme prints on the printer a header for the tabulation of the results, figure A3.3 . The monitor display is cleared and prompts for sample width (mm), sample thickness (mm) and dial reading (0 to 1) appear, figure A3.4 . When these values have been input a prompt to edit the results or continue will appear, figure A3.4 . At this point pressing the 'E' key allows the values of width, thickness and dial reading to be re-entered, pressing the 'C' key continues the programme. The programme now calculates and displays on the monitor the impact energy (J) and the impact strength in both ($J\ mm^{-2}$) and ($KJ\ M^{-2}$), figure

A3.5 . At this point a prompt to accept the results will appear, pressing the 'N' key allows the results to be rejected from the tabulation and statistical analysis, pressing the 'Y' key tabulates the results in the correct column, figure A3.3 and saves the results for later statistical analysis. A prompt to continue with more results will then appear, pressing the 'Y' key allows a new set of width, thickness and dial readings to be entered as before. Pressing the 'N' key submits the results for statistical analysis where the highest, lowest, average and standard deviation of the impact energy and impact strengths are calculated, and printed on the line printer, figure A3.3 . At the end a prompt to continue with more results appears. Pressing the 'Y' key returns the programme to the begining so a new sample name and tup mass can be entered. Pressing the 'N' key stops the programme. A simplified diagram showing the use of the impact testing programme is shown in figure A3.6 .

Table A3.1 . Variables used in impact testing programme.

Variable	Function
N$	Sample name
M	Mass of impacting tup
D()	Array for results storage
E()	Array for statistical analysis
W	Sample width
T	Sample thickness
D	Dial reading
FT	Energy of impact (ft lb)
J	Energy of impact (J)
S	Impact strength (J mm^{-2})
COUNT	Number of samples
HIGH	Maximum value
LOW	Minimum value
AVE	Average value
DVE	Standard deviation

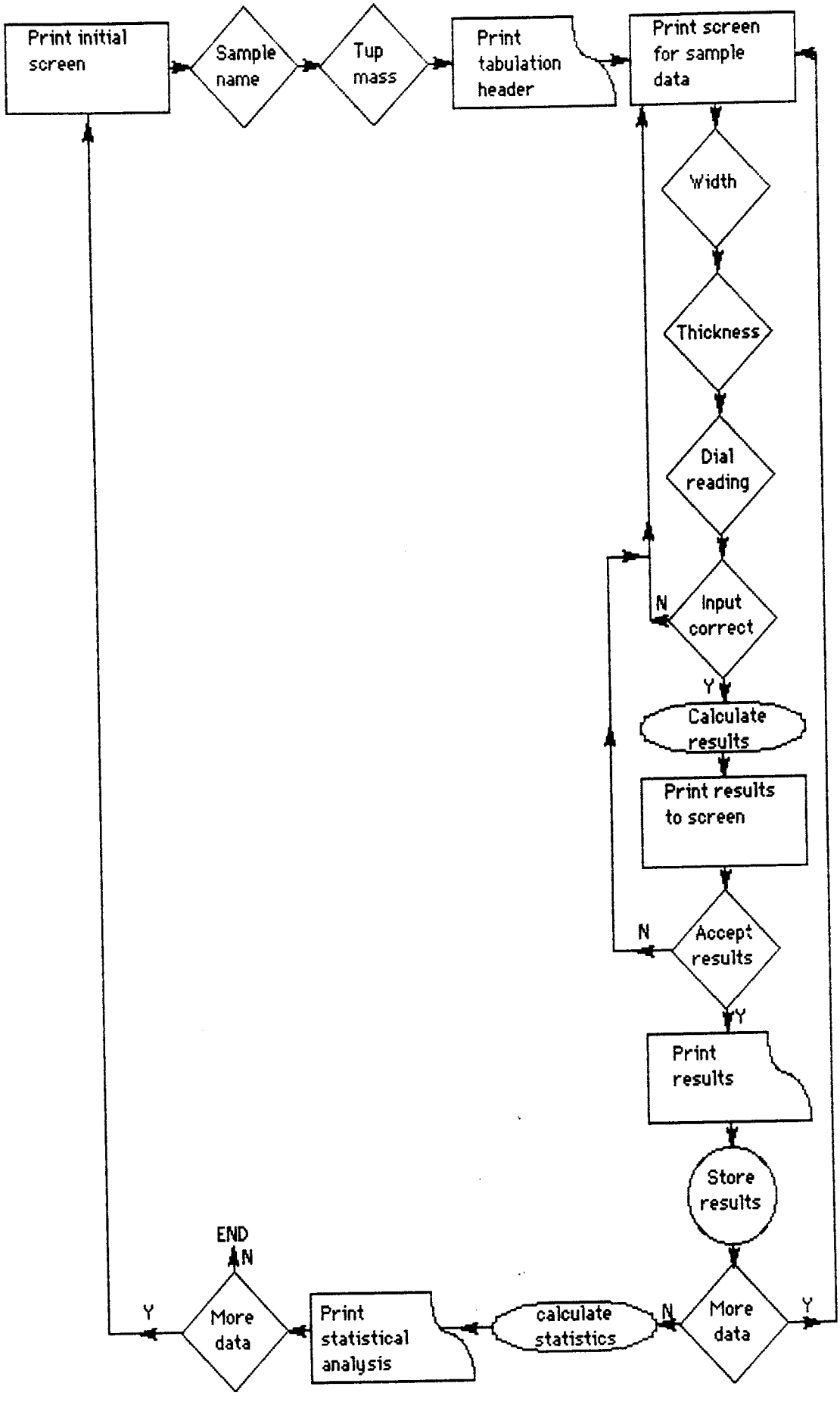


Figure A3.1 . Simplified flow diagram of impact testing programme.

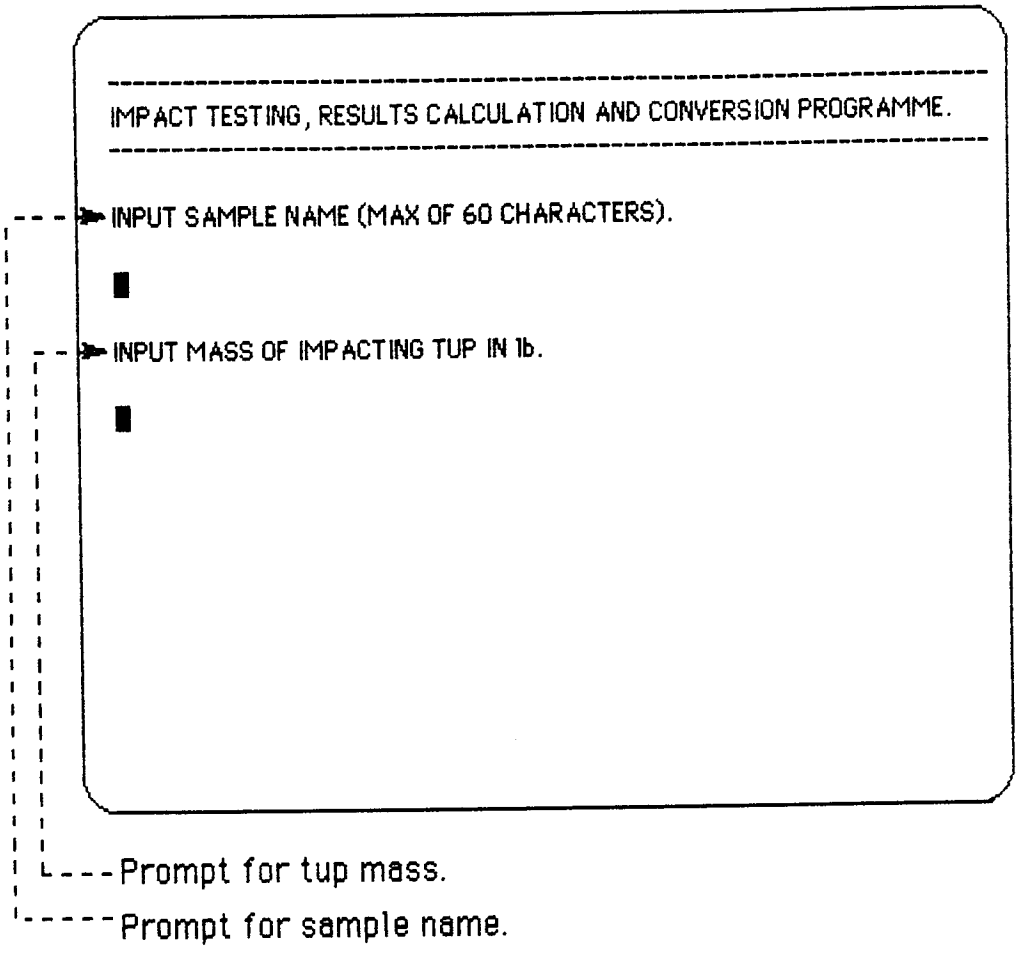


Figure A3.2 . Initial screen of impact testing programme.

****

IMPACT TESTING SAMPLE RESULTS.

****

SAMPLE NAME=EXAMPLE
MASS OF IMPACTING TUP= 2lb

****

SAMPLE WIDTH (mm)	SAMPLE THICKNESS (mm)	DIAL READING	IMPACT ENERGY (J)	IMPACT STRENGTH (J/mm^2)	IMPACT STRENGTH (KJ/M^2)
12.67	3.08	.15	.4067	.010423	10.42
12.69	3.1	.15	.4067	.010339	10.33
12.69	3.1	.15	.4067	.010339	10.33
12.69	3.09	.14	.3769	.009681	9.68

****

ANALYSIS OF RESULTS.

****

IMPACT ENERGY J.

HIGHEST= .406746
LOWEST =.37963
AVERAGE=.3999
STD DVE =.013

IMPACT STRENGTH J/mm^2

HIGHEST = .0104231
LOWEST= 9.68144E-03
AVERAGE=.0101
STD DVE =0

Figure A3.3 . Printed output from impact testing programme.

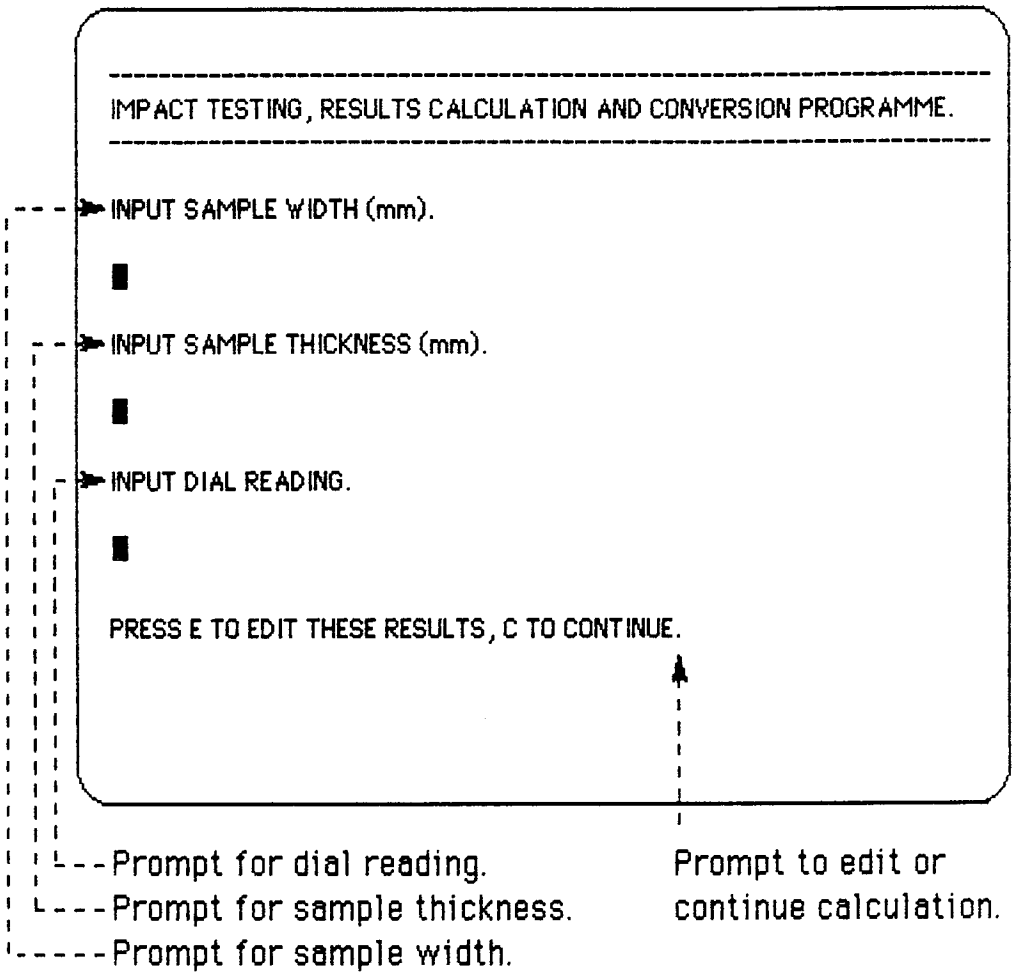


Figure A3.4. Data input screen from impact testing programme.

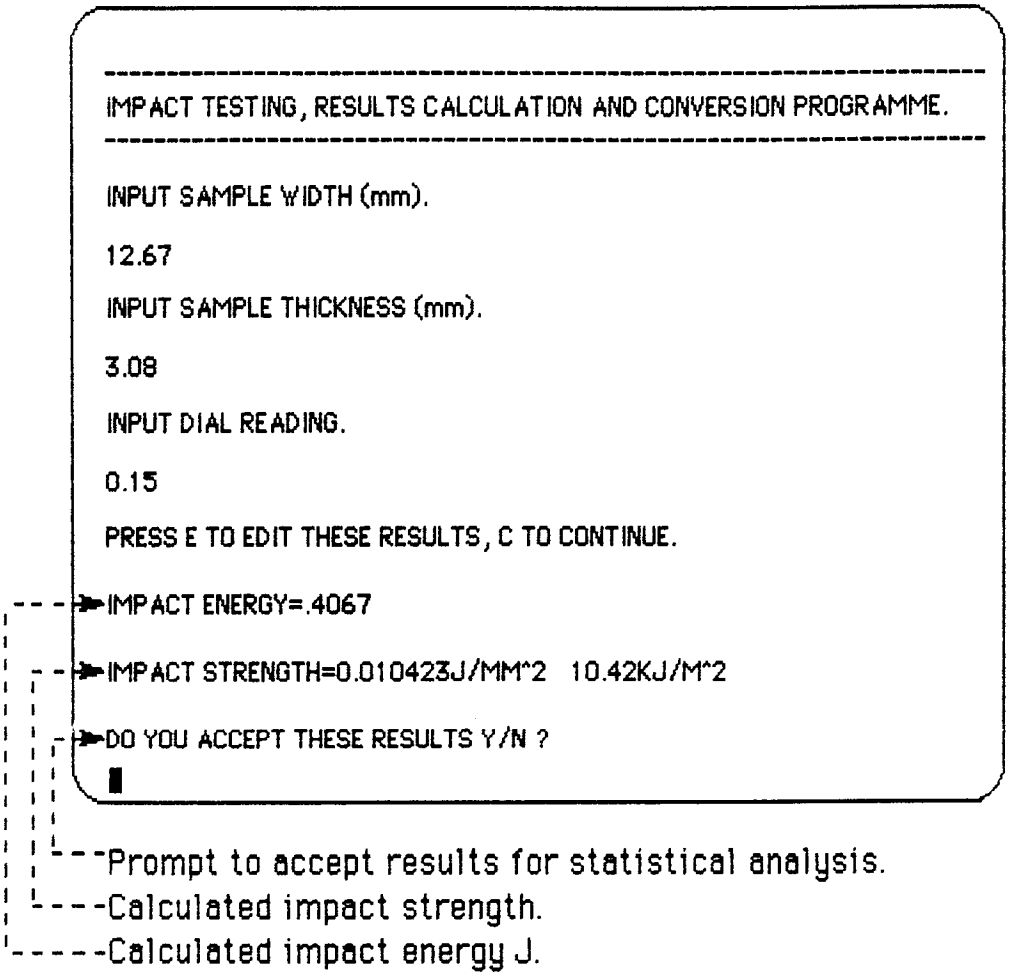


Figure A3.5 . calculation results screen from impact testing programme

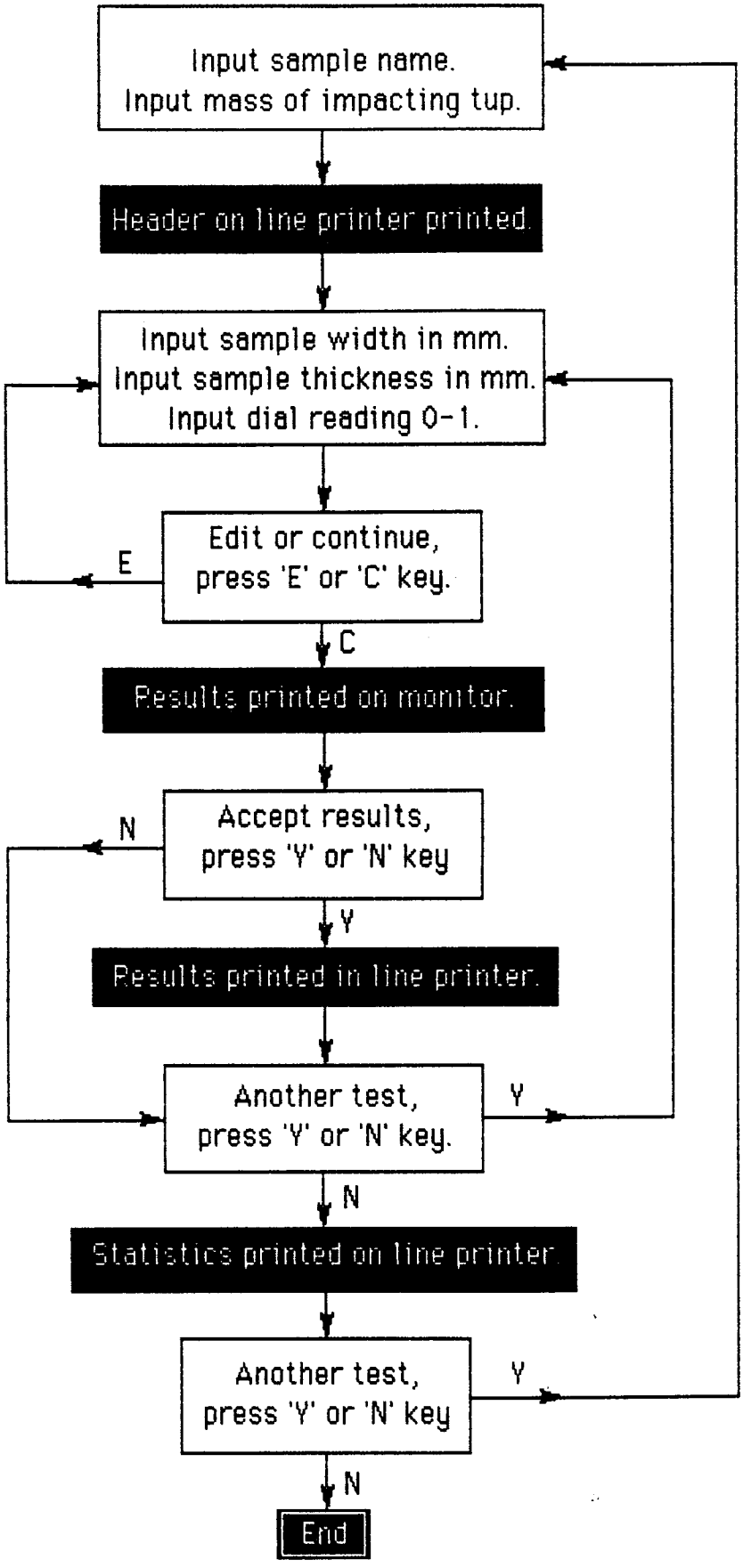


Figure A3.6 . Use of impact testing programme.

APPENDIX 4

Ultraviolet data manipulation programme.

1 Ultraviolet data manipulation programme.

The ultraviolet data manipulation programme (UVDMP) has been designed to allow data collected from the Beckmann DU7 spectrometer via the Beckmann mass storage accessory (BMSA) to be analysed, displayed and manipulated in ways not possible using the DU7 alone.

1.1 The Beckmann mass storage accessory.

The Beckmann mass storage accessory (BMSA) transfers data from the DU7 ultraviolet spectrometer via an RS232C serial interface to an Apple IIe computer running the BMSA software under CP/M 80. The data is stored on 5 $^{1}/_{4}$" floppy discs in the form of a random access data file. The exact format of the file depends upon the nature of the data being stored. Data files stored by the BMSA may be transferred back to the DU7 for use at any time.

2. The structure of the ultraviolet data manipulation programme.

The ultraviolet data manipulation programme (UVDMP) has been structured to allow the largest possible amount of free memory to be available at any time so that large data files can be accommodated. The central programme of the UVDMP is the main menu, this allows a particular routine to be selected by a single key press. The routine programme is loaded into memory, replacing the main menu. The routine programme then loads into memory in the required sequence a series of function programmes. The function programmes carry out calculations which are common to many routine programmes, such as loading the required data file into memory, figure A4.1. There are two other programmes also accessed by the main menu, these are the disc utilities programme and the help programme.

3. The function programmes.

The function programmes are accessed by the routine programmes and their purpose is to carry out the commonly recurring operations. The UVDMP has been written in this fashion so as to avoid repeation in order to save disc and ram space. In order to illustrate how each function programme operates on the data a demonstration file, table A4.1 and table A4.2, has been set up, this file represents a wavelength scan in absorbance mode. The common variables used by the function programmes are listed in table A4.3, the input and output variable in table A4.4.

3.1 Single file name.

The single file name programme is found in all routine programmes its function is to collect a single file name (the file that is to be manipulated) and to add the required disc file name extensions. There is an error trap present so that any disc errors such as a corrupted file give a report and return to the main menu. The monitor display is shown in figure A4.2. The programme requires no input variables and outputs two variables, (**M$**), the file name without extensions and (**N$**), the file name with extensions. Table A4.3, table A4.4, listing 1.

```
      10    REM GET SINGLE FILE NAME
(A)   20    ON ERROR GOTO 130
      30    HOME
(B)   40    FILES "B:*.DAT"
      50    PRINT
      60    PRINT "-----------------------------------"
      70    PRINT
      80    PRINT "INPUT NAME OF FILE TO BE USED?"
      90    PRINT
(C)   100   INPUT M$
(D)   110   LET N$="B:"+M$"+".DAT"
(E)   120   CHAIN P$,L1,ALL
(F)   130   HOME
      140   PRINT
      150   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS
            AND" : PRINT "FILE NAMES USED."
      160   PRINT
      170   PRINT "PRESS ANY KEY TO CONTINUE."
      180   GET K$
      190   IF K$="" THEN GOTO 180
      200   LOAD "MENU",R
```

Listing 1. The get single file name function programme.

(A) This line sets the error trap at line 130, see (F)

(B) This line prints on the monitor the available data files.

(C) This line collects the required file name and stores it as (**M$**).

(D) This line adds the required extensions to (**M$**) and stores the result as (**N$**).

(E) This line returns to the routine programme (**P$**) at the correct line (**L1**) preserving all the variables (**ALL**).

(F) The programme beyond this point gives an error report if required and returns

the programme to the main menu, see (A)

3.1.1 Multiple file name.

The multiple file name programme works in a similar way to the single file name programme except that it is designed to collect from 2 to 20 names. The number of file names to be collected can be set by the routine programme or where no specific number of files are required by the user within the function programme. The monitor display produced by this programme is shown in figure A4.3. The programme requires one input value (**NUM**), the number of data files to be used and outputs an array (**B$()**) which contains all the file names with the required extensions, table A4.3, table A4.4, listing 2.

```
     10   REM MULTIPLE FILE NAME
(A)  20   ON ERROR GOTO 260
     30   HOME
(B)  40   FILES "B:*.DAT"
     50   PRINT
     60   PRINT "---------------------------------"
     70   PRINT
(C)  80   IF NUM<>0 THEN GOTO 140
(D)  90   PRINT "HOW MANY FILES DO YOU WISH TO USE,
          (MAX OF 20)."
     100  INPUT NUM
     110  IF NUM>20 THEN PRINT "NUMBER OF FILES HAS
          BEEN SET TO 20." : LET NUM=20
     120  LET NUM=INT(NUM)
     130  IF NUM<1 THEN PRINT "NUMBER OF FILES HAS
          BEEN SET TO 2." : LET NUM=2
(E)  140  DIM B$(15,NUM)
(F)  150  FOR C=1 TO NUM
     160  UTAB(12)
     170  PRINT TAB(4); "INPUT FILE"; C; "";
     180  INPUT N$
     190  LET N$="B:"+N$+".DAT"
     200  FOR J=1 TO LEN N$
     210  LET M$=MID$(N$,J,1)
     220  LET B$(J,C)=M$
     230  NEXT J
     240  NEXT C
```

```
(G)   250   CHAIN P$,LI,ALL
(H)   260   HOME
      270   PRINT
      280   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS
            AND" : PRINT "FILE NAMES USED."
      290   PRINT
      300   PRINT "PRESS ANY KEY TO CONTINUE."
      310   GET K$
      320   IF K$="" THEN GOTO 310
      330   LOAD "MENU",R
```

Listing 2. The get multiple file names function programme.

(A) This line sets the error trap at line 260, see (H).

(B) This line prints on the monitor the available data files.

(C) This line checks to see if the number of files is set by the routine programme (**NUM>0**) or by the user (**NUM=0**). If the number of files is set by the routine programme then section (D) is missed.

(D) This section of programme allows the number of files to be defined by the user.

(E) This line dimensions the array (**B$()**) in which the file names are stored.

(F) This section of programme as far as (G) collects the file names (**N$**), adds the required extension to the file name and stores the name in (**B$()**).

(G) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(H) The programme beyond this point gives an error report if required and returns the programme to the main menu, see (A).

3.2 File type.

The file type programme is found in all routine programmes, its function is to collect the file header information which defines what type the file is and store this information. The file type information is stored in the second and third records of the data file as two characters, table A4.5. The programme first opens the data file, collects the characters which are stored as (**A$**) and (**B$**), the file is then closed. The programme requires one input variable the file name (**N$**) and outputs two string variables which contain the identifying characters (**A$,B$**), table A4.3, table A4.4, listing 3.

```
      10    REM FILE TYPE
(A)   20    ON ERROR GOTO 110
(B)   30    OPEN "R",#1,N$,2
      40    FIELD #1,2 AS H$
(C)   50    GET #1,2
(D)   60    LET A$=H$
(E)   70    GET #1,3
(F)   80    LET B$=H$
(G)   90    CLOSE #1
(H)   100   CHAIN P$,LI,ALL
(I)   110   HOME
      120   PRINT
      130   PRINT "AN ERROR HAS OCCURRED DURING THE
            EHECUTION OF THIS ROUTINE, CHECK ALL DISCS
            AND" : PRINT "FILE NAMES USED."
      140   PRINT
      150   PRINT "PRESS ANY KEY TO CONTINUE."
      160   GET K$
      170   IF K$="" THEN GOTO 160
      180   LOAD "MENU",R
```

Listing 3. The file type function programme.

(A) This line sets the error trap at line 110, see (I).

(B) This section of programme opens (**OPEN**) a random access file ("**R**"), labels this as the first file (**#1**), the data file opened is (**N$**) and each data section is two bytes (**2**) long. The next line sets a field (**FIELD**) for the data file (**#1**) with two bytes and each variable is assigned as (**H$**).

(C) This line collects (**GET**) the second data record from file (**#1**).

(D) This line swaps the file value (**H$**) into the string variable (**A$**).

(E) This line collects (**GET**) the third data record from file (**#1**).

(F) This line swaps the file value (**H$**) into the string variable (**B$**).

(G) This line closes (**CLOSE**) the file (**#1**).

(H) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(I) The programme beyond this point gives an error report if required and returns the programme to the main menu, see (A).

3.3 Identify file.

The identify file type programme is found in all routine programmes, its function is to identify the type of data file from the variables (**A$**) and (**B$**) and according to the type of file set the data starting position (**J%**), the data multiplication factor (**DIV%**) and assign the variable (**SCAN**) table A4.5, which from then on is used to define the file type. The programme requires two input variables (**A$**) and (**B$**) and outputs the variables (**J%**), (**DIV%**) and (**SCAN**). Table A4.2, table A4.3, table A4.4, listing 4.

```
      10    REM IDENTIFY FILE
(A)   20    ON ERROR GOTO 350
(B)   30    LET A$=LEFT$(A$,1)
      40    LET B$=LEFT$(B$,1)
      50    REM SCAN IN ABS MODE
(C)   60    IF A$="S" AND B$="A" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=1 : GOTO 340
      70    REM SCAN IN TRANS MODE
(D)   80    IF A$="S" AND B$="T" THEN LET J%=7 : LET
            DIV%=100 : LET SCAN=2 : GOTO 340
      90    REM TIME DRIVE ABS MODE
(E)   100   IF A$="T" AND B$="A" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=3 : GOTO 340
      110   REM TIME DRIVE TRANS MODE
(F)   120   IF A$="T" AND B$="T" THEN LET J%=7 : LET
            DIV%=100 : LET SCAN=4 : GOTO 340
      130   REM KINETICS SCAN ABS ONLY
(G)   140   IF A$="T" AND B$="K" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=5 : GOTO 340
      150   REM LOG10 ABS
(H)   160   IF A$="L" AND B$="A" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=8 : GOTO 340
      170   REM FIRST DERIVATIVE
(I)   180   IF A$="D" AND B$="1" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=9 : GOTO 340
      190   REM SECOND DERIVATIVE
(J)   200   IF A$="D" AND B$="2" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=10 : GOTO 340
      210   REM THIRD DERIVATIVE
(K)   220   IF A$="D" AND B$="3" THEN LET J%=7 : LET
            DIV%=10000 : LET SCAN=11 : GOTO 340
      230   REM FOURTH DERIVATIVE
(L)   240   IF A$="D" AND B$="4" THEN LET J%=7 : LET
```

```
          DIV%=10000 : LET SCAN=12 : GOTO 340
     250  REM ADDED SPECTRA
(M)  260  IF A$="D" AND B$="A" THEN LET J%=7 : LET
          DIV%=10000 : LET SCAN=13 : GOTO 340
     270  REM SUBTRACTED SPECTRA
(N)  280  IF A$="U" AND B$="A" THEN LET J%=7 : LET
          DIV%=10000 : LET SCAN=14 : GOTO 340
     290  REM FIXED WAVELENGTH ABS MODE
(O)  300  IF A$="A" THEN LET J%=3 : LET DIV%=10000 : LET
          SCAN=6 : GOTO 340
     310  REM FIXED WAVELENGTH TRANS MODE
(P)  320  IF A$="T" THEN LET J%=3 : LET DIV%=100 : LET
          SCAN=7 : GOTO 340
(Q)  330  LET SCAN=100
(R)  340  CHAIN P$,L1,ALL
(S)  350  HOME
     360  PRINT
     370  PRINT "AN ERROR HAS OCCURRED DURING THE
          EXECUTION OF THIS ROUTINE, CHECK ALL DISCS
          AND" : PRINT "FILE NAMES USED."
     380  PRINT
     390  PRINT "PRESS ANY KEY TO CONTINUE."
     400  GET K$
     410  IF K$="" THEN GOTO 400
     420  LOAD "MENU",A
```

Listing 4. The identify file programme.

(A) This line sets the error trap at line 350, see (S).

(B) These lines define the strings (**A$**) and (**B$**) as single characters.

(C) This line defines a wavelength scan in absorbance mode, for this type of file the data record starts at the seventh character hence (**J%=7**), the data multiplication factor is 10000 hence (**DIV%=10000**) and the file definition variable (**SCAN**) is 1. When all the variables have been set the programme goes to line 340 which returns to the routine programme. The lines (D-N) function in a similar way except where the scan is in transmittance mode then (**DIV%=100**), also the value of (**SCAN**) varies according to the file type, table A4.5.

(D-N) See (C).

(O) This line functions in a similar way to the others see (C) except that (**DIV%=3**) for single wavelength scans.

(P) see (O).

(Q) This line gives a default setting for (**SCAN**) of 100 for unknown file types.

(R) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(S) The programme beyond this point gives an error report if required and returns the programme to the main menu, see (A).

3.4 File header.

The file header routine collects the data from the file header not already collected by the file type routine, (section 3.2). Most files have 6 variables in the file header except for fixed wavelength scans which have 2 variables. Where there are 6 variables the first is the number of data points (**PTS**) ie the number of variables after the header. The second and third variables are used by the file type routine (section 3.2). The fourth variable is the starting wavelength or wavelength X 10 (**SWL**) depending on the type of file, table A4.6. The fifth variable is the ending wavelength or total time (**EWL**) depending on the type of file, table A4.6. The sixth variable is the scan speed (**SP**).

Where there are two variables in the header, ie, for single wavelength scans then the first is the number of data points (**PTS**) and the second is used by the file type routine. The programme requires one input variable, the file name with extensions (**N$**) and outputs up to 4 variables (**PTS**), (**SWL**), (**EWL**) and (**SP**). Table A4.2, table A4.3, table A4.4, listing 5.

```
     10   REM FILE HEADER
(A)  20   ON ERROR GOTO 210
(B)  30   OPEN "R",#1,N$,2
     40   FIELD #1,2 AS H$
(C)  50   IF SCAN=6 OR SCAN=7 THEN GOTO 150
(D)  60   GET #1,1
(E)  70   LET PTS=CVI(H$)
(F)  80   GET #1,4
(G)  90   LET SWL=CVI(H$)
(H)  100  GET #1,5
(I)  110  LET EWL=CVI(H$)
(J)  120  GET #1,6
(K)  130  LET SP=CVI(H$)
(L)  140  GOTO 200
(M)  150  GET #1,1
```

```
(N)   160   LET PTS=CUI(H$)
(O)   170   LET SWL=0
      180   LET EWL=0
      190   LET SP=0
(P)   200   CHAIN P$,LI,ALL
(Q)   210   HOME
      220   PRINT
      230   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS
            AND" : PRINT "FILE NAMES USED."
      240   PRINT
      250   PRINT "PRESS ANY KEY TO CONTINUE."
      260   GET K$
      270   IF K$="" THEN GOTO 260
      280   LOAD "MENU",R
```

Listing 5. The file header programme.

(A) This line sets the error trap at line 210, see (Q).

(B) This section of programme opens (**OPEN**) a random access file ("**R**"), labels this as the first file (**#1**), the data file opened is (**N$**) and each data section is two bytes (**2**) long. The next line sets a field (**FIELD**) for the data file (**#1**) with two bytes and each variable is assigned as (**H$**).

(C) This line sets the trap for files with only two variables in the header and sends the programme to line 150.

(D) This line collects the first variable in the file.

(E) This line converts the collected first variable which is a string variable to a numeric variable in this case (**PTS**). The lines F-K and M-N also collect and convert variables in the same way.

(F-K) See (D),(E).

(L) This line sends the programme section for files with more than two variables onto line 200, see (P).

(M-N) See (D),(E).

(O) These lines set the variables (**SWL**), (**EWL**) and (**SP**) to 0 for files with only two variables in the header.

(P) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(Q) The programme beyond this point gives an error report if required and returns

the programme to the main menu, see (A).

3.5 Load array

The load array programme dimensions two arrays (**Y()**) and (**S()**) to hold the data collected from the file (**N$**). The array which is normally used and manipulated is (**Y()**), the (**S()**) array is used where the data may be saved as another data file. The programme requires the following input variable, the file name (**N$**), the number of data points (**PTS**), the data record start position (**J%**), the data multiplication factor (**DIV%**) and the data offset (**OFFSET**). The programme outputs two arrays (**Y()**) and (**S()**) which both contain the file data. Table A4.2, table A4.3, table A4.4, listing 6.

```
      10    REM LOAD ARRAY
(A)   20    ON ERROR GOTO 150
(B)   30    OPEN "R",#1,N$,2
      40    FIELD #1,2 AS H$
(C)   50    IF P$="OVER" OR P$="COMPARE" OR P$="ADD" OR
            P$="SUB" OR P$="AVERAGE" OR P$="LAP" THEN
            LET FLAG=FLAG+1 : IF FLAG>1 THEN ERASE Y : ERASE S
(D)   60    DIM Y(PTS)
(E)   70    DIM S(PTS)
(F)   80    FOR C=1 TO PTS
(G)   90    GET #1,J%
(H)   100   LET Y(C)=(CVI(H$)+OFFSET)/DIV%
(I)   110   LET S(C)=Y(C)
(J)   120   LET J%=J%+1
(K)   130   NEXT C
(L)   140   CLOSE #1
(M)   150   CHAIN P$,LI,ALL
(N)   160   HOME
      170   PRINT
      180   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      190   PRINT
      200   PRINT "PRESS ANY KEY TO CONTINUE."
      210   GET K$
      220   IF K$="" THEN GOTO 210
      230   LOAD "MENU",R
```

Listing 6. The load array programme

(A) This line sets the error trap at line 160, see (N).

(B) This section of programme opens (**OPEN**) a random access file ("**R**"), labels this as the first file (**#1**), the data file opened is (**N$**) and each data section is two bytes (**2**) long. The next line sets a field (**FIELD**) for the data file (**#1**) with two bytes and each variable is assigned as (**H$**).

(C) This line erases the arrays (**Y()**) and (**S()**) if they have already been used once by the routine programme. This occurs only in the case of routine programmes which use more than one data file.

(D) This line dimensions (**DIM**) the array (**Y()**) to have (**PTS**) number of data points.

(E) This line does the same as (C) to the array (**S()**).

(F) This line starts the data collection loop which is (**PTS**) steps long.

(G) This line collects the "Cth" data point, (**J%**) of the file (**#1**).

(H) This adjusts the collected variable and adjusts it from its stored level to its actual numerical level and stores it in the array (**Y()**).

(I) This line sets the array (**S()**) value to be the corresponding (**Y()**) value.

(J) This line adds one to the value of (**J%**) so that the next data record will be collected in the next loop.

(K) This line returns the programme to line 80 (F) to continue the data collection loop until (**PTS**) steps have been executed.

(L) This line closes (**CLOSE**) the file (**#1**).

(M) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(N) The programme beyond this point gives an error report if required, see (A).

3.6 Zero values

The zero values programme converts where necessary any negative values in the array (**Y()**) to zero. The programme requires three input values, the file type variable (**SCAN**) and the arrays (**Y()**) and (**S()**). The programme outputs two variables, the adjusted arrays (**Y()**) and (**S()**). Table A4.2, table A4.3, table A4.4, listing 7.

```
10      REM ZERO VALUES
```

```
(A)   20    ON ERROR GOTO 80
(B)   30    IF SCAN=8 OR SCAN=9 OR SCAN=10 OR SCAN=11 OR
            SCAN=12 THEN GOTO 70
(C)   40    FOR C=1 TO PTS
(D)   50    IF Y(C)<0 THEN Y(C)=0 : LET S(C)=0
(E)   60    NEXT C
(F)   70    CHAIN P$,L1,ALL
(G)   80    HOME
      90    PRINT
      100   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      110   PRINT
      120   PRINT "PRESS ANY KEY TO CONTINUE."
      130   GET K$
      140   IF K$="" THEN GOTO 210
      150   LOAD "MENU",R
```

Listing 7. The zero values programme.

(A) This line sets the error trap at line 80, see (G).

(B) This line tests the value of scan to see if the values in (**Y()**) need to be zeroed. If not the programme jumps to line 70, see (F).

(C) This line starts the loop which is (**PTS**) steps long, see (E).

(D) This line tests to see if the value of (**Y()**) is less than zero, if it is, then the value is set at zero.

(E) This line returns the loop set at line 40, see (C).

(F) This line returns to the routine programme (**P$**) at the correct line (**L1**) preserving all the variables (**ALL**).

(G) The programme beyond this point gives an error report if required, see (A).

3.7 Maximum and minimum values.

The maximum and minimum values programme finds the maximum and minimum values in the array (**Y()**). The programme requires two input variables, the number of data points (**PTS**) and the array (**Y()**). The programme outputs two variables (**YMAX**), the maximum value in (**Y()**) and (**YMIN**), the minimum value in (**Y()**). Table A4.2, table A4.3, table A4.4, listing 8.

```
     10    REM MAXIMUM AND MINIMUM VALUES
(A)  20    ON ERROR GOTO
(B)  30    LET YMAX=Y(1)
     40    LET YMIN=Y(1)
(C)  50    FOR C=1 TO PTS
(D)  60    IF Y(C)>YMAX THEN YMAX=Y(C)
(E)  70    IF Y(C)<YMIN THEN YMIN=Y(C)
(F)  80    NEXT C
(G)  90    CHAIN P$,LI,ALL
     100   HOME
     110   PRINT
     120   PRINT "AN ERROR HAS OCCURRED DURING THE
           EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
           PRINT "FILE NAMES USED."
     130   PRINT
     140   PRINT "PRESS ANY KEY TO CONTINUE."
     150   GET K$
     160   IF K$="" THEN GOTO 210
     170   LOAD "MENU",R
```

Listing 8.

(A) This line sets the error trap at line 100, see (H).

(B) These lines set arbitrary value for (**YMAX**) and (**YMIN**).

(C) This line starts the loop which is (**PTS**) steps long which tests for the (**YMAX**) and (**YMIN**) values, see (F).

(D) This line tests the current (**YMAX**) value against the (**Y()**) array value, if the (**Y()**) value is greater, then it becomes (**YMAX**).

(E) This line tests the current (**YMIN**) value against the (**Y()**) array value, if the (**Y()**) value is less, then it becomes (**YMIN**).

(G) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variable (**ALL**).

(H) The programme beyond this point gives and error report if required, see (A).

3.8 Scale maximum and minimum.

The scale maximum and minimum programme adjusts the values of (**YMAH**) and (**YMIN**) to give better scaled graphs, it is only used where a graph is going to be plotted. The programme requires two input values, (**YMAH**) and (**YMIN**), and outputs these values again once they have been adjusted. Table A4.2, table A4.3, table A4.4, listing 9.

```
     10   REM SCALE MAXIMUM AND MINIMUM VALUES
(A)  20   ON ERROR GOTO 290
(B)  30   IF SCAN=2 OR SCAN=4 OR SCAN=7 THEN GOTO 100
(C)  40   IF SCAN=8 OR SCAN=9 OR SCAN=10 OR SCAN=11 OR
          SCAN=12 THEN GOTO 200
(D)  50   LET A=4.5-YMAX
     60   LET B=A/0.25
     70   LET B=FIX(B)
     80   YMAX=4.5-(B*0.25)
(E)  90   GOTO 140
(F)  100  LET A=200-YMAX
     110  B=A/5
     120  LET B=FIX(B)
     130  LET YMAX=200-(B*5)
(G)  140  IF SCAN<>8 THEN YMIN=0 GOTO 280
(H)  150  LET A=YMIN-(-0.35)
     160  LET B=A/0.05
     170  LET B=FIX(B)
     180  LET YMIN=-0.35-(B*0.05)
(I)  190  GOTO 280
(J)  200  LET A=1.6-YMAX
     210  LET B=A/0.1
     220  LET B=FIX(B)
     230  LET YMAX=1.6-(B*0.1)
     240  LET A=YMIN+(-0.1)
     250  LET B=A/0.1
     260  LET B=FIX(B)
     270  LET YMIN=0+(B*0.1)
     280  CHAIN P$,L1,ALL
     290  HOME
     300  PRINT
     310  PRINT "AN ERROR HAS OCCURRED DURING THE
          EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
          PRINT "FILE NAMES USED."
     320  PRINT
```

```
330   PRINT "PRESS ANY KEY TO CONTINUE."
340   GET K$
350   IF K$="" THEN GOTO 340
360   LOAD "MENU",R
```

Listing 9.

(A) This line sets the error trap at line 290, see (L).

(B) This line tests the value of (**SCAN**), if (**SCAN**) is 2, 4 or 7 then the programme goes to line 100, see (F).

(C) This line tests the value of (**SCAN**), if (**SCAN**) is 8, 9, 10, 11 or 12 then the programme goes to line 200, see (J).

(D) These lines adjust the value of (**YMAH**) if (**SCAN**) is 1, 3, 5 or 6.

(E) This line sends the programme to line 140, see (G).

(F) These lines adjusts the value of (**YMAH**), see (B).

(G) This line again tests the value of (**SCAN**), if (**SCAN**) is 8 then the programme continues, see (H). If (**SCAN**) is not 8 then the programme goes to line 280, see (K).

(H) These lines adjust the value of (**YMIN**), see (G).

(I) This line sends the programme to line 280, see (K).

(J) These lines adjust the values of (**YMAH**) and (**YMIN**), see (C).

(K) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(L) The programme beyond this point gives an error report if required, see (A).

3.9 Plot and label single axis

The plot and label single axis programme is used to plot annotate a single X-Y axis which occupies the whole monitor screen. Special software is required to annotate the axis since the Apple IIe in high resolution graphics mode does not permit the simultaneous printing of both text and graphics. The solution applied to this problem has been to plot the text required as individual pixels, the display produced is shown in Figure A4.4. The programme requires number input variables and outputs number variables, Listing 10.

```
        10    REM PLOT AND LABEL SINGLE AXIS
(A)     20    ON ERROR GOTO 1100
(B)     30    TEXT
        40    HGR
        50    HCOLOR=3
(C)     60    HPLOT 32,159 TO 35,0
(D)     70    HPLOT 35,159 TO 279,159
(E)     80    FOR C=35 TO 279 STEP 4
        90    HPLOT C,0 : HPLOT C,40 : HPLOT C,120
        100   NEXT C
(F)     110   FOR C=0 TO 159 STEP 4
        120   HPLOT 84,C : HPLOT 133,C : HPLOT 182,C : HPLOT : 231,C
              : HPLOT 279,C
        130   NEXT C
        140   REM LABLE AXIS
(G)     150   DIM A(125,2)
(H)     160   FOR C=1 TO 124
        170   READ A
        180   LET A(C,1)=A
        190   NEXT C
(I)     200   DATA, 2,1,2,2,2,2,1,2,3,2,1,3,3,1,2,1,1,2,3,1,2,3,3,1,
              2,3,3,3,1,2,3
        210   DATA 1,3,1,3,1,2,3,3,3,3,1,2,3,1,1,2,3,3,3,1,2,3,1,2,3,
              1,1,1,2,3,1
        220   DATA 3,1,2,3,1,2,3,1,3,3,3,3,3,1,2,3,1,3,1,2,3,1,3,1,3,
              1,2,3,1,2,3
        230   DATA1,3,1,2,3,3,3,1,2,3,1,2,3,1,3,1,3,1,3,1,3,1,3,1,2,3,1,2,
              1,2,1,2,3
(J)     240   FOR C=1 TO 124
        250   READ A
        260   LET A(C,2)=A
        270   NEXT C
(K)     280   DATA 1,2,2,3,4,5,6,6,6,1,2,2,3,4,4,5,6,6,6,1,1,1,2,3,3,
              3,4,5,6,6,6
        290   DATA 1,1,2,2,3,3,3,4,5,6,1,1,1,2,3,3,3,4,5,6,6,6,1,1,1,
              2,3,4,4,4,5
        300   DATA 5,6,6,6,1,1,1,2,2,3,4,5,6,1,1,1,2,2,3,3,3,4,4,5,5,
              6,6,6,1,1,1
        310   DATA 2,2,3,3,3,4,5,6,6,6,1,1,1,2,2,3,3,4,4,5,5,6,6,6,3,
              3,4,4,3,3,3
        320   REM POSITION AND PRINT CHARACTERS
(L)     330   LET P1=0 : LET P2=0
(M)     340   LET Z$=STR$(YMAX)
(N)     350   LET FLAG=1
```

```
(O)   360   FOR C=1 TO LEN(Z$)
(P)   370   LET Y$=MID$(Z$,C,1)
(Q)   380   IF Y$="1" THEN LET A=1 : LET B=9 : GOSUB 1000
      390   IF Y$="2" THEN LET A=10 : LET B=19 : GOSUB 1000
      400   IF Y$="3" THEN LET A=20 : LET B=31 : GOSUB 1000
      410   IF Y$="4" THEN LET A=32 : LET B=41 : GOSUB 1000
      420   IF Y$="5" THEN LET A=42 : LET B=53 : GOSUB 1000
      430   IF Y$="6" THEN LET A=54 : LET B=66 : GOSUB 1000
      440   IF Y$="7" THEN LET A=67 : LET B=75 : GOSUB 1000
      450   IF Y$="8" THEN LET A=76 : LET B=90 : GOSUB 1000
      460   IF Y$="9" THEN LET A=91 : LET B=103 : GOSUB 1000
      470   IF Y$="0" THEN LET A=104 : LET B=118 : GOSUB 1000
      480   IF Y$="." THEN LET A=119 : LET B=122 : GOSUB 1000
      490   IF Y$="-" THEN LET A=123 : LET B=124 : GOSUB 1000
(R)   500   NEXT C
(S)   510   LET FLAG=FLAG+1
(T)   520   IF FLAG>2 THEN CHAIN P$,L1,ALL
(U)   530   IF FLAG=2 THEN LET Z$=STR$(YMIN) : LET P1=0 : LET
            P2=152 : GOTO 360
(V)  1000   REM PLOT CHARACTERS ON SCREEN
     1010   FOR N=A TO B
     1020   LET H1=A(N,1)
     1030   LET Y1=A(N,2)
     1040   HPLOT H1+P1,Y1+P2
     1050   NEXT N
     1060   LET P1=P1+5
     1070   RETURN
(W)  1100   HOME
     1110   PRINT
     1120   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
     1130   PRINT
     1140   PRINT "PRESS ANY KEY TO CONTINUE."
     1150   GET K$
     1160   IF K$="" THEN GOTO 1150
     1170   LOAD "MENU",A
```

Listing 10.

(A) This line sets the error trap at line 110, see (W).

(B) These lines clear the monitor screen and put the computer into high resolution graphics mode and defines the colour of the plotted points.

(C) This line plots the Y axis.

(D) This line plots the X axis.

(E) These lines plot the grid X axis lines.

(F) These lines plot the grid Y axis lines.

(G) This line dimensions the array (**A()**) in which the coordinates of the characters to be plotted are stored.

(H) This line loads the X coordinate of the character into the array (**A()**).

(I) These lines contain the X corrdinates of the characters.

(J) This line loads the Y coordinate of the character into the array (**A()**).

(K) These lines contain the Y coordinates of the characters.

(L) This line defines the initial character plotting position.

(M) This line converts (**YMAH**) from a numeric variable to a string variable (**Z$**).

(N) This line defines the control variable (**FLAG**) which is used to define the number and position of the character being plotted.

(O) This line starts a loop which is as long as the number of characters in (**Z$**), see (R).

(P) This line selects each individual character of (**Z$**) in sequence and stores it as (**Y$**).

(Q) These lines identify the charactger (**Y$**). Once the character is identified the start position A and the end position B of the character data in the array (**A()**) are set. The programme then goes to line 1000, see (V).

(P) This line returns the loop set at line 360, see (O).

(S) This line incruments (**FLAG**).

(T) This line tests the value of (**FLAG**), if (**FLAG>2**) then the programme returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(U) This line tests the value of (**FLAG**), if (**FLAG=2**) then (**YMIN**) is converted to a string variable (**Z$**) and the programme goes to line 360, see (O).

(V) This subroutine plots the characters onto the monitor screen.

(W) The programme beyond this point gives and error report if required, see (A).

3.9.1 Plot and label twin axis.

The plot and label twin axis programme is used to plot and annotate twin X-Y axis which occupy half the monitor screen each. Special software if required to annotate the axis since the Apple IIe in high resolution graphics mode does not permit the simultaneous printing of both text and graphics. The solution applied to this problem has been to plot the text required as individual pixels, the display produced is shown in

figure A4.5. The programme requires number input variables and outputs number variables, listing 11.

```
      10    REM PLOT AND LABEL TWIN AXIS
(A)   20    ON ERROR GOT 1100
(B)   30    TEXT
      40    HGR
      50    HCOLOR=3
(C)   60    HPLOT 35,0 TO 35,75
(D)   70    HPLOT 35,85 TO 35,159
(E)   80    HPLOT 35,75 TO 279,75
(F)   90    HPLOT 35,159 TO 279,159
(G)   100   FOR C=35 TO 279 STEP 4
      110   HPLOT C,0 : HPLOT C,36 : HPLOT C,85 : HPLOT C,121
      120   NEXT C
(H)   130   FOR C=0 TO 159 STEP 4
      140   HPLOT 84,C : HPLOT 133,C : HPLOT 182,C : HPLOT 231,C :
            HPLOT 279,C
      150   HPLOT 84,C+85 : HPLOT 133,C+85 : HPLOT 182,C-85 :
            HPLOT 231,C+85 : HPLOT 279,C-85
      160   NEXT C
      170   REM LABLE AXIS
(I)   180   DIM A(125,2)
(J)   190   FOR C=1 TO 124
      200   READ A
      210   LET A(C,1)=A
      220   NEXT C
(K)   230   DATA, 2,1,2,2,2,2,1,2,3,2,1,3,3,1,2,1,1,2,3,1,2,3,3,1,
            2,3,3,3,1,2,3
      240   DATA 1,3,1,3,1,2,3,3,3,3,1,2,3,1,1,2,3,3,3,1,2,3,1,2,3,
            1,1,1,2,3,1
      250   DATA 3,1,2,3,1,2,3,1,3,3,3,3,3,1,2,3,1,3,1,2,3,1,3,1,3,
            1,2,3,1,2,3
      260   DATA1,3,1,2,3,3,3,1,2,3,1,2,3,1,3,1,3,1,3,1,3,1,2,3,1,2,
            1,2,1,2,3
(L)   270   FOR C=1 TO 124
      280   READ A
      290   LET A(C,2)=A
      300   NEXT C
(M)   310   DATA 1,2,2,3,4,5,6,6,6,1,2,2,3,4,4,5,6,6,6,1,1,1,2,3,3,
            3,4,5,6,6,6
      320   DATA 1,1,2,2,3,3,3,4,5,6,1,1,1,2,3,3,3,4,5,6,6,6,1,1,1,
```

```
          2,3,4,4,4,5
     330  DATA 5,6,6,6,1,1,1,2,2,3,4,5,6,1,1,1,2,2,3,3,3,4,4,5,5,
          6,6,6,1,1,1
     340  DATA 2,2,3,3,3,4,5,6,6,6,1,1,1,2,2,3,3,4,4,5,5,6,6,6,3,
          3,4,4,3,3,3
     350  REM POSITION AND PRINT CHARACTERS
(N)  360  LET P1=0 : LET P2=0
(O)  370  LET FLAG=0
     380  LET YMAX=D(1,5)
(P)  390  LET Z$=STR$(YMAX)
(Q)  400  FOR C=1 TO LEN(Z$)
(R)  410  LET Y$=MID$(Z,C,1)
(S)  420  IF Y$="1" THEN LET A=1 : LET B=9 : GOSUB 1000
     430  IF Y$="2" THEN LET A=10 : LET B=19 : GOSUB 1000
     440  IF Y$="3" THEN LET A=20 : LET B=31 : GOSUB 1000
     450  IF Y$="4" THEN LET A=32 : LET B=41 : GOSUB 1000
     460  IF Y$="5" THEN LET A=42 : LET B=53 : GOSUB 1000
     470  IF Y$="6" THEN LET A=54 : LET B=66 : GOSUB 1000
     480  IF Y$="7" THEN LET A=67 : LET B=75 : GOSUB 1000
     490  IF Y$="8" THEN LET A=76 : LET B=90 : GOSUB 1000
     500  IF Y$="9" THEN LET A=91 : LET B=103 : GOSUB 1000
     510  IF Y$="0" THEN LET A=104 : LET B=118 : GOSUB 1000
     520  IF Y$="." THEN LET A=119 : LET B=122 : GOSUB 1000
     530  IF Y$="-" THEN LET A=123 : LET B=124 : GOSUB 1000
(T)  540  NEXT C
(U)  550  LET FLAG=FLAG+1
(V)  560  IF FLAG=1 THEN LET YMAX=D(1,6) : LET P1=0 : LET
          P2=75 : GOTO 390
     570  IF FLAG=2 THEN YMAX=D(2,5) : LET P1=0 : LET
          P2=85 : GOTO 390
     580  IF FLAG=3 THEN LET YMAX=D(2,6) : LET P1=0 : LET
          P2=150 : GOTO 390
     590  IF FLAG=4 THEN LET YMAX=D(1,3) : LET P1=35 : LET
          P2=75 : GOTO 390
     600  IF FLAG=5 THEN LET YMAX=D(1,2) : LET P1=35 : LET
          P2=253 : GOTO 390
     610  PRINT TAB(11); D(2,3); TAB(76); D(2,2)
(W)  620  CHAIN P$,LI,ALL
(X)  1000 REM PLOT CHARACTERS ON SCREEN
     1010 FOR N=A TO B
     1020 LET X1=A(N,1)
     1030 LET Y1=A(N,2)
     1040 HPLOT X1+P1,Y1+P2
     1050 NEXT N
```

```
      1060  LET P1=P1+5
      1070  RETURN
(Y)   1100  HOME
      1110  PRINT
      1120  PRINT "AN ERROR HAS OCCURRED DURING THE
            EHECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      1130  PRINT
      1140  PRINT "PRESS ANY KEY TO CONTINUE."
      1150  GET K$
      1160  IF K$="" THEN GOTO 1150
      1170  LOAD "MENU",R
```

Listing 11.

(A) This line sets the error trap at line 1100, see (Y).

(B) These lines clear the monitor screen, put the computer into high resolution graphics mode and defines the colour of the plotted points.

(C) This line plots the upper graph X axis.

(D) This line plots the lower graph X axis.

(E) This line plots the upper graph Y axis.

(F) This line plots the lower graph Y axis.

(G) These lines plot the grid X axis lines.

(H) These lines plot the grid Y axis lines.

(I) This line dimensions the array (**A()**) in which the coordinates of the characters to be plotted are stored.

(J) This line loads the X coordinate of the character into the array (**A()**).

(K) These lines contain the X coordinates of the characters.

(L) These line loads the Y coordinate of the character into the array (**A()**).

(M) These lines contain the Y coordinates of the characters.

(N) This line defines the intital character plotting position.

(O) This line defines the control variable (**FLAG**) which is used to define the number and position of the character being plotted.

(P) This line converts (**YMAX**) from a numeric variable to a string variable (**Z$**).

(Q) This line starts a loop which is as long as the number of characters in (**Z$**), see (T).

(R) This line selects each individual character of (**Z$**) in sequence and stores it as (**Y$**).

(S) These lines identify the character (**Y$**). Once the character is identified the

start position (**A**) and the end position (**B**) of the character data in the array (**A()**) are set. The programme then goes to line 1000, see (X).

(T) This line returns the loop set at lin 400, see (Q).

(U) This line increments (**FLAG**).

(V) These lines test the value of (**FLAG**), depending on its value the number to be printed is defined and its position set.

(W) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(X) This subroutine plots the characters onto the monitor screen.

(Y) The programme beyond this point gives an error report if required, see (A).

3.10 Scale and plot graph on single axis.

The plot on single axis programme scales and plots data on a single axis. The programme requires four input variables, the number of data points (**PTS**), the array (**Y()**) which contains the points to be plotted, the value (**YSCALE**) the factor by which the array (**Y()**) is adjusted to fit the axis and the maximum value of the array (**Y()**), (**YMAX**). The display produced by this routine is shown in figure A4.6.The programme outputs one variable, the array (**Y()**) with adjusted values. Table A4.2, table A4.3, table A4.4, listing 12.

```
     10   REM SCALE AND PLOT SINGLE AXIS
(A)  20   ON ERROR GOTO 220
(B)  30   HGR2
     40   HCOLOR=3
(C)  50   LET XSCALE=242/PTS
(D)  60   FOR C=1 TO PTS
     70   LET Y(C)=Y(C)*YSCALE
     80   NEXT C
(E)  90   LET UYMAX=YSCALE*YMAX
     100  LET SHIFTY=UYMAX-159
(F)  110  IF SHIFTY=0 THEN GOTO 150
(G)  120  FOR C=1 TO PTS
     130  LET Y(C)=Y(C)-SHIFTY
     140  NEXT C
(H)  150  LET H=XSCALE
(I)  160  HPLOT 279-H,159-Y(1)
(J)  170  FOR C=1 TO PTS
```

```
        180   HPLOT TO 279-H,159-Y(C)
(K)     190   LET H=HSCALE
        200   NEHT C
(L)     210   CHAIN P$,LI,ALL
(M)     220   HOME
        230   PRINT
        240   PRINT "AN ERROR HAS OCCURRED DURING THE
              EHECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
              PRINT "FILE NAMES USED."
        250   PRINT
        260   PRINT "PRESS ANY KEY TO CONTINUE."
        270   GET K$
        280   IF K$="" THEN GOTO 270
        290   LOAD "MENU",A
```

Listing 12.

(A) This line sets the error trap at line 220, see (M).

(B) These lines put the computer into high resolution graphics mode and defines the plotted colour.

(C) This line sets the increment on the X axis.

(D) These lines scale the array (**Y()**) for plotting.

(E) These lines test for any round off error in the value of (**YSCALE**).

(F) If there is no round off error then the programme goes to line 150, see (H).

(G) These lines correct (**Y()**) for any round off error.

(H) This line sets the X axis increment (**H**).

(I) This line plots the first data point.

(J) These lines plot the graph by plotting from the last point plotted ot the next.

(K) This line incements the X axis value.

(L) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variable (**ALL**).

(M) The programme beyond this point gives an error report if required, see (A).

3.10.1 Scale and plot graph on twin axis.

The plot on twin axis programme scales and plots the data on twin axis. The programme requires five input variables, the number of data points (**PTS**), the array (**Y()**) which contains the points to be plotted, the value (**YSCALE**), the factor by which the array (**Y()**) is adjusted to fit the axis, the maximum value of the array (**Y()**), (**YMAX**) and the variable (**POST**) which defines on which axis the graph is to be plotted.

The display produced by this routine is shown in figure A4.7. The programme outputs one variable the array (**Y()**) with adjusted values. Table A4.3, table A4.4, listing 13.

```
     10    REM SCALE AND PLOT SINGLE AXIS
(A)  20    ON ERROR GOTO 220
(B)  30    HGR 2
     40    HCOLOR=3
(C)  50    LET HSCALE=242/PTS
(D)  60    FOR C=1 TO PTS
     70    LET Y(C)=Y(C)*YSCALE
     80    NEXT C
(E)  90    LET UYMAX=YSCALE*YMAX
     100   LET SHIFTY=UYMAX-74
(F)  110   IF SHIFTY=0 THEN GOTO  150
     120   FOR C=1 TO PTS
     130   LET Y(C)=Y(C)-SHIFTY
     140   NEXT C
(H)  150   LET X=HSCALE
(I)  160   IF POST=1 THEN HPLOT 279-X,74-Y(1)
(J)  170   IF POST=2 THEN HPLOT 279-X,159-(75-(159-(Y1)+74))
     180   FOR C=1 TO PTS
(K)  190   IF POST=1 THEN HPLOT TO 279-X,74-Y(C)
(L)  200   IF POST=2 THEN HPLOT TO 279-X,159-(74-(159-(Y(1)
           +74)))
(M)  210   LET X=X+HSCALE
     220   NEXT C
(N)  230   CHAIN P$.L1,ALL
(O)  240   HOME
     250   PRINT
     260   PRINT "AN ERROR HAS OCCURRED DURING THE
           EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
           PRINT "FILE NAMES USED."
     270   PRINT
     280   PRINT "PRESS ANY KEY TO CONTINUE."
     290   GET K$
     300   IF K$="" THEN GOTO 270
     310   LOAD "MENU",R
```

Listing 13.

(A) This line sets the error trap at line 240, see (O).

(B) These lines put the computer into high resolution graphics mode and define the

plotted colour.

(C) This line sets the increment on the X axis.

(D) These lines scale the array (**Y()**) for plotting.

(E) These lines test for any round off error in the value of (**YSCALE**).

(F) If there is no round off error then the programme goes to line 150, see (H).

(G) These lines correct (**Y()**) for any round off error.

(H) This line set the X axis increment (**H**).

(I) If (**POST=1**) then this line plots the first point on the upper axis.

(J) If (**POST=2**) then this line plots the first point on the lower axis.

(K) If (**POST=1**) then this line plots the graph on the upper axis.

(L) If (**POST=2**) then this line plots the graph on the lower axis.

(M) This line increments the X axis value.

(N) This line returns to the routine programme (**P$**) at the the correct line (**L1**) preserving all the variable (**ALL**).

(O) The programme beyond this point gives an error report if required, see (A).

3.11 Save file.

The save file programme saves on disc a data file which in some cases can be directly transferred back to the DU7. The programme requires five input variables, the value of (**SCAN**), the number of data points (**PTS**) the starting wavelength (**SWL**), the ending wavelength (**EWL**) and the scan speed (**SP**). The monitor display is shown in figure A4.8.Table A4.1, table A4.2, listing 14.

```
     10   REM SAVE FILE
(A)  20   ON ERROR GOTO 690
(B)  30   TEXT
     40   HOME
     50   PRINT : PRINT
(C)  60   PRINT TAB(4) : "DO YOU WISH TO SAVE THIS FILE (Y/N)"
     70   GET A$
     80   IF A$="" THEN GOTO 70
     90   IF A$"N" THEN LOAN"MENU",A
    100   IF A$<>"Y" THEN GOTO 70
    110   PRINT
    120   RESET
    130   PRINT TAB(4); "PUT DISC FOR DATA IN DRIVE 'B' AND
          PRESS ANY KEY."
```

```
        140   GET A$
        150   IF A$="" THEN GOTO 140
(D)     160   HOME
        170   FILES "B:*.DAT"
        180   PRINT
        190   PRINT "----------------------------------------"
        200   PRINT
(E)     210   PRINT TAB(4); "INPUT NAME FOR FILE (NO MORE THAN 8
              CHARACTERS)."
(F)     220   INPUT F$
(G)     230   IF LEN(F$)>8 THEN PRINT "FILE NAME TOO LONG" :
              PRINT : PRINT "PRESS ANY KEY TO CONTINUE." : GET A$ :
              GOTO 160
        240   IF LEN(F$)=0 THEN GOTO 160
(H)     250   LET F$="B:"+F$+".DAT"
(I)     260   IF SCAN=1 THEN LET A$="S" : LET B$="A" : LET J%=7 :
              LET DIV%=10000
        270   IF SCAN=2 THEN LET A$="S" : LET B$="T" : LET J%=7 :
              LET DIV%=100
        280   IF SCAN=3 THEN LET A$="T" : LET B$="A" : LET J%=7 :
              LET DIV%=10000
        290   IF SCAN=4 THEN LET A$="T" : LET B$="T" : LET J%=7 :
              LET DIV%=100
        300   IF SCAN=5 THEN LET A$="T" : LET B$="K" : LET J%=7 :
              LET DIV%=10000
        310   IF SCAN=6 THEN LET A$="S" : LET J%=3 : LET DIV%=
              10000
        320   IF SCAN=7 THEN LET A$="T" : LET J%=3 : LET DIV%=
              100
        330   IF SCAN=8 THEN LET A$="L" : LET B$="A" : LET J%=7 :
              LET DIV%=10000
        340   IF SCAN=9 THEN LET A$="D" : LET B$="1" : LET J%=7 :
              LET DIV%= 10000
        350   IF SCAN=10 THEN LET A$="D" : LET B$="2" : LET J%=7 :
              LET DIV%=10000
        360   IF SCAN=11 THEN LET A$="D" : LET B$="3" : LET J%=7 :
              LET DIV%=10000
        370   IF SCAN=12 THEN LET A$"D" : LET B$="4" : LET J%=7 :
              LET DIV%=10000
        380   IF SCAN=13 THEN LET A$"D" : LET B$="A" : LET J%=7 :
              LET DIV%=10000
        390   IF SCAN=14 THEN LET A$"U" : LET B$="A" : LET J%=7 :
              LET DIV%=10000
(J)     400   IF SCAN=6 OR SCAN=7 THEN GOTO 630
```

```
        410   OPEN "R",#1,F$,2
        420   FIELD #1,2,A$ H$
(L)     430   LSET H$=MKI$(PTS)
        440   PUT #1,1
        450   LSET H$=MKI$(SWL)
        460   PUT #1,4
        470   LSET H$=MKI$(EWL)
        480   PUT #1,5
        490   LSET H$=MKI$(SP)
        500   PUT #1,6
        510   LSET H$=A$
        520   PUT #1,2
        530   LSET H$=B$
        540   PUT #1,3
(M)     550   FOR C=1 TO PTS
        560   LET H=(S(C)*DIV%)-12233
        570   LSET H$=MKI$(H)
        580   PUT #1,J%
        590   LET J%=J%+1
        600   NEHT C
(N)     610   CLOSE #1
(O)     620   CHAIN P$,LI,ALL
(P)     630   OPEN "R",#1,F$,2
        640   FIELD #1,2 AS H$
(Q)     650   LSET H$=MKI$(PTS)
        660   PUT #1,1
        670   LSET H$=A$
        680   PUT #1,2
(R)     690   GOTO 540
(S)     700   HOME
        710   PRINT
        720   PRINT "AN ERROR HAS OCCURRED DURING THE
              EHECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
              PRINT "FILE NAMES USED."
        730   PRINT
        740   PRINT "PRESS ANY KEY TO CONTINUE."
        750   GET K$
        760   IF K$="" THEN GOTO 750
        770   LOAD "MENU",R
```

Listing 14. Save file.

(A) This line sets the error trap at line 700, see (S).

(B) These lines clear the monitor screen.

(C) These lines find if the file is to be saved, if the 'Y' key is pressed then the programme continues with the saving. If the 'N' key is pressed then the programme ends execution and loads the main menu.

(D) These lines clear the monitor screen and display the files currently on the data disc.

(E) This line is the prompt for the name of the data file which is to be saved.

(F) This line collects the new file name as (**F$**).

(G) These lines test that the inputed name (**F$**) is suitable as a file name, if (**F$**) is not suitable then the programme goes to line 160, see (D).

(H) This line adds the necessary extentions to the file name (**F$**).

(I) These lines test the value of (**SCAN**) and set (**A$**), (**B$**), (**J%**) and (**DIU%**) accordingly.

(J) This line tests to see if the file is a single wavelength scan if so then the programme goes to a special saving routine at line 630, see (P).

(K) This section of programme opens (**OPEN**) a random access file (**"R"**), labels this as the first file (**#1**), the data file opened is (**F$**) and each data section is two bytes (2). The next line sets a field (**FIELD**) for the data file (**#1**) with two bytes and each variable is assigned as (**H$**).

(L) These lines set the file header.

(M) These lines store the array (**S()**) into the data file.

(N) This line closes the data file (**F$**).

(O) This line returns to the routine programme (**P$**) at the correct line (**LI**) preserving all the variables (**ALL**).

(P) If the file is a single wavelength type. This section of programme opens (**OPEN**) a random access file (**"R"**), labels this as the first file (**#1**), the data file opened is (**F$**) and each data section is two bytes (2). The next line sets field (**FIELD**) for the data file (**#1**) with two bytes and each variable is assigned as (**H$**).

(Q) These lines set the file header for a single wavelength file.

(R) This line sends the single wavelength routine to line 540, see (M).

(S) The programme beyond this point gives an error report if required, see (A).

Table A4.1. Codes used to describe the function programmes.

Roututine programme.	Code.
Single file name.	SN
Multiple file name.	MN
File type.	FT
Identify file.	IF
File header.	FH
Load array.	LA
Zero values.	ZV
Maximum and minimum.	MM
Scale maximum and minimum.	SM
Plot and label single axis.	PS
Plot and label twin axis.	PT
Scale and plot graph, single axis.	SS
Scale and plot graph, twin axis.	ST
Save file.	SF

Table A4.2 Demonstration file illustrating the manipulation of a wavelength scan in absorbance mode for plotting by the function programmes.

Data position in array.	FT	IF	FH	LA	ZV	MM	SM	SS
1 (PTS)	-	-	10	10	10	10	10	10
2 (A$)	S	S	S	S	S	S	S	S
3 (b$)	A	A	A	A	A	A	A	A
4 (SWL)	-	-	890	890	890	890	890	890
5 (EWL)	-	-	900	900	900	900	900	900
6 (SP)	-	-	1200	1200	1200	1200	1200	1200
7	-	-	-	-.001	0.000	0.000	0.000	0.000
8	-	-	-	0.200	0.200	0.200	0.200	18
9	-	-	-	0.704	0.704	0.704	0.704	63
10	-	-	-	0.902	0.902	0.902	0.902	81
11	-	-	-	1.101	1.101	1.101	1.101	100
12	-	-	-	1.502	1.502	1.502	1.502	136
13	-	-	-	1.015	1.015	1.015	1.015	92
14	-	-	-	1.000	1.000	1.000	1.000	90
15	-	-	-	0.721	0.721	0.721	0.721	65
16	-	-	-	0.411	0.411	0.411	0.411	37
SCAN	-	1	1	1	1	1	1	1
YMAX	-	-	-	-	-	1.502	1.75	1.75
YMIN	-	-	-	-	-	0.000	0	0
YSCALE	-	-	-	-	-	0	0	90.85

Table A4.3 Main variables used in the function programmes.

Variable	Function
M$	File name without extensions.
N$	File name with extensions.
NUM	Number of data files.
B$()	Multiple file name with extensions.
A$,B$	File type identification characters.
J%	Start of data file record.
DIV%	Data multiplication factor.
SCAN	File type identification variable.
PTS	Number of data points in file.
SWL	The starting wavelength.
EWL	The ending wavelength.
SP	Scan speed.
Y()	Array containing data for manipulation.
S()	Array containing data for saving.
YMAX	Maximum value in array Y().
YMIN	Minimum value in array Y().

Table A4.4 Input and output variables used by the function programmes.

Programme	Input variables	output variables
Single file name "NAME"		N$, M$.
Multiple file name "MNAME"		B$()
File type "TYPE"	N$	A$, B$
Identify file "IDENT"	A$, B$	J%, DIV%, SCAN
File header "HEADER"	N$, SCAN	PTS, SWL, EWL, SP
Load array "ARRAY"	N$, PTS, J%, DIV%	Y(), S()
Zero values "ZERO"	SCAN, PTS, Y()	Y()
Maximum & minimum "MAXMIN"	PTS, Y()	YMAX, YMIN
Scale maximum & minimum "AMAX"	SCAN, YMAX, YMIN	YMAX, YMIN
Plot & label single axis "AXIS"	YMAX, YMIN	
Plot & label twin axis "TAXIS"	YMAX, YMIN	
Scale & plot single axis "PLOTSP"	PTS, YMAX, Y(), YSCALE	
Scale & plot twin axis "SPLOTSP"	PTS, POST, Y(), YMAX, YSCALE	
Save spectrum "STORE"	SCAN, PTS, SWL, EWL, SP	

Table A4.5 File identification variables and scan values used by the file type programme.

File identification variables.		File type	Scan number	DU7 compatable
A$	B$			
S	A	Wavelength scan, absorbance mode	1	Yes
S	T	Wavelength scan, transmittance mode	2	Yes
T	A	Time drive, absorbance mode.	3	Yes
T	T	Time drive, transmittance mode	4	Yes
T	K	Kinetics scan, absorbance mode	5	Yes
A		Fixed wavelength, absorbance mode	6	Yes
T		Fixed wavelength transmittance mode	7	Yes
L	A	Log absorbance	8	No
D	1	First derivative	9	No
D	2	Second derivative	10	No
D	3	Third derivative	11	No
D	4	Fourth derivative	12	No
D	A	Added spectra, absorbance mode	13	No
D	U	Subtracted spectra, absorbance mode	14	No

Table A4.6 Variables collected by the file header programme and their position in the header.

File identification variables.		File type	Scan number	DU7 compatable
A$	B$			
S	A	Wavelength scan, absorbance mode	1	Yes
S	T	Wavelength scan, transmittance mode	2	Yes
T	A	Time drive, absorbance mode.	3	Yes
T	T	Time drive, transmittance mode	4	Yes
T	K	Kinetics scan, absorbance mode	5	Yes
A		Fixed wavelength, absorbance mode	6	Yes
T		Fixed wavelength transmittance mode	7	Yes
L	A	Log absorbance	8	No
D	1	First derivative	9	No
D	2	Second derivative	10	No
D	3	Third derivative	11	No
D	4	Fourth derivative	12	No
D	A	Added spectra, absorbance mode	13	No
D	U	Subtracted spectra, absorbance mode	14	No

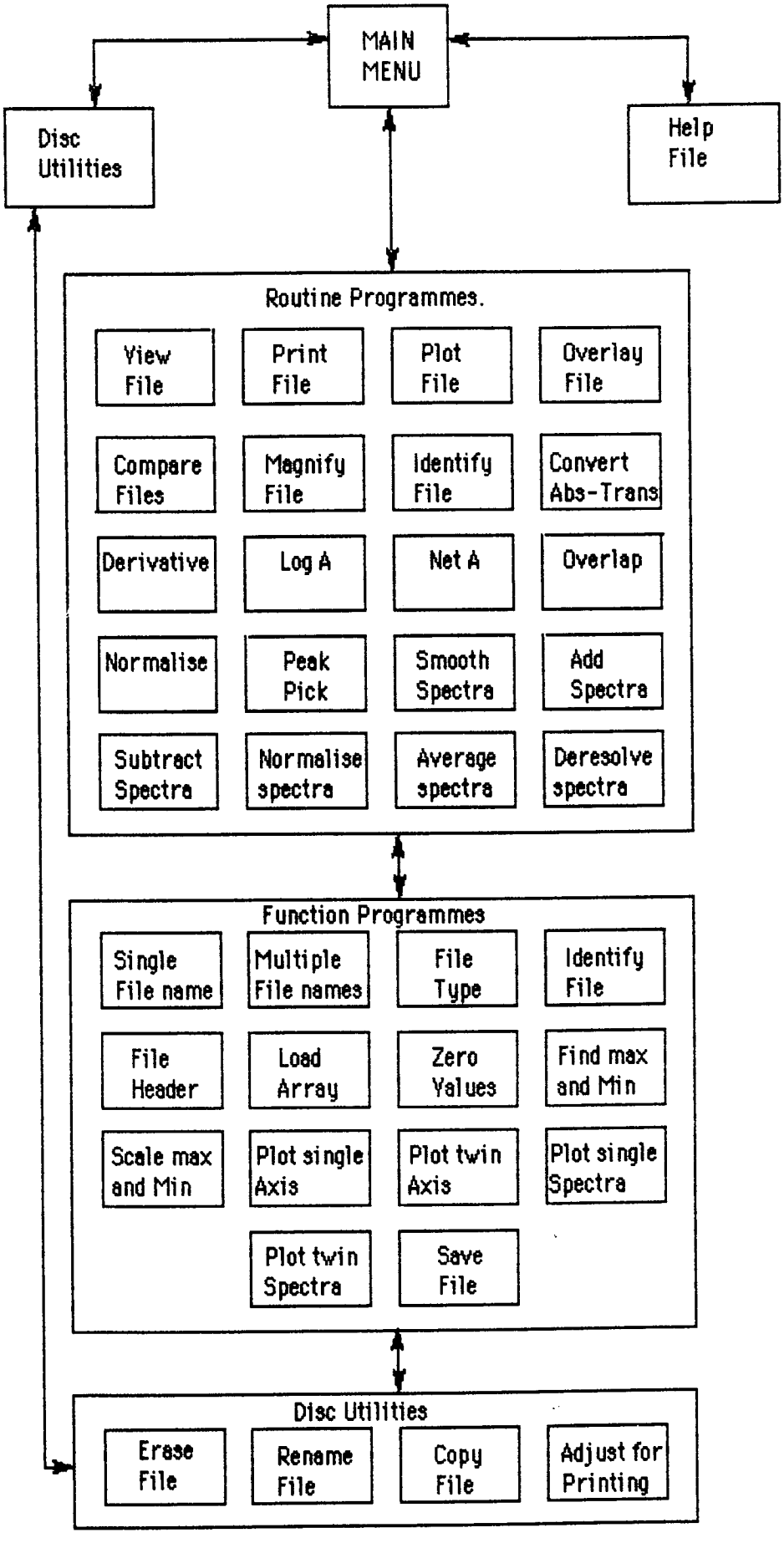


Figure A4.1 Simplified structure of the UVDMP.

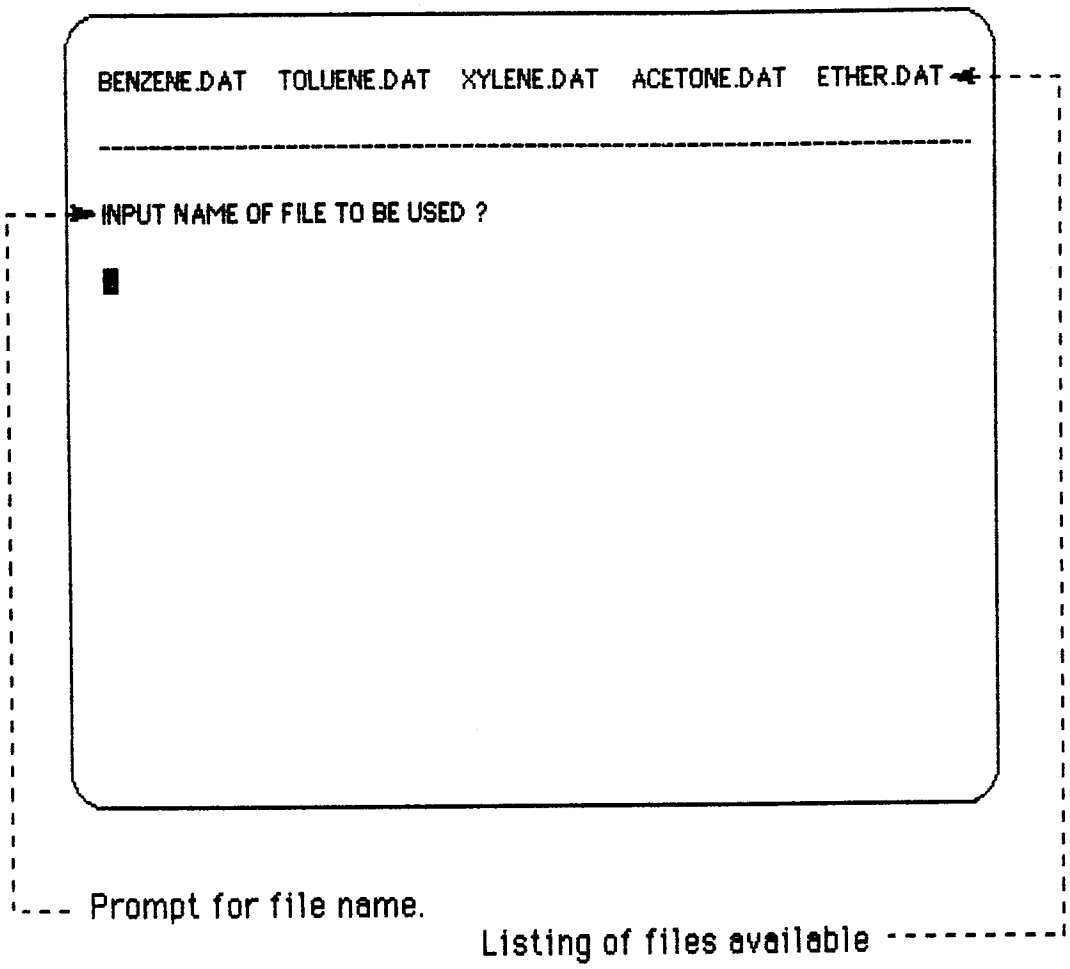


Figure A4.2 Display from single file name programme.

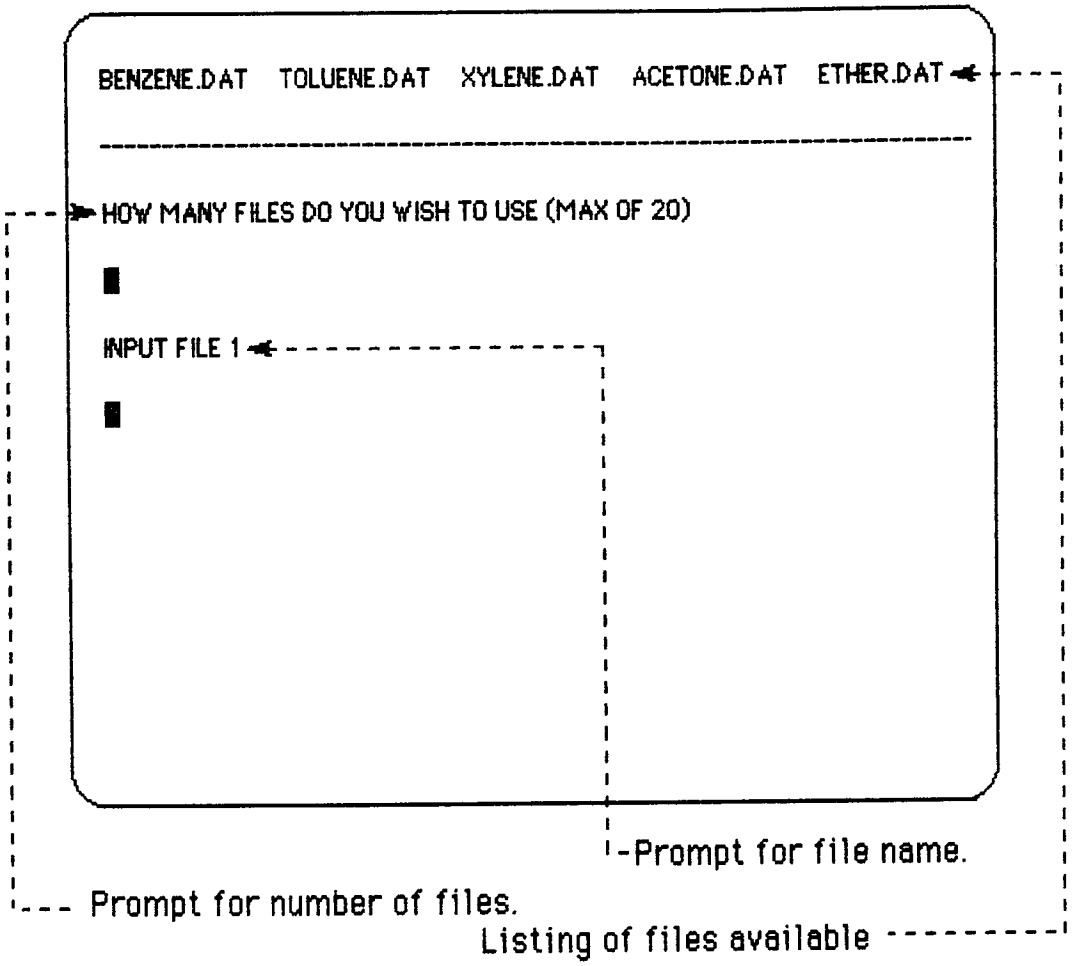


Figure A4.3 Display from the multiple file name programme.

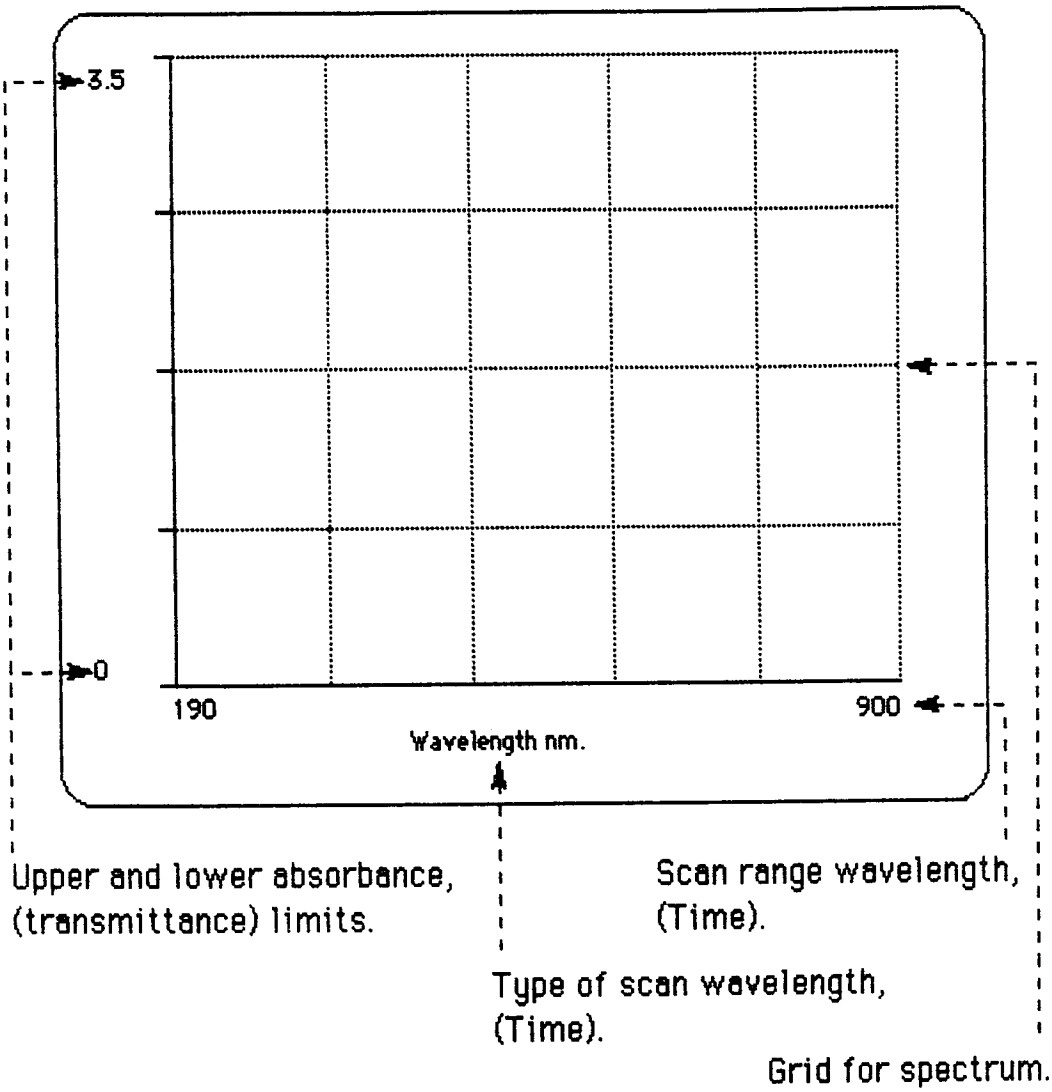


Figure A4.4 Display from plot and label single axis programme.

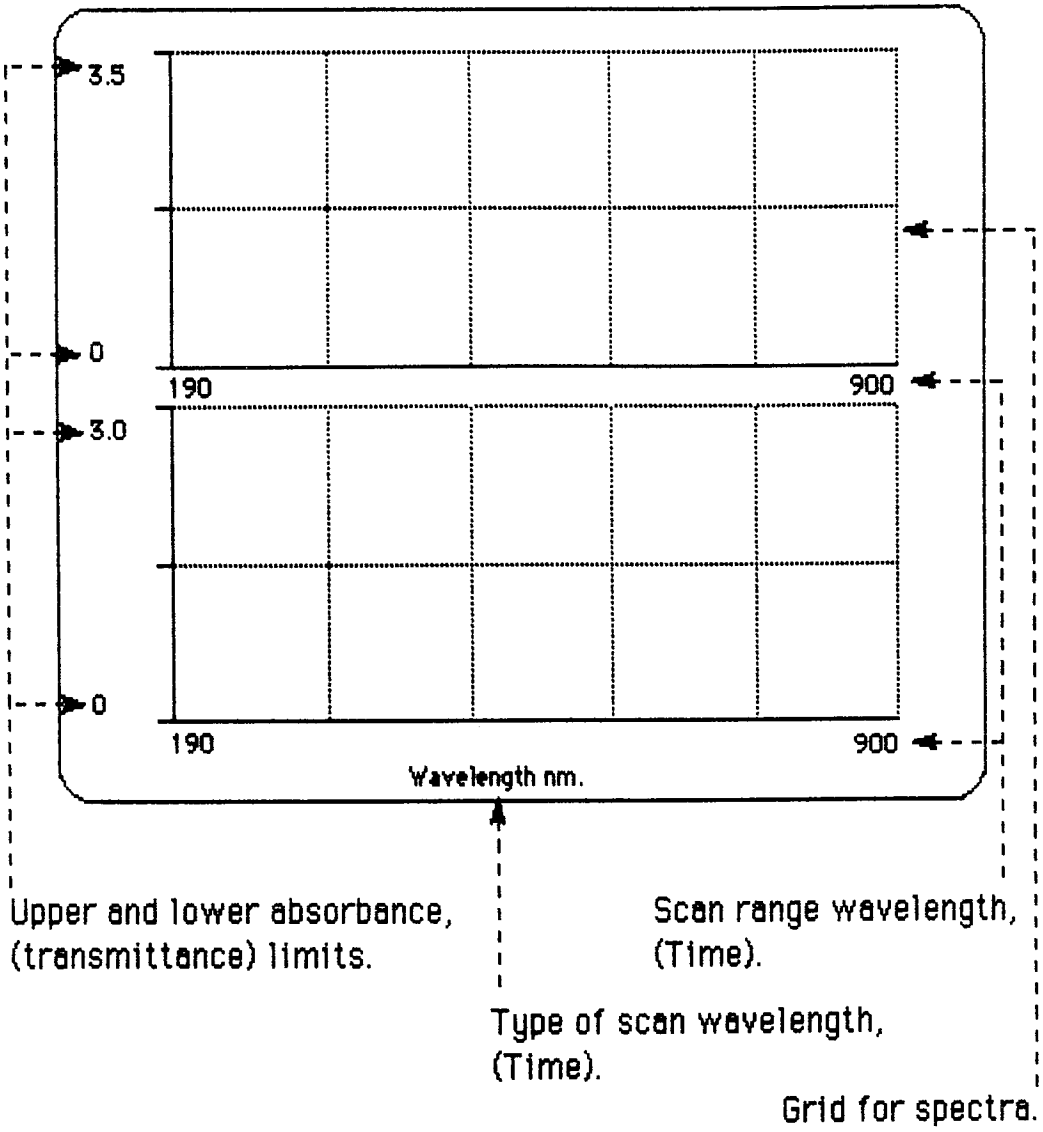
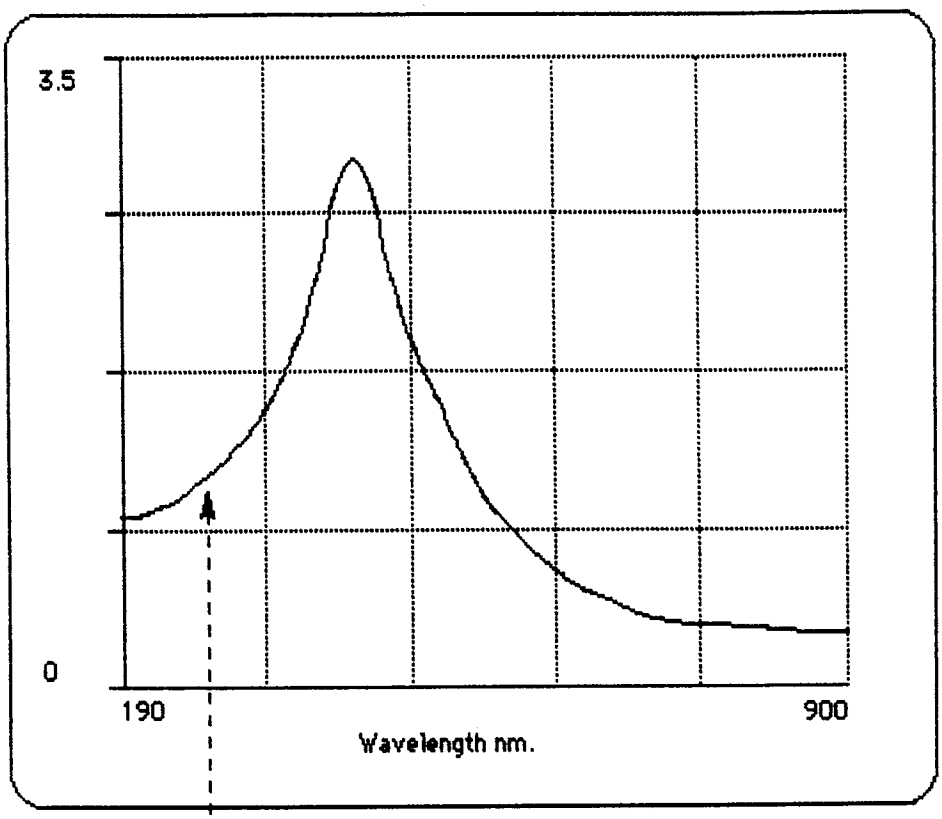
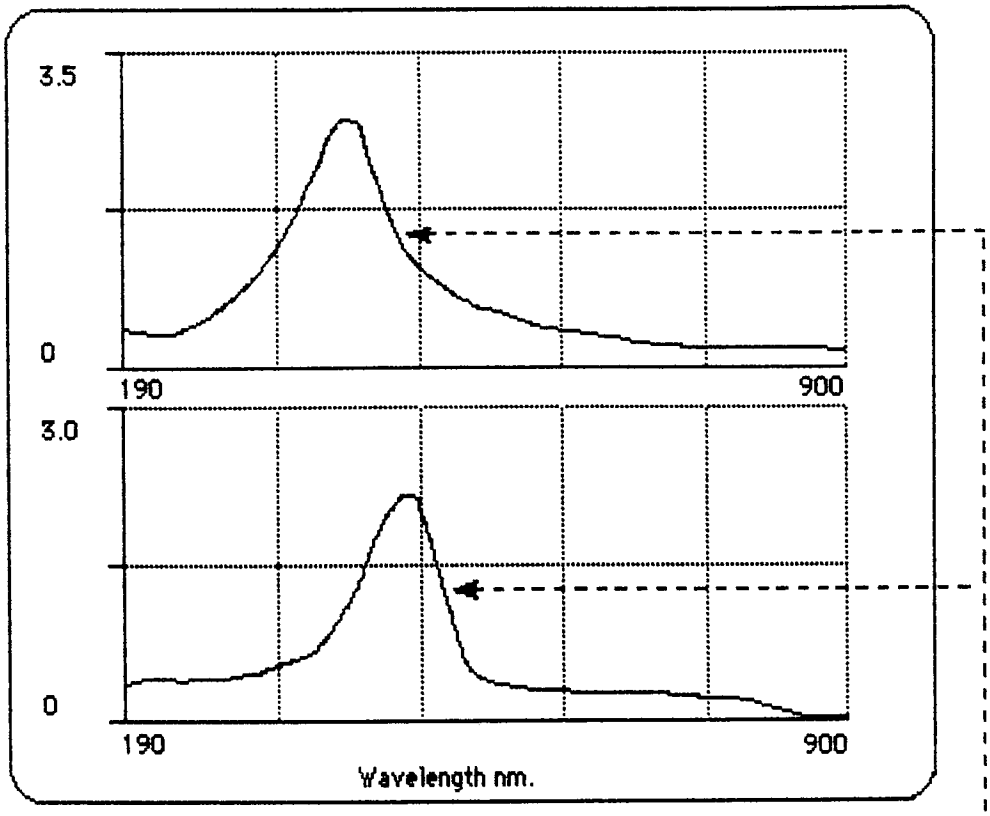


Figure A4.5 Display from plot and label twin axis programme.



Spectrum, NB the screen has a limited resolution giving the spectrum a "steped" appearance.

Figure A4.6 Display from scale and plot single axis programme.



Spectra, NB poor screen resolution gives "steped" appearance.

Figure A4.7 Display from plot graph on twin programme.

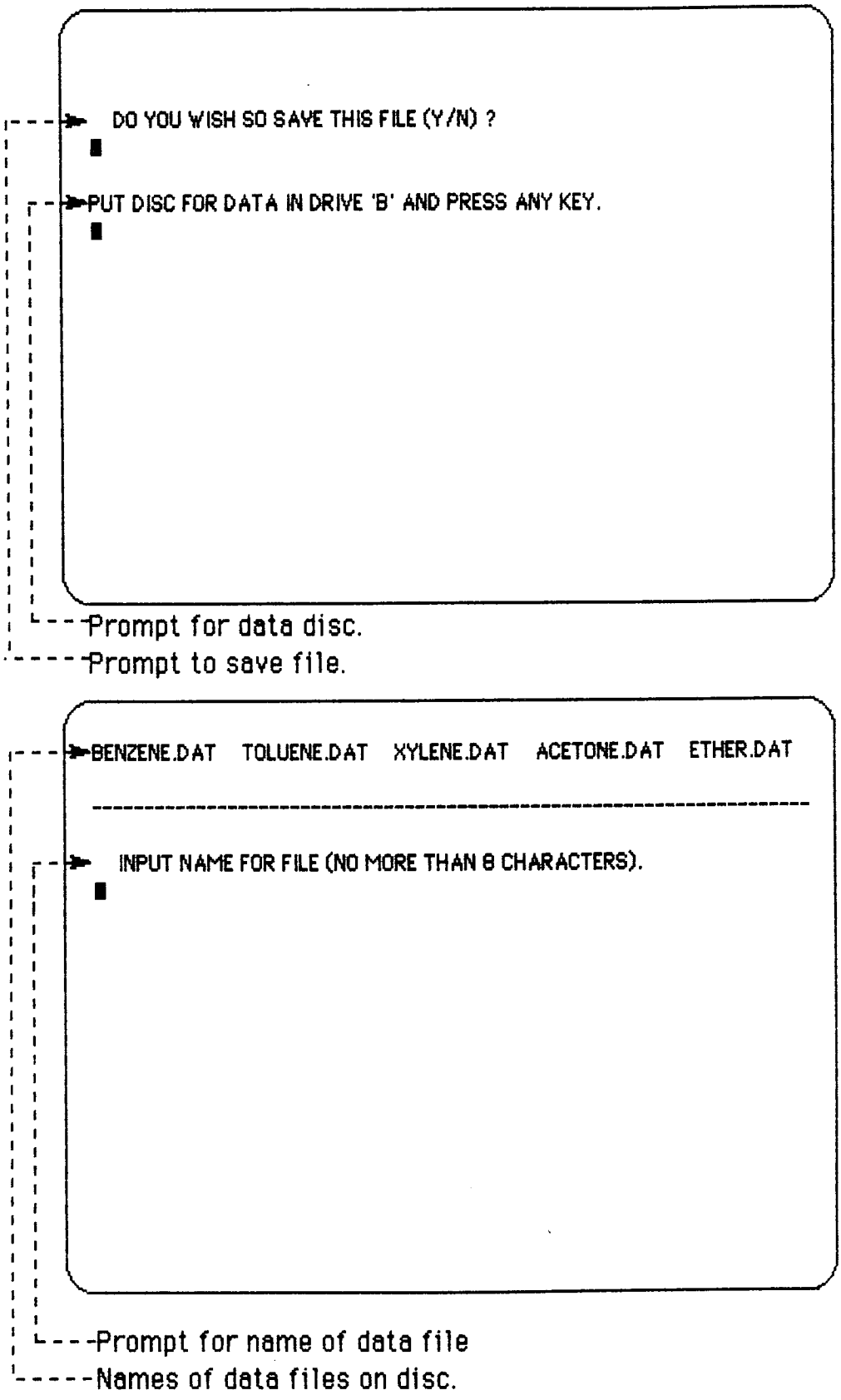


Figure A4.8 Display from save file programme.

4.0 The routine programmes.

The routine programmes carry out the various operations of the UVDMP by accessing the various function programmes, to carry out common recurring calculations and then manipulating the data according to their own purpose. All the routine programmes are accessed by a single key press via the main menu. Each listing is accompanied by a table which shows the file types used, the key press required to access and the user input required.

4.1 View file.

The view file programme emulates one of the BMSA routines which allows the spectral data in the form of a numerical file to ba displayed on the monitor screen, figure A4.9, table A4.7, listing 14.

Table A4.7 View file.

File types used.	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
All	SN, FT, IF, FH, LA, ZV.	File name	1	1

```
      10    REM VIEW FILE
(A)   20    ON ERROR GOTO 540
      30    LET OFFSET=12233
(B)   40    LET P$="A:VIEW"
      50    LI=60 : CHAIN "A:NAME",10,ALL
      60    HOME
      70    LI=80 : CHAIN "A:TYPE",10,ALL
      80    LI=90 : CHAIN "A:IDENT",10,ALL
      90    PRINT TAB (27);"CALCULATING PLEASE WAIT."
      100   LI=100 : CHAIN "A:HEADER",10,ALL
      110   LI=120 : CHAIN "A:ARRAY",10,ALL
      120   LI=130 : CHAIN "A:ZERO",10,ALL
      130   HOME
(C)   140   PRINT "FILE NAME-";M$
      150   PRINT "DATA POINTS-";PTS
      160   PRINT "MODE"
(D)   170   IF SCAN=1 THEN PRINT "WAVELENGTH SCAN,
            ABSORBANCE."
```

```
      180   IF SCAN=2 THEN PRINT "WAVELENGTH SCAN, %
            TRANSMITTANCE."
      190   IF SCAN=3 THEN PRINT "TIME DRIVE, ABSORBANCE."
      200   IF SCAN=4 THEN PRINT "TIME DRIVE, %
            TRANSMITTANCE"
      210   IF SCAN=5 THEN PRINT "KINETICS SCAN, ABSORBANCE."
      220   IF SCAN=6 THEN PRINT "FIXED WAVELENGTH,
            ABSORBANCE."
      230   IF SCAN=7 THEN PRINT "FIXED WAVELENGTH, %
            TRANSMITTANCE."
      240   IF SCAN=8 THEN PRINT "LOG, ABSORBANCE."
      250   IF SCAN=9 THEN PRINT "1st DERIVATIVE."
      260   IF SCAN=10 THEN PRINT "2nd DERIVATIVE."
      270   IF SCAN=11 THEN PRINT "3rd DERIVATIVE."
      280   IF SCAN=12 THEN PRINT "4th DERIVATIVE."
      290   IF SCAN=13 THEN PRINT "ADDED SPECTRA,
            ABSORBANCE."
      300   IF SCAN=14 THEN PRINT "SUBTRACTED SPECTRA,
            ABSORBANCE."
(E)   400   IF SCAN<>3 AND SCAN<>4 AND SCAN<>5 AND SCAN<>6
            AND SCAN<>7 THEN PRINT TAB(10); "START WVL";
            TAB(25); "END WVL"; TAB(35); "SPEED" : PRINT TAB(10);
            SWL; TAB(25); EWL; TAB(35); SP
(F)   410   IF SCAN=3 OR SCAN=4 OR SCAN=5 THEN PRINT TAB(10);
            "TOTAL TIME'; TAB(25);"WAVELENGTH; TAB(35);"SPEED":
            PRINT TAB(10); EWL;TAB(25); SWL/10; TAB(35); SP
      420   LET N=0
(G)   430   FOR I=1 TO PTS
      440   LET N=N+1
(H)   450   IF DIV%=10000 THEN PRINT USING " ##.####"; Y(I)
(I)   460   IF DIV%=100 THEN PRINT USING " ###.##"; Y(I)
      470   IF N=8 THEN PRINT
      480   IF N=8 THEN LET N=0
      490   NEXT I
      500   PRINT
      510   PRINT "PRESS ANY KEY TO CONTINUE."
      520   GET K$
      530   IF K$="" THEN GOTO 520
      540   LOAD "A:MENU",R
(K)   550   HOME
      560   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      570   PRINT
```

```
580    GET K$
590    IF K$="" THEN GOTO 580
600    LOAD "A:MENU",R
```

Listing 14. View file.

(A) This line sets the error trap at line 550, see (K).

(B) This line sets the value of (**P$**) to (**A:VIEW**) so that the function programmes load on completion the correct routine programme.

(C) These lines print on the monitor the file name and number of data points.

(D) These lines print on the monitor the scan mode according to the value of (**SCAN**).

(E) If the scan is not a time drive or fixed wavelength then the starting wavelength, finishing wavelength and scan speed are printed.

(F) For time drive scans this line prints the total time, wavelength and speed.

(G) This line starts the loop which prints out the data values.

(H) This line sets the printer template for values of (**DIV%**) of 10000 and prints the value.

(I) This line sets the printer template for values of (**DIV%**) of 100 and prints the value.

(J) These lines pause the programme and on a key press load the main menu back into memory.

(K) The lines beyond this point give an error report if required.

4.2 Print file.

The print file programme emulates one of the BMSA routines which allows the spectral data in the form of a numerical file to be dumped to a printer, figure A4.10, table A4.8, listing 15.

Table 4.8 Print file.

File types used.	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
All	SN, FT, IF, FH, LA, ZV.	File name	2	1

```
        10    REM PRINT FILE
(A)     20    ON ERROR GOT 540
        30    LET OFFSET=12233
(B)     40    LET P$="A:PRINT"
        50    LI=60 : CHAIN "A:NAME",10,ALL
        60    HOME
        70    LI=80 : CHAIN "A:TYPE",10,ALL
        80    LI=90 : CHAIN "A:IDENT",10,ALL
        90    PRINT TAB(27); "CALCULATING, PLEASE WAIT."
        100   LI=110 : CHAIN "A:HEADER",10,ALL
        110   LI=120 : CHAIN "A:ARRAY",10,ALL
        120   LI=130 : CHAIN "A:ZERO",10,ALL
        130   HOME
(C)     140   LPRINT "FILE NAME-"; M$
        150   LPRINT "DATA POINTS-"; PTS
        160   LPRINT "MODE."
(D)     170   IF SCAN-1 THEN LPRINT "WAVELENGTH SCAN,
              ABSORBANCE."
        180   IF SCAN=2 THEN LPRINT "WAVELENGTH SCAN, %
              TRANSMITTANCE."
        190   IF SCAN=3 THEN LPRINT "TIME DRIVE, ABSORBANCE."
        200   IF SCAN=4 THEN LPRINT "TIME DRIVE, %
              TRANSMITTANCE."
        210   IF SCAN=5 THEN LPRINT "KINETICS SCAN,
              ABSORBANCE."
        220   IF SCAN=6 THEN LPRINT "FIXED WAVELENGTH,
              ABSORBANCE."
        230   IF SCAN=7 THEN LPRINT "FIXED WAVELENGTH, %
              TRANSMITTANCE."
        240   IF SCAN=8 THEN LPRINT "LOG, ABSORBANCE."
        250   IF SCAN=9 THEN LPRINT "1ST DERIVATIVE."
        260   IF SCAN=10 THEN LPRINT "2ND DERIVATIVE."
        270   IF SCAN=11 THEN LPRINT "3RD DERIVATIVE."
        280   IF SCAN=12 THEN LPRINT "4TH DERIVATIVE."
        290   IF SCAN=13 THEN LPRINT "ADDED SPECTRA,
              ABSORBANCE,"
        300   IF SCAN=14 THEN LPRINT "SUBTRACTED SPECTRA,
              ABSORBANCE."
(E)     400   IF SCAN<>3 AND SCAN<>4 AND SCAN<>5 AND SCAN<>6
              AND SCAN<>7 THEN LPRINT TAB(10); "START
              WVL"; TAB(25); "END WVL"; TAB(35); "SPEED" : LPRINT
              TAB(10); SWL; TAB(25); EWL; TAB(35); SP
(F)     410   IF SCAN=3 OR SCAN=4 OR SCAN=5 THEN LPRINT
```

```
            TAB(10); "TOTAL TIME"; TAB(25); "WAVELENGTH";
            TAB(35); "SPEED" : LPRINT TAB(10); EWL;
            TAB(25); SWL/10; TAB (35); SP
      420   LET N=0
(G)   430   FOR I=1 TO PTS
      440   LET N=N+1
(H)   450   IF DIV%=10000 THEN LPRINT USING " ##.####"; Y(I)
(I)   460   IF DIV%=100 THEN LPRINT USING " ###.##"; Y(I)
      470   IF N=9 THEN LPRINT
      480   IF N=8 THEN LET N=0
      490   NEXT I
      500   LPRINT
(J)   510   PRINT "PRESS ANY KEY TO CONTINUE."
      520   GET K$
      530   IF K$="" THEN GOTO 520
      540   LOAD "A:MENU",R
(K)   550   HOME
      560   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTING, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      570   PRINT
      580   GET K$
      590   IF K$="" THEN GOT 580
      600   LOAD "A:MENU",R
```

Listing 15. Print file.

(A) This line sets the error trap at line 550, see (K).

(B) This line sets the value of (**P$**) to (**A:PRINT**) so that the function programmes load on completion the correct routine programme.

(C) These lines print on the monitor the file name and number of data points.

(D) These lines print on the monitor the scan mode according to the value of (**SCAN**).

(E) If the scan is not a time drive or fixed wavelength then the starting wavelength, finishing wavelength and scan speed are printed.

(F) For time drive scans, this line prints the total time, wavelength and speed.

(G) This line starts the loop which prints out the data values.

(H) This line sets the printer template for values of (**DIV%**) of 10000 and prints the value.

(I) This line sets the printer template for values of (**DIV%**) of 100 and prints the value.

(J) These lines pause the programme and on a key press load the main menu back

into memory.

(K) The lines beyong this point give an error report if required.

4.3 Plot file.

The plot file programme displays on the monitor the spectrum in the form of an XY graph. The limits of the axis are automatically selected to optimise the display. The display produced is shown in figure A4.6, table A4.9, listing 16.

Table A4.9 Plot file.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
Not 6, 7	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	File name	3	1

```
     10   REM PLOT SINGLE SPECTRUM.
(A)  20   ON ERROR GOTO 260
     30   LET OFFSETT=12233
(B)  40   LET P$="A:PLOT"
(C)  50   LI=60 : CHAIN "A:NAME",10,ALL
     60   HOME
     70   PRINT TAB(27); "CALCULATING PLEASE WAIT."
     80   LI=90 : CHAIN "A:TYPE",10,ALL
     90   LI=100 : CHAIN "A:INDENT",10,ALL
     100  IF SCAN=100 THEN PRINT "SPECTRUM IS OF AN
          UNKNOWN TYPE AND CANNOT BE PLOTTED." : GOTO 220
     110  IF SCAN=6 OR SCAN=7 THEN PRINT "FIXED WAVELENGTH
          SCANS CANNOT BE PLOTTED." : GOTO 220
(D)  120  LI=130 : CHAIN "A:HEADER",10,ALL
     130  LI=140 : CHAIN "A:ARRAY",10,ALL
     140  LI=150 : CHAIN "A:ZERO",10,ALL
     150  LI=160 : CHAIN "A:MAXMIN",10,ALL
     160  LI=170 : CHAIN "A:AMAX",10,ALL
(E)  170  LET YSCALE=159/(YMAX-YMIN)
(F)  180  LI-190 : CHAIN "A:AXIS",10,ALL
     190  LI=200 : CHAIN "A:PLOTSP",10,ALL
```

```
(G)   200   IF SCAN=1 OR SCAN=2 OR SCAN=9 OR SCAN=10 OR
            SCAN=11 OR SCAN=12 OR SCAN=13 OR SCAN=14 THEN
            PRINT TAB(11); EWL; TAB(76); SWL : PRINT TAB(33);
            "WAVELENGTH NM."
(H)   210   IF SCAN=3 OR SCAN=4 OR SCAN=5 THEN PRINT
            TAB(11); "0";=; TAB(76);EWL; : PRINT TAB(33);"TIME"
(I)   220   PRINT "PRESS ANY KEY TO CONTINUE.
      230   GET K$
      240   IF K$="" THEN GOTO 230
      250   LOAD "A:MENU,R
      260   HOME
(J)   270   PRINT "AN ERROR HAS OCCURRED DURING THE
            EHECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      280   PRINT
      290   GET K$
      300   IF K$="" THEN GOTO 290
      310   LOAD "A:MENU",R
```

Listing 16. Plot file.

(A) This line gives an error report if required, see J.

(B) This line sets the value of (**P$**) to (**A:PLOT**).

(C) These lines collect the file name, identify the file type and checks that it is a type that can be plotted.

(D) These lines collect the file header information, load the array, zero the values, calculate and alter the maximum and minimum values.

(E) This line calculates the values of (**YSCALE**).

(F) These lines plot the axis and graph.

(G) For wavelength scans, this line lables the X axis.

(H) For time drive spectra, this line lables the X axis.

(I) These lines pause the programme until a key is pressed, then which the scan is cleared and the main menu loaded.

(J) These lines give an error report if required, see (A).

4.4 Overlay files.

The overlay files programme allows upto 20 spectra to be plotted in an overlaid form on an X Y graph. The limits of the axis are automatically selected to optimise the display. The display produced is illustrated in figure A4.11, table A4.10, listing 17.

Table A4.10 Overlay files.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
Not 6, 7	MN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	Number of files. File names.	4	1

```
     10   REM OVERLAY SPECTRA
(A)  20   ON ERROR GOTO 650
     30   LET OFFSET=12233
(B)  40   LET P$="OVER"
     50   LI=60 : CHAIN "A:MNAME",10,ALL
     60   HOME
     70   PRINT TAB(27); "CALCULATING PLEASE WAIT."
     75   DIM P(20)
     76   DIM D(NUM,7)
(C)  80   LET I=1
     85   LET N$=""
     90   FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEXT K
     100  LI=110 : CHAIN "A:TYPE",10,ALL
     110  LI=115 : CHAIN "A:IDENT",10,ALL
     155  LET D(1,7)=J%
     120  LET P(I)=SCAN
(D)  130  LET I=I+1 : IF I<NUM THEN GOTO 85
     140  REM CHECK ALL SPECTRA ARE OF THE SAME TYPE.
(E)  150  FOR I=1 TO NUM
     160  IF P(I)<>SCAN THEN HOME : PRINT "SPECTRA ARE NOT
          ALL OF SAME TYPE, PROGRAMME CANNOT CONTINUE." :
          GOTO 600
     170  NEXT I
     180  REM COLLECT ALL HEADER INFORMATION
(F)  200  LET I=1
     210  LET N$=""
     220  FOR J=1 TO 15 : LET N$=N$+B$(J,I) : NEXT J
     230  LI=240 : CHAIN "A:HEADER",10,ALL
     240  LET D(I,1)=PTS
     250  LET D(I,2)=SWL
     260  LET D(I,3)=EWL
     265  LET D(I,4)=SP
```

```
        269   LET J%=INT(D(I,7))
        270   LI=272 : CHAIN "A:ARRAY",10,ALL
        272   LI=273 : CHAIN "A:ZERO",10,ALL
        273   LI=274 : CHAIN "A:MAHMIN",10,ALL
        274   LET D(I,5)=YMAH
        275   LET D(I,6)=YMIN
        280   LET I=I+1 : IF I<=NUM THEN GOT 210
        290   IF SCAN<>1 AND SCAN<>2 THEN GOTO 360
        300   REM CHECK FOR MAH AND MIN WAVELENGTHS OF SCAN
(J)     310   FOR I=1 TO NUM
        320   IF D(I,2)>SWL THEN SWL=D(I,2)
        330   IF D(I,3)<EWL THEN EWL=D(I,3)
        340   NEHT I
        350   GOTO 400
        360   REM FIND TIME FOR TIME DRIVE SCANS
        370   FOR I=1 TO NUM
        380   IF D(I,3)>EWL THEN EWL=D(I,3)
        390   NEHT I
        400   REM FIND YMAH AND YMIN IN ALL FILES
        420   LET YMAH=D(1,5) : LET YMIN=D(1,6)
(K)     430   FOR I=1 TO NUM
        440   IF D(I,5)>YMAH THEN YMAH=D(1,5)
        450   IF D(1,6)<YMIN THEN YMIN=D(I,6)
        460   NEHT I
(L)     475   LI=480 : CHAIN "A:AMAH",10,ALL
(M)     480   LET YSCALE=159/(YMAH-YMIN)
(N)     490   LI=500 : CHAIN "A:AHIS",10,ALL
(O)     500   LET I=1
        510   LET N$=""
        520   FOR J=1 TO 15 : LET N$=N$+B$+B$(J,I) : NEHT J
        525   LET PTS=D(I,1)
        526   LET J%=INT(D(I,7))
        530   LI=540 : CHAIN "A:ARRAY",10,ALL
        540   LI=550 : CHAIN "A:ZERO",10,ALL
        550   LET PTS=D(I,1)
        560   LI=570 : CHAIN "A:PLOTSP",10,ALL
        570   LET I=I+1 : IF I<=NUM THEN GOTO 510
(P)     580   IF SCAN=1 OR SCAN=2 OR SCAN=8 OR SCAN=9 OR
              SCAN=10 OR SCAN=11 OR SCAN=12 OR SCAN=13 OR
              SCAN=14 THEN PRINT TAB(11); EWL; TAB(76); SWL; :
              PRINT TAB(33); "WAVELENGTH nm."
        590   IF SCAN=3 OR SCAN=4 OR SCAN=5 THEN PRINT
              TAB(11):"0"; TAB(76);EWL; : PRINT TAB(33); "TIME."
(Q)     600   PRINT "PRESS ANY KEY TO CONTINUE."
```

```
610   GET K$
620   IF K$="" THEN GOTO 610
630   TEXT
640   LOAD "A:MENU",R
650   HOME
660   PRINT "AN ERROR HAS OCCURRED DURING THE
      EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND " :
      PRINT "FILE NAMES USED."
670   PRINT
680   GET K$
690   IF K$="" THEN GOTO 680
700   LOAD "A:MENU",R
```

Listing 17. Overlay files.

(A) This line gives and error report if required, see (R).

(B) This line sets the value of (**P$**) to "over".

(C) This line starts the loop which collects the file type data which is stored in the arrays (**P()**) and (**D()**).

(D) This line ends the loop.

(E) These lines check that the spectra are all the same type so they can be overlayed, if not an error report is given and the programme returns to the main menu.

(F) This loop collects the header information and stores it in the array (**D()**) along with the maximum and minimum values.

(G) This line tests for the limits of the X axis.

(H) This line tests for the limits of the Y axis.

(I) This line adjusts the maximum value.

(J) This line sets the value of Y scale.

(K) This line draws the graph axis.

(L) These lines load, zero and plot each graph in turn.

(M) These lines lable the X axis as required.

(N) These line pause the programme until a key is pressed after which the main menu if loaded.

(R) These lines give an error report if required, see (A).

4.5 Compare files.

The compare file programme allows two files to be simultaneously compared on separate axis one above the other. The files can be of different types. The display

produced is illustrated in figure A4.7, table A4.11, listing 18.

Table A4.11 Compare files.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
Not 6, 7	MN, FT, IF, FH, LA, ZV, MM, SM, PT, ST.	File names.	5	1

```
        10    REM COMPARE TWO FILES
(A)     20    ON ERROR GOTO 420
        30    LET OFFSET=12233
(B)     40    LET P$="COMPARE"
(C)     50    LET NUM=2
        60    LI=70 : CHAIN "A:MNAME",10,ALL
        80    PRINT TAB(27); "CALCULATING, PLEASE WAIT."
        90    DIM P(2)
        100   DIM D(2,8)
(D)     110   LET I=1
        120   LET N$=""
        130   FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEXT K
        140   LI=150 : CHAIN "A:TYPE",10,ALL
        150   LI=160 : CHAIN "A:IDENT",10,ALL
        160   LET D(I,7)=J%
        165   LET D(I,8)=DIV%
        170   LET P(I)=SCAN
        180   LI=181 : CHAIN "A:HEADER",10,ALL
        181   LET D(I,1)=PTS
        182   LET D(I,2)=SWL
        183   LET D(1,3)=EWL
        184   LET D(I,4)=SP
        190   LI=200 : CHAIN "A:ARRAY",10,ALL
        200   LI=210 : CHAIN "A:ZERO",10,ALL
        210   LI=220 : CHAIN "A:MAXMIN",10,ALL
        220   LI=230 : CHAIN "A:MAX",10,ALL
        230   LET D(I,5)=YMAX
        240   LET D(I,6)=YMIN
        250   LET I=I+1 : IF I<=NUM THEN GOTO 120
```

```
(E)   260   LI=270 : CHAIN "A:TAXIS",10,ALL
      270   REM PLOT
(F)   280   LET I=1
      290   LET N$=""
      300   FOR K=1 TO 15 : LET N$=N$+B$(K,1) : NEXT K
      302   LET PT$=D(I,1)
      304   LET J%=INT(D(I,7))
      305   LET DIV%=INT(D(I,8))
      306   IF I=1 THEN LET POST=1
      308   IF I>1 THEN LET POST=2
      309   LET SCAN=P(I)
      310   LI=315 : CHAIN "A:ARRAY",10,ALL
      315   LI=320 : CHAIN "A:ZERO",10,ALL
      320   LET YMAX=D(1,5)
      330   LET YMIN=D(I,6)
      340   LET YSCALE=74/(YMAX-YMIN)
      350   LI=360 : CHAIN "A:PLOTSP",10,ALL
      360   LET I=I+1 : IF I<=NUM THEN GOTO 290
(F)   370   PRINT "PRESS ANY KEY TO CONTINUE."
      380   GET K$
      390   IF K$="" THEN GOTO 380
      400   TEXT
      410   LOAD "MENU",R
(H)   420   HOME
      430   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      440   PRINT
      450   GET K$
      460   IF K$="" THEN GOTO 450
      470   LOAD "A:MENU",R
```

Listing 18. Compare files.

(A) This line gives an error report if required, see (H).

(B) This line sets the value of (**P$**) to compare.

(C) This line sets the number of file names (**NUM**) to be collected.

(D) These lines collect the file type, Indent, Header , Maximum and Minimum values from the two selected files.

(E) This line plots the twin axis on the monitor scree.

(F) These lines collect the data for and plot the two graphs, the first named one on the upper graph and the second on the lower.

(G) These lines pause the programme until a key is pressed, after which the programme returns to the main menu.

(H) These lines give an error report if requires, see (A).

4.6 Magnify file.

The magnify file programme allows an area of a spectra to be highlighted and examined in detail, this smaller spectra can be saved so that other operations can be carried out quicker on the smaller file. The monitor display for this programme is shown in figure A4.12. The monitor display produced is the same as for plot file, figure A4.6, table A4.12, listing 19.

Table A4.12 Magnify file.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
Not 6, 7	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS, SF	File name. Starting, ending wavelength.	8	1

```
        10    REM MAGNIFY SPECTRUM
(A)     20    ON ERROR GOTO 810
        30    LET OFFSET=12233
(B)     40    LET P$="MAG"
        50    LI=60 : CHAIN "A:NAME",10,ALL
        60    HOME
        70    PRINT TAB(27); "CALCULATING PLEASE WAIT."
(C)     80    LI=90 : "A:TYPE",10,ALL
        90    LI=100 : CHAIN "A:IDENT",10,ALL
(D)     100   IF SCAN=1 OR SCAN=2 OR SCAN=8 OR SCAN=9 OR
              SCAN=10 OR SCAN=11 OR SCAN=12 OR SCAN=13 OR
              SCAN=14 THEN GOTO 120
        110   PRINT : PRINT "SPECTRUM MUST BE EITHER A
              WAVELENGTH SCAN IN ABSORBANCE OR
              TRANSMITTANCE" : PRINT "OR A LOG 10 ABSORBANCE,
              OR A DERIVATIVE, OR AN ADDED OR SUBTRACTED
              SPECTRUM"
        115   PRINT : PRINT "PRESS ANY KEY TO CONTINUE." : GET K$
              : LOAD "MENU",R
```

```
(F)   120   LI=130 : CHAIN "A:HEADER",10,ALL
      130   HOME
      140   PRINT "FILE NAME-"; M$
      150   PRINT "DATA POINTS-"; PTS
      160   PRINT
      170   PRINT "MODE"
      180   IF SCAN=1 THEN PRINT "WAVELENGHT SCAN,
            ABSORBANCE."
      190   IF SCAN=2 THEN PRINT "WAVELENGTH SCAN,
            TRANSMITTANCE."
      200   IF SCAN=8 THEN PRINT "LOG ABSORBANCE."
      210   IF SCAN=9 THEN PRINT "1ST DERIVATIVE."
      220   IF SCAN=10 THEN PRINT "2ND DERIVATIVE."
      230   IF SCAN=11 THEN PRINT "3RD DERIVATIVE."
      240   IF SCAN=12 THEN PRINT "4TH DERIVATIVE."
      250   IF SCAN=13 THEN PRINT "ADDED SPECTRA,
            ABSORBANCE."
      260   IF SCAN=14 THEN PRINT "SUBTRACTED SPECTRA,
            ABSORBANCE."
      270   PRINT
      280   PRINT "STARTING WAVELENGTH-"; SWL; "nm.'
      290   PRINT
      300   PRINT "ENDING WAVELENGTH-"EWL; "nm."
      310   PRINT
      320   PRINT "SCAN SPEED-"; SP; "nm/min."
      330   VTAB(14)
(G)   340   PRINT "NEW STARTING WAVELENGTH-";
      350   INPUT SWL1
      360   IF SWL1<>INT(SWL1) OR SWL1>SWL OR SWL1<=EWL
            THEN VTAB(14) : PRINT "
                 " : GOTO 330
      370   VTAB(16)
(H)   380   PRINT "NEW ENDING WAVELENGTH-";
      390   INPUT EWL1
      400   IF EWL<>INT(EWL1) OR EWL1>SWL OR EWL1>SWL1 OR
            EWL1<EWL THEN VTAB(16) :
            PRINT"                                    " : GOTO 370
      410   HOME
(I)   420   PRINT TAB(27); "CALCULATING PLEASE WAIT."
      430   LI=440 : CHAIN "A:ARRAY",10,ALL
      440   LI=450 : CHAIN "A:ZERO",10,ALL
(J)   450   LET PTS1=PTS-1
      460   LET WVL-(SWL-EWL)/PTS1
      470   LET XRANGE=(SWL1-EWL1)
```

```
        480   LET PTS1=(HRANGE/WVL)+1
        490   ERASE S
        500   DIM S(PTS1)
(K)     510   FOR I=1 TO PTS
        520   LET SPOS=SWL-(WVL*I)-WVL
        530   IF SPOS=SWL1 THEN LET SPOS=I : GOTO 550
        540   NEXT I
        550   FOR I=1 TO PTS
        560   LET EPOS=EWL-(WVL*I)-WVL
        570   IF EPOS=EWL1 THEN LET : GOTO 590
        580   NEXT I
        585   LET COUNT=0
        590   FOR I=SPOS TO EPOS
        620   NEXT I
(I)     630   ERASE Y
        640   DIM Y(PTS1)
        650   FOR I=1 TO PTS1
        660   LET Y(I)=S(I)
        670   NEXT I
(M)     680   LET PTS=PTS1
        690   LET SWL=SWL1
        700   LET EWL=EWL1
(N)     710   LI=720 : CHAIN " A:MAXMIN:,10,ALL
        720   LI=730 : CHAIN "A:AMAX",10,ALL
        730   LET YSCALE=159/(YMAX-YMIN)
        740   LI=750 : CHAIN "A:AXIS",10,ALL
        750   LI=760 : CHAIN "A:PLOTSP",10,ALL
        760   PRINT TAB(11); EWL; TAB(76); SWL : PRINT
              TAB(33); "WAVELENGTH nm."
(O)     770   PRINT "PRESS ANY KEY TO CONTINUE."
        780   GET K$
(P)     790   LI=800 : CHAIN "A:STORE",10,ALL
        800   LOAD "MENU",R
(Q)     810   HOME
        820   PRINT "AN ERROR HAS OCCURRED DURING THE
              EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
              PRINT "FILE NAMES USED."
        830   PRINT
        840   GET K$
        850   IF K$="" THEN GOTO 840
        860   LOAD "A:MENU",R
```

Listing 19. Magnify file.

(A) This line gives an error report if requires, see (Q).

(B) This line sets the value of (**P$**) to (**MAG**).

(C) These lines collect the file type and identification data.

(D) This line checks that the file is of a suitable type of magnification, ie, a wavelength scan.

(E) If the scan is not of a permitted type then these lines print an error message and return to the main menu on a key press.

(F) These lines collect and print the file header information and print the file name, number of data points, the scan mode, the maximum and minimum wavelength and the scan speed.

(G) These lines print a prompt for a new starting wavelength, tests that it is a permitted wavelength and if not re-prompts for a new input.

(H) These lines perform the same function as (G) for the new ending wavelength.

(I) These lines collect and zero the array data.

(J) These lines calculate the new number of data points.

(K) These lines transfer the data from the (**Y()**) array to the (**S()**) array.

(L) These lines erase the old (**U()**) array, dimension as new (**Y()**) array and transfer data from the (**S()**) array to the (**Y()**) array.

(M) These lines redefine new values of (**PTS**), (**SWL**) and (**EWL**).

(N) These lines prepare and plot the new recognised spectrum on the monitor.

(O) These lines pause the programme until a key is pressed.

(P) This line accesses the routine to allow the new spectrum to be saved.

(Q) This line gives an error message if required, see (A).

4.7 Identify file.

The identify file programme gives information as to the nature of the file chosen. The programme displays on the monitor the file name, number of data points, the scan mode, the starting wavelength, the ending wavelength, (or total time and wavelength for kinetics scans), the scan speed, maximum and minimum values. The display produced is shown in figure A4.13, table A4.13, listing 20.

Table A4.13 Identify file.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
Not 6, 7	SN, FT, IF, FH, LA, ZV, MM.	File name	1	2

```
     10   REM IDENTIFY FILE TYPE
(A)  20   ON ERROR GOTO 610
     30   LET OFFSET=12233
(B)  40   LET P$="FIND"
(C)  50   LI=60 : CHAIN "A:NAME",10,ALL
     60   HOME
     70   LI=80 : CHAIN : "A:TYPE,10,ALL
     80   LI=90 : CHAIN "A:IDENT",10,ALL
     90   PRINT TAB(27); "CALCULATING PLEASE WAIT."
     100  LI=10 : CHAIN "A: HEADER",10,ALL
     110  LI=120 : CHAIN "A:ARRAY",10,ALL
     120  LI=125 : CHAIN "A:ZERO",10,ALL
     125  LI=130 : CHAIN "A:MAXMIN",10,ALL
(D)  130  HOME
     140  PRINT "FILE NAME-";M$
     150  PRINT "DATA POINTS-";PTS
     160  PRINT "MODE."
     170  IF SCAN=1 THEN PRINT "WAVELENGTH SCAN,
          ABSORBANCE."
     180  IF SCAN=2 THEN PRINT "WAVELENGTH SCAN, %
          TRANSMITTANCE."
     190  IF SCAN=3 THEN PRINT "TIME DRIVE, ABSORBANCE."
     200  IF SCAN=4 THEN PRINT "TIME DRIVE, %
          TRANSMITTANCE."
     210  IF SCAN=5 THEN PRINT "KINETICS SCAN, ABSORBANCE."
     220  IF SCAN=6 THEN PRINT "FIXED WAVELENGTH,
          ABSORBANCE."
     230  IF SCAN=7 THEN PRINT "FIXED WAVELENGTH, %
          TRANSMITTANCE."
     240  IF SCAN=8 THEN PRINT "LOG, ABSORBANCE."
     250  IF SCAN=9 THEN PRINT "1ST DERIVATIVE."
     260  IF SCAN=10 THEN PRINT "2ND DERIVATIVE."
```

```
290   IF SCAN=13 THEN PRINT "ADDED SPECTRA,
      ABSORBANCE."
300   IF SCAN=14 THEN PRINT "SUBTRACTED SPECTRA,
      ABSORBANCE."
400   IF SCAN<>3 AND SCAN<>4 AND SCAN<>5 AND SCAN<>6
      AND SCAN<>7 THEN PRINT TAB(10); "START WVL";
      TAB(25); "END WVL"; TAB(35); "SPEED" : PRINT
      TAB(10); SWL; TAB(25); EWL; TAB(35); SP
410   IF SCAN=3 OR SCAN=4 OR SCAN=5 THEN PRINT TAB(10);
      "TOTAL TIME"; TAB(25); "WAVELENGTH"; TAB(35);
      SPEED" : PRINT TAB(10); EWL; TAB(25); SWL/10;
      TAB(35); SP
500   PRINT "MAXIMUM VALUE-"; YMAX
510   PRINT "MINIMUM VALUE-"; YMIN
560   PRINT
570   PRINT "PRESS ANY KEY TO CONTINUE."
580   GET K$
590   IF K$="" THEN GOTO 580
600   LOAD "A:MENU",R
610   HOME
620   PRINT "AN ERROR HAS OCCURRED DURING THE
      EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
      PRINT "FILE NAMES USED."
630   PRINT
640   GET K$
650   IF K$="" THEN GOTO 640
660   LOAD "A:MENU",R
```

(E) (F)

Listing 20. Identify file.

(A) This line gives and error message if required, see F.

(B) This line sets the value of (**P$**) to (**FIND**).

(C) These lines collect the file name, all the header information, load and zero the array and find the maximum and minimum values.

(D) These lines print the file name, data points, scan mode, starting and ending wavelength or wavelength on line for kinetics scans followed by the scan speed and the Maximum and Minimum values.

(E) These lines pause the programme until a key is pressed after which the programme returns to the main menu.

(F) These lines give an error report if required, see A.

4.8 Derivative programme.

The derivative programme calculates the first, second, third or fourth derivative of a wavelength scan in absorbance mode. The derivative is calculated using a simple algorythmn which assumes that the line between two adjacent points of the spectrum is straight. Therefore the derivative which is the slope of the curve resolves itself to a simple triangle, figure A14, table A4.14, listing 21.

Table A4.14 Derivative programme.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS, SF.	File name.	2	2

```
     10   REM DERIVATIVE
(A)  20   ON ERROR GOTO 580
     30   LET OFFSET=12233
(B)  40   LET P$="A:DERV"
     50   LI=60 : CHAIN "A:NAME"10,ALL
     60   HOME
(C)  70   LI=80 : CHAIN "A:TYPE",10,ALL
     80   LI=90 : CHAIN "A:IDENT",10,ALL
(D)  90   IF SCAN=1 THEN GOTO 110
(E)  100  PRINT : PRINT "DERIVATIVE FUNCTION WILL ONLY
          WORK WITH WAVELENGTH SCANS IN ABSORBANCE
          MODE." : PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
          GET K$ : LOAD "A:MENU",R
(F)  110  PRINT TAB(32);"DERIVATIVE MENU."
     120  PRINT "-----------------------------------"
     130  PRINT : PRINT
     140  PRINT TAB(4); "(1)-CALCULATE AND DISPLAY 1ST
          DERIVATIVE."
     150  PRINT
     160  PRINT TAB(4); "(2)-CALCULATE AND DISPLAY 2ND
          DERIVATIVE."
     170  PRINT
     180  PRINT TAB(4); "(3)-CALCULATE AND DISPLAY 3RD
          DERIVATIVE."
```

```
        190   PRINT
        200   PRINT TAB(4); "(4)-CALCULATE AND DISPLAY 4TH
              DERIVATIVE."
        210   PRINT
        220   GET A$
(G)     230   IF A$="" THEN GOTO 220
        240   IF A$="1" THEN LET U=1 : GOTO 290
        250   IF A$="2" THEN LET U=2 : GOTO 290
        260   IF A$="3" THEN LET U=3 : GOTO 290
        270   IF A$="4" THEN LET U=4 : GOTO 290
        280   GOTO 220
(H)     290   LI=300 : CHAIN "A:HEADER",10,ALL
        300   LI=310 : CHAIN "A:ARRAY",10,ALL
        310   LI=320 : CHAIN "A:ZERO",10,ALL
        320   HOME : PRINT TAB(27); "CALCULATING PLEASE WAIT."
(I)     322   LET SCAN=8+U
        325   REM CALCULATE DERIVATIVE
        330   LET HRANGE=SWL-EWL
        340   LET HINC=HRANGE/PTS
(J)     350   FOR N=1 TO U
        360   LET S(1)=0
(K)     370   FOR I=1 TO PTS-1
        380   LET S(I+1)=(Y(I)-Y(I+1))/HINC
        390   LET S(1)=0
        400   LET S(PTS)=0
        410   NEXT I
        420   FOR I=1 TO PTS
        430   LET Y(I)=S(I)
        440   NEXT I
(M)     450   NEXT N
(N)     460   LI=470 : CHAIN "A:MAXMIN",10,ALL
        470   LI=480 : CHAIN "A:AMAX",10,ALL
        480   YSCALE=159/(YMAX-YMIN)
        490   LI=500 : CHAIN "A:AXIS",10,ALL
        500   LI=510 : CHAIN "A:PLOTSP",10,ALL
        510   PRINT TAB(11); EWL; TAB(76); SWL; : PRINT U;
              "DERIVATIVE"; TAB(33); "WAVELENGTH nm."
(O)     520   PRINT "PRESS ANY KEY TO CONTINUE"
        530   GET K$
        540   IF K$="" THEN GOTO 530
        550   TEXT
(P)     560   LI=570 : CHAIN "A:STORE",10,ALL
        570   LOAD "A:MENU",R
(Q)     580   HOME
```

```
590   PRINT "AN ERROR HAS OCCURRED DURING THE
      EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
      PRINT "FILE NAMES USED."
600   PRINT
610   GET K$
620   IF K$="" THEN GOTO 610
630   LOAD "A:MENU",R
```

Listing 21. Derivative programme.

(A) This line gives an error message if required, see Q.

(B) This line sets the value of (**P$**) to (**DERV**).

(C) These lines collect the file type data.

(D) This line checks that the file is a wavelength scan in absorbance mode.

(E) If the file is not of the correct type then this line prints an error message, pause the programme and on a key press, returns to the main menu.

(F) These lines print the derivative menu.

(G) These lines accept the key press from the derivative menu and set the value of (**U**) accordingly.

(H) These lines collect and zero the array data.

(I) This line sets the new value of scan for the selected derivative.

(J) This line starts the derivative calculation loop.

(K) These lines calculate a single derivative.

(L) These lines store the new derivative file in the array (**Y()**).

(M) This line ends the derivative calculation loop.

(N) These lines plot the new derivative.

(O) These lines pause the programme until a key is pressed.

(P) This line allows the derivative file to be saved.

(Q) This line gives an error message if required, see A.

4.9 Log absorbance.

The log absorbance programme emulates a function available on the DU7 but in addition allows the new file created to be saved onto a floppy disc. The log absorbance programme simply converts all the absorbance values from a wavelength scan into their logramithic equivalent value and displays the resulting file on the screen. The monitor appears as figure A4.6, table A4.15, listing 22.

Table A4.15 Log absorbance.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	File name.	2	2

```
      10    REM LOG A PROGRAMME
(A)   20    ON ERROR GOTO 330
      30    LET OFFSET=12233
(B)   40    LET P$="A:LOGA"
      50    LI=60 : CHAIN "A:NAME",10,ALL
      60    HOME
      70    PRINT TAB(27); "CALCULATING PLEASE WAIT."
(C)   80    LI=90 : CHAIN "A:TYPE",10,ALL
      90    LI=100 : CHAIN "A:IDENT",10,ALL
(D)   100   IF SCAN=1 THEN GOTO 120
(E)   110   PRINT : PRINT "ONLY WAVELENGTH SCANS IN
            ABSORBANCE MODE MAY BE USED." : PRINT : PRINT
            "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
            "MENU",R
(F)   120   LI=130 : CHAIN "A:HEADER",10,ALL
      130   LI=140 : CHAIN "A:ARRAY",10,ALL
      140   LI=150 : CHAIN "A:ZERO",10,ALL
      150   REM CALCULATE LOG A
(G)   155   LET SCAN=8
(H)   160   FOR I=1 TO PTS
      170   IF Y(I)=LOG(Y(I))
(I)   185   LET S(I)=Y(I)
(J)   190   NEXT I
(K)   200   LI=210 : CHAIN "A:MAXMIN",10,ALL
      210   LI=220 : CHAIN "A:AMAX",10,ALL
      220   YSCALE=159/(YMAX-YMIN)
      230   LI=240 : CHAIN "A:AXIS,10,ALL
      240   LI=250 : CHAIN "A:PLOTSP",10,ALL
      250   PRINT TAB(11); EWL; TAB(76); SWL; : PRINT TAB(33);
            "WAVELENGTH nm."
(L)   270   PRINT ANY KEY TO CONTINUE."
      280   GET K$="" THEN GOTO 280
      300   TEXT
```

```
      310   CHAIN "A:STORE,10,ALL
      320   LOAD "A:MENU", R
(M)   330   HOME
      340   PRINT "AN ERROR HAS OCCURRED DURING THE
            EHECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      350   PRINT
      360   GET K$
      370   IF K$="" THEN GOTO 360
      380   LOAD "A:MENU",R
```

Listing 22. Log absorbance.

(A) This line sets the error trap at line 330, see M.

(B) This line sets the value of (**P$**) to (**LOG A**).

(C) These lines collect the header information.

(D) This line tests to see if the scan is of the correct type and wavelength scan in absorbance mode.

(E) If the scan is not of the correct type this line prints on error message, pauses the programme and on a key press returns to the main menu.

(F) These lines store the data into the array and zeros any negative values.

(G) This line sets the value of (**SCAN**) to 8.

(H) This line starts the loop which counts the array value to it log value.

(I) This line stores the log values in the saving array (**S()**).

(J) This line ends the log calculation loop.

(K) These lines carry out the necessary calculations to plot the log graph.

(L) These lines pause the programme until a key is pressed after which the main menu is loaded.

(M) These lines give an error message if required, see A.

4.10 Overlap.

The overlap programme calculates as a percentage the degree of similarity between two spectra. The programme calculates the average of the sum of the square of the difference between all the points on the spectra and reports the result as a percentage, figure A4.15, table A4.16, listing 23.

Table A4.16 Overlap programme.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	File name	3	2

```
      10    REM OVERLAP
(A)   20    ON ERROR GOTO 730
      30    LET OFFSETT=12233
(B)   40    LET P$="LAP"
(C)   50    LET NUM=2
      60    LI=70 : CHAIN "A:MNAME",10,ALL
      70    HOME
      80    PRINT TAB(27); "CALCULATING PLEASE WAIT."
(D)   90    DIM D(2,9)
      100   LET I=1
(E)   110   LET N$=""
      120   FOR K=1 TO 15 : LET N$=N$+B$(K,1) : NEXT K
      130   LI=140 : CHAIN "A:TYPE",10,ALL
      140   LI=150 : CHAIN "A:IDENT",10,ALL
      150   LET D(1,7)=J%
      160   LET D(1,8)=DIV%
      170   LET D(1,9)=SCAN
(F)   180   IF SCAN<>1 THEN PRINT "ONLY WAVELENGTH SCANS IN
            ABSORBANCE MODE MAY BE USED." : PRINT : PRINT
            "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
            "MENU",R
(G)   190   LI=200 : CHAIN "A:HEADER",10,ALL
      200   LET D(1,1)=PTS
      210   LET D(1,2)=SWL
      220   LET D(1,3)=EWL
      230   LET D(1,4)=SP
      240   LET I=1 : IF 1<NUM THEN GOTO 110
(H)   250   IF D(1,1)=D(2,1) AND D(1,2)=D(2,2) AND D(1,3)=D(2,3)
            AND D(1,4)=(2,4) THEN GOTO 270
(I)   260   PRINT : PRINT "FILES MUST BE COLLECTED UNDER
            IDENTICAL CONDITIONS." : PRINT : PRINT "PRESS ANY
            KEY TO CONTINUE." : GET K$ : LOAD "MENU",R
```

```
(J)   270   LET I=1
      280   LET N$=""
      290   FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEHT K
      300   LI=310 : CHAIN "A:ARRAY",10,ALL
      310   LI=320 : CHAIN "A:ZERO",10,ALL
      320   LI=330 : CHAIN "A:MAHMIN",10,ALL
      330   LI=340 : CHAIN "A:MAH",10,ALL
      340   LET D(1,5)=YMAH
      350   LET D(1,6)=YMIN
      355   IF I>1 THEN GOTO 400
      360   IF I=1 THEN DIM Z(PTS) DIM Z(PTS) : LET J%=7
      370   FOR N=1 TO PTS
      380   LET Z(N)=Y(N)
      390   NEHT N
(K)   400   LET I=1+1 : IF I<=NUM THEN GOTO 280
(L)   450   LET YMAH=D(1,5)
      460   IF D(2,5)>YMAH THEN YMAH=D(2,5)
      470   LET YMIN=D(1,6)
      480   IF D(2,6)<YMIN THEN YMIN=D(2,6)
      490   ERASE D
(M)   500   FOR I=1 TO PTS
      510   LET DIFF=DIFF+SQR((Z(I)-Y(I))*(Z(I)-Y(I)))
      520   NEHT I
      525   IF DIFF=0 THEN LET DIFF=100 : GOTO 570
(N)   530   LET DIFF=DIFF/PTS
      540   DIFF=(DIFF/4.5)
      550   IF DIFF=1 THEN LET DIFF=0 : GOTO 570
      560   LET DIFF=ABS((DIFF*100)-100)
(O)   570   LI=580 : CHAIN "AHIS",10,ALL
      580   FOR I-1 TO PTS
      590   LET S(I)=Z(I)
      600   LET Z(I)=Y(I)
      610   LET Z(I)=Y(I)
      620   NEHT
      630   LET I=1
      640   LET N$=""
      650   FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEHT K
      656   IF I=1 THEN GOTO 660
      657   FOR N-1 TO PTS
      658   LET Y(N)=Z(N)
      659   NEHT N
      660   LI=670 : CHAIN "A:PLOTSP",10,ALL
      705   LET 1=I+1 : IF I<=NUM THEN GOTO 640
(P)   710   PRINT "SPECTRA ARE"; DIFF; "% SIMILAR."
```

```
(Q)   720   PRINT "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
            "MENU",R
(R)   730   HOME
      740   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
            PRINT "FILE NAMES USED."
      750   PRINT
      760   GET K$
      770   IF K$="" THEN GOTO 760
      780   LOAD "A:MENU",R
```

Listing 23. Overlap programme.

(A) This line sets the error trap, see R.

(B) This line sets the value of (**P$**) to (**LAP**).

(C) This line sets the number of file names to be collected to 2.

(D) This line sets the array to store the header data.

(E) These lines identify the file type and define values of (**J%**), (**DIV**) and (**SCAN**).

(F) This line ensures that the file isof the correct type, ie, a wavelength scan in absorbance mode. If not, an error message is printed, the programme paused and on a key press returns to the main menu.

(G) These lines collect the header information and store it in the array (**D()**).

(H) This line tests that all header information is the same for both files.

(I) If the header information is not identical this line prints and error message, pauses the programme and on a key press returns to the main menu.

(J) This line starts the loop which collects both data files and stores them in the arrays (**Y()**) and (**Z()**).

(K) This line ends the data file collection loop.

(L) These lines calculate the maximum and minimum Y values.

(M) This loop calculates the positive difference between the two files.

(N) This line calculates the average difference per point.

(O) These lines plot the two spectra.

(P) This line presents the % similarity between the two spectra.

(Q) This line pauses the programme until a key is pressed.

(R) This line is the error trap.

4.11 Normalise spectrum.

The normalise spectrum adjusts proportionally the spectrum such that the maximum value corresponds to some arbitary value. This programme allows for better display of files in for example a library disc, figure A4.16, table A4.17, listing 24.

Table A4.17 Normalise spectrum.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	File name, new maximum.	3	2

```
     10   REM NORMALISE SPECTRUM
(A)  20   ON ERROR GOTO 450
     30   LET OFFSET=12233
(B)  40   LET P$="NORM"
     50   LI=60 : CHAIN "A:NAME",10,ALL
     60   HOME
     70   PRINT TAB(27); "CALCULATING PLEASE WAIT."
     80   LI=90 : CHAIN "A:TYPE",10,ALL
     90   LI=100 : CHAIN "A:IDENT",10,ALL
(C)  100  IF SCAN=1 THEN GOTO 120
(D)  110  PRINT : PRINT "ONLY WAVELENGTH SCANS IN
          ABSORBANCE MODE MAY BE USED." : PRINT : PRINT
          "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
          "MENU",R
(E)  120  LI=130 : CHAIN "A:HEADER",10,ALL
     130  LI=140 : CHAIN "A:ARRAY",10,ALL
     140  LI=150 : CHAIN "A:ZERO",10,ALL
     150  LI=151 : CHAIN "A:MAXMIN",10,ALL
     160  HOME
     170  PRINT : PRINT
     180  PRINT " INPUT MAXIMUM VALUE TO ADJUST SPECTRUM
          TO."
     190  INPUT TOP
     200  IF TOP<0 OR TOP >4.5 THEN GOTO 160
(G)  210  LET FACT=0-YMIN
     220  FOR I=1 TO PTS
     230  LET Y(I)=Y(I)+FACT
```

```
        240   LET S(I)=Y(I)
        250   NEXT
(H)     260   LET YMAX=YMAX+FACT
        270   LET YMIN=0
        280   LET FACT=TOP/YMAX
(I)     290   FOR I=1 TO PTS
        300   LET Y(I)=Y(I)*FACT
        310   LET S(I)=Y(I)
        320   NEXT I
(J)     330   LET YMAX=TOP
        340   YSCALE=159/(YMAX-YMIN)
(K)     350   LI=190 : CHAIN "A:AXIS",10,ALL
        360   LI=200 : CHAIN "A:PLOTSP",10,ALL
        370   IF SCAN=1 OR SCAN=2 THEN PRINT TAB(11); EWL;
              TAB(76); SWL; : PRINT TAB(33); "WAVELENGTH nm."
        380   PRINT "PRESS ANY KEY TO CONTINUE."
        390   GET K$
        400   IF K$="" THEN GOTO 390
        410   TEXT
        420   HOME
(L)     430   LI=260 : CHAIN "A:STORE",10,ALL
        440   LOAD "A:MENU".R
(M)     450   HOME
        460   PRINT "AN ERROR HAS OCCURRED DURING THE
              EXECUTION OF THIS ROUTINE, CHECK ALL DISCS AND" :
              PRINT "FILE NAMES USED."
        470   PRINT
        480   GET K$
        490   IF K$="" THEN GOTO 480
        500   LOAD "A:MENU",R
```

Listing 24. Normalise spectrum.

(A) This line sets the error trap, see M

(B) This line sets the value of (**P$**) to (**NORM**).

(C) This line ensures that the file is in absorbance mode.

(D) If the scan is not in the correct mode this line prints and error message, pauses the programme and on a key press returns to the main menu.

(E) These lines collect the file data.

(F) These lines allow the maximum absorbance to be set by the user.

(G) These lines adjust the baseline to zero.

(H) These lines calculate the adjustment factor for the maximum value.

(I) These lines adjust the spectrum to the new maximum.

(J) This line sets the new (**YMAX**) value.

(K) These lines plot the new adjusted spectrum.

(L) This line allows the adjusted spectrum to be saved on floppy disc.

(M) This line gives an error message, see A.

4.12 Smooth spectrum.

The smooth spectrum routine cosmetically smooths any spectrum. The routine uses a simple smoothing algorithm which assumes that any point is the average of the points either side of it. The more points that are taken either side the smoother the spectrum. The routine does tend to remove any sharp peaks so should be used only for cosmetic purposes. The smoothing routine is illustrated in figure A4.17. Table A4.18, listing 25.

Table A4.18. Smooth spectrum.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	File name, new name for saveing	4	2

```
     10   REM SMOOTH SPECTRA
(A)  20   ON ERROR GOTO 830
     30   LET OFFSET=12233
(B)  40   LET P$="SMOOTH"
     50   LI=60 : CHAIN "A:NAME",10,ALL
     60   HOME
     70   LI=80 : CHAIN "A:TYPE",10,ALL
     80   LI=90 : CHAIN "A:IDENT",10,ALL
(C)  90   IF SCAN=1 OR SCAN=2 OR SCAN=8 OR SCAN=9 OR
          SCAN=10 OR SCAN=11 OR SCAN=12 OR SCAN=13 OR
          SCAN=14 THEN GOTO 150
```

```
      100   PRINT "DATA CANNOT BE SMOOTHED."
      110   PRINT
      120   PRINT "DATA MUST BE EITHER A WAVELENGTH SCAN ABS
            OR TRANS MODE, LOG A, OR A DERIVATIVE"
      130   PRINT
      140   PRINT "PRESS ANY KEY TO CONTINUE." : GET A$ : LOAD
            "A:MENU",A
(D)   150   REM SMOOTHING MENU
      160   HOME
      170   PRINT TAB(32); "SMOOTHING MENU."
      180   PRINT
      190   PRINT"-----------------------------------------
            ------------------------------------------------"
      200   PRINT : PRINT
      210   PRINT TAB(4); "(1)-SMOOTH OVER 3 POINTS."
      220   PRINT
      230   PRINT TAB(4); "(2)-SMOOTH OVER 5 POINTS."
      240   PRINT
      250   PRINT TAB(4); "(3)-SMOOTH OVER 7 POINTS."
      260   PRINT
      270   PRINT TAB(4); "(4)-SMOOTH OVER 9 POINTS."
      280   PRINT
      290   PRINT TAB(4); "(5)-SMOOTH OVER 11  POINTS."
      300   PRINT
      310   PRINT TAB(4); "(6)-SMOOTH OVER 13 POINTS."
      320   PRINT
      330   PRINT TAB(4); "(7)-SMOOTH OVER 15 POINTS."
      340   PRINT
      350   PRINT TAB(4); "(8)-SMOOTH OVER 17 POINTS."
      360   PRINT
(E)   370   GET A$
      380   IF A$="" THEN GOTO 370
      390   IF A$="1" THEN POINTS=3 : GOTO 500
      400   IF A$="2" THEN POINTS=5 : GOTO 500
      410   IF A$="3" THEN POINTS=7 : GOTO 500
      420   IF A$="4" THEN POINTS=9 : GOTO 500
      430   IF A$="5" THEN POINTS=11 : GOTO 500
      440   IF A$="6" THEN POINTS=13 : GOTO 500
      450   IF A$="7" THEN POINTS=15 : GOTO 500
      460   IF A$="8" THEN POINTS=17 ; GOTO 500
      470   GOTO 370
      500   HOME : PRINT TAB(27); "CALCULATING, PLEASE
```

```
            WAIT."
(F)   510   LI=520 : CHAIN "A:HEADER",10,ALL
      520   LI=530 : CHAIN "A;ARRAY",10,ALL
      530   LI=540 : CHAIN "A:ZERO",10,ALL
(G)   540   REM SMOOTHING ALGORITHM
      550   FOR I=POINTS-(INT(POINTS/2)) TO
            PTS-(INT(POINTS/2)+)
      560   FOR J=1 TO INT(POINTS/2)
      570   LET S(I)=S(I)+Y(I-J)
      580   LET S(I)=S(I)+Y(I+J)
      590   NEXT J
      600   LET S(I)=S(I)/POINTS
      610   NEXT I
(H)   620   REM TRANSFER DATA FROM S TO Y
      630   FOR I=1 TO PTS
      640   LET Y(I)=S(I)
      650   NEXT I
(I)   700   REM PLOT DATA
      710   LI=720 " CHAIN "A:MAXMIN",10,ALL
      720   LI=730 : CHAIN "A:AMAX",10,ALL
      730   YSCALE=159/(YMAX-YMIN)
      740   LI=750 : CHAIN "A:AXIS",10,ALL
      750   LI=760 : CHAIN "A:PLOTSP",10,ALL
      760   PRINT TAB(11); EWL; TAB(76); SWL; : PRINT TAB(33);
            "WAVELENGTH NM."
      780   GET K$
      790   IF K$="" THEN GOTO 280
      800   TEXT
(J)   810   CHAIN "A:STORE",10,ALL
      820   LOAD "A:MENU",R
(K)   830   HOME
      840   PRINT
      850   PRINT "AN ERROR HAS OCCURRED DURING THE
            EXECUTION
            OF THIS ROUTINE, CHECK ALL DISCS AND" : PRINT "FILE
            NAMES USED."
      860   PRINT
      870   PRINT "PRESS ANY KEY TO CONTINUE."
      880   GET K$
      890   IF K$="" THEN GOTO 880
      900   LOAD "MENU",R
```

Listing 25. Smooth spectrum.

(A) This line sets the error trap at line 830, see (K).

(B) This line sets the value of **P$** to "**SMOOTH**"

(C) These lines test to see if the file type is one that can be smoothed, if it is not then an error report is given and the main menu loaded.

(D) These line print the smoothing menu (Figure 4.17)

(E) These lines wait for a key to be pressed and select the corresponding smoothing routine.

(F) These lines load the data array to be smoothed.

(G) These lines contain the smoothing algorithm, Figure 4.18.

(H) These lines store the smoothed data in the array (**(S)**) for smoothing.

(I) These lines plot the smoothed data on the monitor screen.

(J) This line calls the routine which allows the smoothed data to be saved onto a floppy disc.

(K) These lines print an error message see (A).

4.13 Add two spectra.

This programme allows two spectra to be added, the files must be of the same type and collected under the same conditions. The files are displayed in the same way as the display two files programme. The two files to be added are displayed on the upper axis and the added file is displayed on the lower axis. The resulting added file can be saved onto a floppy disc, figure A4.19, table A4.19, listing 26.

Table A4.19. Add two spectra.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	MN, FT, IF, FH, LA, ZV, MM, SM, PT, SS.	File names, new name for saveing	5	2

```
     10   REM ADD TWO FILES
(A)  20   ON ERROR GOTO 490
     30   LET OFFSET=12233
(B)  40   LET P$="ADD"
(C)  50   LET NUM=2
     60   LI=70 : CHAIN "A:MNAME",10,ALL
     70   HOME
     80   PRINT TAB(27); "CALCULATING, PLEASE WAIT."
     90   DIM P(2)
     100  DIM D(2,8)
     110  LET I=1
     120  LET N$=""
     130  FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEHT K
(D)  140  LI=150 : CHAIN "A:TYPE",10,ALL
     150  LI=160 : CHAIN "A:IDENT",10,ALL
     160  LET D(I,7)=J%
     165  LET D(I,8)=DIV%
     170  LET P(I)=SCAN
(E)  175  IF SCAN<>1 THEN PRINT : PRINT "ONLY WAVELENGTH
          SCANS IN ABSORBANCE MODE MAY BE USED." : PRINT :
          PRINT "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
          "MENU",R
(F)  180  LI=181 : CHAIN "A:HEADER",10,ALL
     181  LET D(I,1)=PTS
     182  LET D(I,2)=SWL
     183  LET D(I,3)=EWL
     184  LET D(I,4)=SP
(G)  190  LI=200 : CHAIN "A:ARRAY",10,ALL
     200  LI=210 : CHAIN "A:ZERO",10,ALL
     210  LI=220 : CHAIN "A:MAXMIN",10,ALL
     220  LI=230 : CHAIN "A:MAX",10,ALL
     230  LET D(I,5)=YMAX
     240  LET D(1,6)=YMIN
(H)  244  IF I=1 THEN DIM Z(PTS)
(J)  245  FOR N=1 TO PTS
     246  LET Z(N)=Z(N)=Z(N)+Y(N)
     247  NEHT N
     250  LET I=I+1 : IF I<=NUM THEN GOTO 120
     251  IF D(1,1)=D(2,1) AND D(1,2)=D(2,2) AND D(1,3)=D(2,3)
          AND D(1,4)=D(2,4) THEN GOTO 255
(K)  252  PRINT : PRINT "FILES MUST BE COLLECTED UNDER
          IDENTICAL CONDITIONS." PRINT : PRINT "PRESS ANY
```

```
        KEY TO CONTINUE." : GET K$ : RUN "MENU",R
    255 LET YMAH=D(1,5) : IF D(2,5)>D(1,5) THEN YMAH=D(2,5) :
        LET D(1,5)=YMAH
    256 LET YMIN=0
    257 FOR I=1 TO PTS
    258 LET Y(I)=Z(I)
    259 NEHT I
(L) 260 LI=261 : CHAIN "A:MAHMIN",10,ALL
    261 LET A=9-YMAH
    262 LET B=A/.25
    263 LET B=FIH(B)
    264 LET YMAH=9-(B*.25)
    265 LET D(2,5)=YMAH
    266 LET D(2,6)=0
(M) 271 LI=275 : CHAIN "A:TAHIS",10,ALL
    275 REM PLOT
(N) 280 LET I=1
    290 LET N$=""
    300 FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEHT K
    302 LET PTS=D(1,1)
    304 LET J%INT(D(1,7))
    305 LET DIV%=INT(D(1,8))
    306 LET POST=1
    309 LET SCAN=P(I)
    310 LI=315 : CHAIN "A:ARRAY",10,ALL
    315 LI=340 : CHAIN "A:ZERO",10,ALL
    340 LET YSCALE=74/D(1,5)
    345 LET YMAH=D(1,5)
    350 LI=360 : CHAIN "A:SPLOTSP",10,ALL
    360 LET I=I+1 : IF I<NUM THEN GOTO 290
    370 POST=2
    380 LET YSCALE=74/D(2,5)
    385 LET YMAH=D(2,5) : LET YMIN=D(2,6)
    390 FOR I=1 TO PTS
    400 LET Y(I)=Z(I)
    410 LET S(I)=Z(I)
    420 NEHT I
    430 ERASE Z
(O) 440 LI=450 : CHAIN "A:SPLOTSP",10,ALL
(P) 450 PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
    460 GET K$
    465 LET SCAN=13
```

```
(Q)   470  LI=480 : CHAIN "A:STORE",10,ALL
      480  LOAD "MENU",R
(R)   490  HOME
      500  PRINT
      510  PRINT "AN ERROR HAS OCCURRED DURING THE EHECUTION
           OF THIS ROUTINE, CHECK ALL DISCS AND" : PRINT "FILE
           NAMES USED."
      520  PRINT
      530  PRINT "PRESS ANY KEY TO CONTINUE."
      540  GET K$
      550  IF K$="" THEN GOTO 540
      560  LOAD "MENU",R
```

Listing 26. Add two spectra.

(A) This line sets up the error message at line 490, see (R)

(B) This line sets the value of **P$** to "**ADD**"

(C) This line sets the value of **NUM** to 2.

(D) These lines collect the file header information for two files.

(E) This line checks that the two files are a wavelength scan in absorbance mode, ie SCAN=1, prints an error message if required and on a key press loads the main menu.

(F) This line collects the file header information.

(G) These lines collect the data file, zero the required values, calculate the maximum and minimum and adjust the maximum for plotting.

(H) This line sets up the array **Z()** to store the added file.

(J) This loop adds the array data storing the added data in the array **Z()**.

(K) This line ensures data from both spectra have been collected under the same conditions.

(L) This line calculates the new maximum and minimum values.

(M) This line draws the twin axis on the monitor (figure A4.5).

(N) This loop to line 360 plots the two spectra which have been added on the monitor (figure A4.19).

(O) This line plots the added spectra on the monitor (figure A4.19).

(P) This line pauses the display on the monitor until a key is pressed.

(Q) This line allows the added spectra to be stored on a floppy disc.

(R) These line print the error message, see (A).

4.14 Subtract two spectra.

This programme allows two spectra to be subtracted, the files must be of the same type and collected under the same conditions. The files are displayed in the same way as the display two files programme. The two files to be subtracted are displayed on the upper axis and the resulting file is displayed on the lower axis figure A4.20. The resulting subtracted file can be saved onto a floppy disc. Table A4.20, Listing 27.

Table 4.20. Subtract two spectra.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	MN, FT, IF, FH, LA, ZV, MM, SM, PT, SS.	File names, new name for saveing	6	2

```
      10 REM SUBTRACT TWO FILES
(A)   20 ON ERROR GOTO 490
      30 LET OFFSET=12233
(B)   40 LET P$="SUB"
(C)   50 LET NUM=2
      60 LI=70 : CHAIN "MNAME",10,ALL
      70 HOME
      80 PRINT TAB(27); "CALCULATING, PLEASE WAIT."
      90 DIM P(2)
      100 DIM D(2,8)
(D)   110 LET I=1
      120 LET N$=""
      130 FOR K=1 TO 15 : LET N$=N$+BS(K,I) : NEXT K
      140 LI=150 : CHAIN "A:TYPE",10,ALL
      150 LI=160 : CHAIN "A:IDENT",10,ALL
      160 LET D(1,7)=J%
      165 LET D(1,8)=DIV%
      170 LET P(I)=SCAN
(E)   175 IF SCAN<>1 THEN : PRINT "ONLY WAVELENGTH SCANS IN
          ABSORBANCE MODE MAY BE USED." : PRINT : PRINT
          "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
```

```
        "MENU",R
(F)  180 LI=181 : CHAIN "A:HEADER",10,ALL
     181 LET D(I,1)=PTS
     182 LET D(1,2)=SWL
     183 LET D(I,3)=EWL
     184 LET D(I,4)=SP
(G)  190 LI=200 : CHAIN "A:ARRAY",10,ALL
     200 LI=210 : CHAIN "A:ZERO",10,ALL
     210 LI=220 : CHAIN "A:MAXMIN",10,ALL
     220 LI=230 : CHAIN "A:MAX",10,ALL
     230 LET D(I,5)=YMAX
     240 LET D(I,6)=YMIN
(H)  244 IF I=1 THEN DIM Z(PTS)
(J)  245 FOR N=1 TO PTS
     246 IF I=1 THEN LET Z(N)=Y(N)
     247 IF I=2 THEN LET Z(N)=Z(N)-Y(N)
     248 NEXT N
     250 LET I=I+1 : IF I<NUM  THEN GOTO 120
     251 IF D(1,1)=D(2,1) AND D(1,2)=D(2,2) AND D(1,3)=D(2,3)
         AND D(1,4)=D(2,4) THEN GOTO 255
(K)  252 PRINT : PRINT "FILES MUST BE COLLECTED UNDER
         IDENTICAL CONDITIONS." PRINT : PRINT "PRESS ANY  KEY
         TO CONTINUE." : GET K$ " RUN "MENU",R
     255 LET YMAX=D(1,5) " IF D(2,5)>D(1,5) THEN YMAX=D(2,5)  :
         LET D(1,5)=YMAX
     256 LET YMIN=0
     257 FOR I=1 TO PTS
     258 LET Y(I)=Z(I)
     259 NEXT I
(L)  260 LI=261 : CHAIN "A:MAXMIN",10,ALL
     261 LET A=9-YMAX
     262 LET B=A/.25
     263 LET B=FIX(B)
     264 LET YMAX=9-(B*.25)
     265 LET D(2,5)=YMAX
     266 LET A=YMIN+(-.5)
     267 LET B=A/.5
     268 LET B=FIX(B)
     269 LET YMIN=0+(B*.5)
     270 LET D(2,6)=YMIN
(M)  271 LI=275 : CHAIN "A:TAXIS",10,ALL
     275 REM PLOT
```

```
(N)   280 LET I=1
      290 LET N$=""
      300 FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEHT K
      302 LET PTS=D(1,1)
      304 LET J%=INT(D(1,7))
      305 LET DIV%=INT(D(1,8))
      306 LET POST=1
      309 LET SCAN=P(I)
      310 LI=315 : CHAIN "A:ARRAY",10,ALL
      315 LI=340 : CHAIN "A:ZERO",10,ALL
      340 LET YSCALE=74/D(1,5)
      345 LET YMAX=D(1,5)
(O)   350 LI=360 : CHAIN "A:PLOTSP",10,ALL
      360 LET I=I+1 : IF I<=NUM THEN GOTO 290
      370 POST=2
      380 YSCALE=74/(D(2,5)-D(2,6))
      385 LET YMAX=D(2,5) : LET YMIN=D(2,6)
      390 FOR I=1 TO PTS
      400 LET Y(I)=Z(I)
      410 LET S(I)=Z(I)
      420 NEHT I
      430 ERASE 2
      440 LI=450 : CHAIN "A:PLOTSP",10,ALL
(P)   450 PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
      460 GET K$
      465 LET SCAN=14
(Q)   470 LI=480 : CHAIN "A:STORE",10,ALL
      480 LOAD "MENU",R
(R)   490 HOME
      500 PRINT
      510 PRINT "AN ERROR HAS OCCURRED DURING THE EHECUTION
          OF THIS ROUTINE, CHECK ALL DISCS AND" : PRINT "FILE
          NAMES USED."
      520 PRINT
      530 PRINT "PRESS ANY KEY TO CONTINUE."
      540 GET K$
      550 IF K$="" THEN GOTO 540
      560 LOAD "MENU",R
```

Listing 27. Subtract two spectra.

(A) This line sets up the error message at line 490, see (R)

(B) This line sets the value of **P$** to "**SUB**"

(C) This line sets the value of **NUM** to 2.

(D) These lines collect the file header information for two files.

(E) This line checks that the two files are a wavelength scan in absorbance mode, ie SCAN=1, prints an error message if required and on a key press loads the main menu.

(F) This line collects the file header information.

(G) These lines collect the data file, zero the required values, calculate the maximum and minimum and adjust the maximum for plotting.

(H) This line sets up the array **Z()** to store the subtracted file.

(J) This loop adds the array data storing the subtracted data in the array **Z()**.

(K) This line ensures data from both spectra have been collected under the same conditions.

(L) This line calculates the new maximum and minimum values.

(M) This line draws the twin axis on the monitor (figure A4.5).

(N) This loop to line 360 plots the two spectra which have been subtracted on the monitor (figure A4.20).

(O) This line plots the subtracted spectra on the monitor (figure A4.20).

(P) This line pauses the display on the monitor until a key is pressed.

(Q) This line allows the subtracted spectra to be stored on a floppy disc.

(R) These line print the error message, see (A).

4.15 Average spectra.

This programme allows the average of upto 20 spectra to be calculated and displayed, all the spectra must be of the same type and collected under the same conditions. The files to be averaged are displayed on the upper axis and the resulting file is displayed on the lower axis figure A4.21. The resulting averaged file can be saved onto a floppy disc. Table A4.21, Listing 28.

Table A4.21. Average spectra.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1 only.	MN, FT, IF, FH, LA, ZV, MM, SM, PT, SS.	File names, new name for saveing	7	2

```
      10   REM AVERAGE SPECTRA
(A)   20   ON ERROR GOTO 490
      30   LET OFFSET=12233
(B)   40   LET P$="AVERAGE"
(C)   50   LET NUM=0
      60   LI=70 : CHAIN "A:MNAME",10,ALL
      70   HOME
      80   PRINT TAB(27); "CALCULATING, PLEASE WAIT."
      90   DIM P(NUM)
      100  DIM D(NUM,8)
(D)   110  LET I=1
      120  LET N$=""
      130  FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEXT K
      140  LI=150 : CHAIN "A;TYPE",10,ALL
      150  LI=160 : CHAIN "A:IDENT",10,ALL
      160  LET D(I,7)=J%
      165  LET D(I,8)=DIV%
      170  LET P(I)=SCAN
(E)   175  IF SCAN<>1 THEN PRINT : PRINT "ONLY WAVELENGTH
           SCANS IN ABSORBANCE MODE MAY BE USED." : PRINT :
           PRINT "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
           "MENU",R
(F)   180  LI=181 : CHAIN "A:HEADER",10,ALL
      181  LET D(I,1)=PTS
      182  LET D(I,2)=SWL
      183  LET D(I,3)=EWL
      184  LET D(I,4)=SP
(G)   190  LI=200 : CHAIN "A:ARRAY",10,ALL
      200  LI=210 : CHAIN "A:ZERO",10,ALL
      210  LI=220 : CHAIN "A:MAXMIN",10,ALL
```

```
        220   LI=230 : CHAIN "A:AMAX",10,ALL
        230   LET D(1,5)=YMAX
        240   LET D(1,6)=YMIN
(H)     244   IF I=1 THEN DIM Z(PTS)
(J)     245   FOR N=1 TO PTS
        246   LET Z(N)=Z(N)+Y(N)
        247   NEXT N
        250   LET I=I+1 : IF I<=NUM THEN GOTO 120
(K)     251   FOR I=1 TO NUM
        252   IF D(1,1)<>D(I,1) OR D(1,2)<>D(1,2) OR D(1,3)<>D(1,3)
              OR D(1,4)<>D(I,4) THEN GOTO 255
        253   NEXT I
        254   GOTO 256
        255   PRINT : PRINT "FILES MUST BE COLLECTED UNDER
              IDENTICAL CONDITIONS." : PRINT : "PRESS ANY KEY TO
              CONTINUE." : GET K$ : LOAD "MENU",R
        256   LET YMAX=D(1,5)
        257   FOR I=1 TO NUM
        258   IF D(I,5)>YMAX THEN YMAX D(I,5)
        259   NEXT I
        260   FOR I=1 TO PTS
        261   LET Y(I)=Z(I)/NUM
        262   NEXT I
(L)     263   LI=264 : CHAIN "A:MAXMIN",10,ALL
        264   LET D(2,5)=YMAX
        265   LET D(2,6)=0
(M)     271   LI=275 : CHAIN "A:THIS",10,ALL
        275   REM PLOT
(N)     280   LET I=1
        290   LET N$=""
        300   FOR K=1 TO 15 : LET N$=N$+B$(K,I) : NEXT K
        302   LET PTS=D(I,1)
        304   LET J%INT(D(I,7))
        305   LET DIV%=INT(D(I,8))
        306   POST=1
        309   LET SCAN=P(I)
        310   LI=315 : CHAIN "A:ARRAY",10,ALL
        315   LI=340 : CHAIN "A:ZERO",10,ALL
        340   LET YSCALE=74/D(1,5)
        345   LET YMAX=D(1,5)
(O)     350   LI=360 : CHAIN "A:SPLOTSP",10,ALL
        360   LET I=I+1 : IF I<=NUM THEN GOTO 290
```

```
      370   POST=2
      380   LET YSCALE-74/D(2,5)
      385   LET YMAH=D(2,5) : LET YMIN=D(2,6)
      390   FOR I=1 TO PTS
      400   LET Y(I)=Z(I)/NUM
      410   LET S(I)=Z(I)/NUM
      420   NEHT I
      430   ERASE Z
(P)   440   LI=450 : CHAIN "A:SPLOTSP",10,ALL
      450   PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
      460   GET K$
      465   LET SCAN=1
(Q)   470   LI=480 : CHAIN ""A:STORE",10,ALL
      480   LOAD "MENU",R
      486   LI=490 : CHAIN "A:AMAH",10,ALL
(R)   490   HOME
      500   PRINT
      510   PRINT "AN ERROR HAS OCCURRED DURING THE EHECUTION
            OF THIS ROUTINE, CHECK ALL DISCS AND" : PRINT "FILE
            NAMES USED."
      520   PRINT
      530   PRINT "PRESS ANY KEY TO CONTINUE."
      540   GET K$
      550   IF K$="" THEN GOTO 540
      560   LOAD "MENU",R
```

(A) This line sets up the error message at line 490, see (R)

(B) This line sets the value of **P$** to "**AVERAGE**"

(C) This line sets the value of **NUM** to 0.

(D) These lines collect the file header information for upto 20 files.

(E) This line checks that the files collected are a wavelength scan in absorbance mode, ie **SCAN=1**, prints an error message if required and on a key press loads the main menu.

(F) This line collects the file header information.

(G) These lines collect the data file, zero the required values, calculate the maximum and minimum and adjust the maximum for plotting.

(H) This line sets up the array **Z()** to store the averaged file.

(J) This loop adds the array data storing the averaged data in the array **Z()**.

(K) This line ensures data from the spectra have been collected under the same

conditions.

(L) This line calculates the new maximum and minimum values.

(M) This line draws the twin axis on the monitor (figure A4.5).

(N) This loop to line 360 plots the spectra which have been averaged on the monitor (figure A4.21).

(O) This line plots the averaged spectra on the monitor (figure A4.21).

(P) This line pauses the display on the monitor until a key is pressed.

(Q) This line allows the averaged spectra to be stored on a floppy disc.

(R) These line print the error message, see (A).

4.16. Adjust baseline.

The adjust baseline programme allows a new minimum value to be selected for a spectrum and adjusts the whole spectrum in line with that new minimum. The programme can use any wavelength scan, the new adjusted spectrum is displayed as a normal wavelength scan (figure A4.6). The adjusted file is stored in the same mode as the original spectrum, table A4.22, listing 29.

Table A4.22. Adjust baseline.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1, 2, 13, 14.	SN, FT, IF, FH, LA, ZV, MM, SM, PT, PS.	File name, new baseline new file name.	8	2

```
     10   REM BASELINE
(A)  20   ON ERROR GOTO 270
     30   LET OFFSET=12233
(B)  40   LET P$="BASE"
(C)  50   LI=60 : CHAIN "A:NAME",10,ALL
     60   HOME
     70   PRINT TAB(27); "CALCULATING, PLEASE WAIT."
(D)  80   LI=90 : CHAIN  "A:TYPE",10,ALL
```

```
     90   LI=100 : CHAIN "A:IDENT",10,ALL
     100  IF SCAN=1 OR SCAN=2 OR SCAN=13 OR SCAN=14 THEN
          GOTO 120
     110  PRINT : PRINT "ONLY WAVELENGTH SCANS IN
          ABSORBANCE OR TRANSMITTANCE MODES MAY BE USED."
          : PRINT : PRINT : PRESS ANY KEY TO CONTINUE." : GET
          K$ : LOAD "MENU",A
(E)  120  LI=130 : CHAIN "A:HEADER",10,ALL
     130  LI=140 : CHAIN "A:ARRAY",10,ALL
     140  LI=150 : CHAIN "A:ZERO",10,ALL
     150  LI=151 : CHAIN "A:MAXMIN",10,ALL
(F)  151  HOME
     152  PRINT : PRINT
     153  INPUT "INPUT NEW BASELINE VALUE.-";FACT
     154  IF SCAN=1 OR SCAN=13 OR SCAN=14 AND
          FACT+YMAX<=4.5 THEN GOTO 156
     155  PRINT "NEW MAXIMUM VALUE IS TOO LARGE." : PRINT
          "PRESS ANY KEY TO CONTINUE." : GET A$ : GOTO 151
     156  IF SCAN=2 AND FACT+YMAX<=100 THEN GOTO 161
     157  PRINT "NEW MAXIMUM VALUE IS TOO LARGE." : PRINT
          "PRESS ANY KEY TO CONTINUE." : GET A$ : GOTO 151
     161  LET FACT=0-YMIN
(G)  162  FOR I=1 TO PTS
     163  LET Y(I)=Y(I)+FACT
     164  LET S(I)=Y(I)
     165  NEXT I
(H)  166  LET YMAX=YMAX+FACT
     167  LET YMIN=FACT
(I)  169  LI=170 : CHAIN "A:AMAX",10,ALL
     170  YSCALE=159/(YMAX-YMIN)
     180  LI=190 : CHAIN "A:AXIS",10,ALL
     190  LI=200 : CHAIN "A:PLOTSP",10,ALL
     200  IF SCAN=1 OR SCAN=2 THEN PRINT TAB(11); EWL;
          TAB(76); SWL; : PRINT TAB(33); "WAVELENGTH nm."
     220  PRINT "PRESS ANY KEY TO CONTINUE."
     230  GET K$
     240  IF K$="" THEN GOTO 230
     245  TEXT
(J)  250  LI=260 : CHAIN "A:STORE",10,ALL
     260  LOAD "A:MENU",A
(K)  270  HOME
     280  PRINT
```

```
290  PRINT "AN ERROR HAS OCCURRED DURING THE EXECUTION
     OF THIS ROUTINE, CHECK ALL DISCS AND" : PRINT "FILE
     NAMES USED."
300  PRINT
310  PRINT "PRESS ANY KEY TO CONTINUE."
320  GET K$
330  IF K$="" THEN GOTO 320
340  LOAD "MENU",R
```

Listing 29. Adjust baseline.

(A) This line sets the error message at line 270, see (K).

(B) This line sets the value of **P$** to "**BASE**".

(C) This line collects the information on the file to be adjusted.

(D) These lines collect the file header information, check the file is of a compatible type and if necessary print an error message.

(E) These lines collect the file to be adjusted, zero any negative values and calculate the maximum and minimum values of the file.

(F) These lines collect the new baseline value (FACT), checks that this value is valid, if not an error message is printed and a new value prompted for.

(G) This loop adjusts the spectrum to the new baseline.

(H) This line calculates the new **YMAX** value.

(I) This line displays the new spectrum on the monitor (figure A4.6).

(J) This line allows the adjusted spectrum to be saved on floppy disc.

(K) These lines print an error message if required, see (A).

4.17 Deresolve spectrum.

The deresolve spectrum programme allows data files to be compacted. The programme reduces the number of data points in high resolution spectra freeing disc space and speeding up the operation of the UVDMP programmes. The deresolved spectra can be saved like any other file, the deresolution process cannot be reversed, it is therefore recommended that the original files are retained if this is required. The monitor display of this programme is shown in figure A4.22, table A4.23, listing 33.

Table A4.23. Deresolve spectrum.

File types used. (SCAN value)	Routine programmes accessed.	User input required	User access.	
			Key	Menu page
1, 2, 8, 9, 10, 11, 12, 13, 14.	SN, FT, IF, FH, LA, ZV, MM, SM, PS, SS.	File names, new name for saveing	1	3

```
     10   REM DERESOLVE
(A)  20   ON ERROR GOTO 500
     30   LET OFFSET=12233
(B)  40   LET P$="DER"
(C)  50   LI=60 : CHAIN "A:NAME",10,ALL
     60   LI=70 : CHAIN "A:TYPE",10,ALL
     70   LI=80 : CHAIN "A:IDENT",10,ALL
(D)  80   IF SCAN=1 OR SCAN=2 OR SCAN=8 OR SCAN=9 OR
          SCAN=10 OR SCAN=11 OR SCAN=12 OR SCAN=13 OR
          SCAN=14 THEN GOTO 100
     90   HOME : PRINT : PRINT "FILE UNSUITABLE, ONLY
          WAVELENGTH SCANS MAY BE DERESOLVED." : PRINT :
          PRINT "PRESS ANY KEY TO CONTINUE." : GET K$ : LOAD
          "MENU",R
(E)  100  LI=110 : CHAIN "A:HEADER",10,ALL
(F)  110  IF SP<>1200 THEN GOTO 130
     120  HOME : PRINT : PRINT "SPECTRUM IS ALREADY ON
          MINIMUM RESOLUTION." : PRINT : PRINT "PRESS ANY
          KEY TO CONTINUE." : GET K$ : LOAD "MENU",R
(G)  130  HOME
     140  PRINT TAB(32); "DERESOLUTION MENU."
     150  PRINT "----------------------------------------
          ----------------------"
     160  PRINT
     170  PRINT TAB(4); "CURRENT SCAN SPEED-"; SP; " nm/min."
     180  PRINT
     190  PRINT TAB(4); "CURRENT RESOLUTION-"; SP/1200; "
          nm."
     200  PRINT : PRINT
     210  PRINT TAB(4); " (1)-DERESOLVE TO 1 nm."
```

```
     220  PRINT
     230  PRINT TAB(4); " (2)-DERESOLVE TO 0.5 nm."
     240  PRINT
     250  PRINT TAB(4); " (3)-DERESOLVE TO 0.25 nm."
     260  PRINT
     270  PRINT TAB(4); "(4)-DERESOLVE TO 0.1 nm."
     280  PRINT
     290  GET A$
     300  IF A$="1" THEN LET SP1=1200 : GOTO 350
     310  IF A$-"2" AND SP<600 THEN LET SP1=600 : GOTO 350
     320  IF A$="3" AND SP<300 THEN LET SP1=300 : GOTO 350
     330  IF A$="4" AND SP<120 THEN LET SP1=120 : GOTO 350
     340  GOTO 130
     350  LET RANGE=SWL-EWL
     352  HOME
     354  PRINT TAB(27); "CALCULATING, PLEASE WAIT."
(H)  360  LET PTS1=(RANGE/(SP1/1200))+1
(I)  370  DIM S(PTS1)
(J)  380  LET STP=((1200/SP)/(1200/SP1))
     400  OPEN "R",#1,N$,2
     410  FIELD #1,2 AS H$
     420  FOR I=1 TO PTS1
     440  GET #1,J%
     450  LET S(I)=(CVI(H$)+OFFSET)/DIV%
     455  LET J%=J%+STP
     460  NEXT I
     465  CLOSE #1
(K)  470  LET SP=SP1
     475  LET PTS=PTS1
(L)  480  LI=490 : CHAIN "A:STORE',10,ALL
     490  LOAD "MENU",R
(M)  500  HOME
     510  PRINT
     520  PRINT "AN ERROR HAS OCCURRED DURING THE EHECUTION
          OF THIS ROUTINE, CHECK ALL DISCS AND" : PRINT "FILE
          NAMES USED."
     530  PRINT
     540  PRINT "PRESS ANY KEY TO CONTINUE."
     550  GET K$
     560  IF K$="" THEN GOTO 550
     570  LOAD "MENU",R
```

Listing 33. Deresolve spectrum.

(A) This line sets the error trap at line 500, see (M).

(B) This line sets the value of **P$** to "**DER**".

(C) These lines collect the name of the file to be deresolved, collect the identity data and assign the value of **SCAN**.

(D) These lines test the value of **SCAN** to ensure the file can be deresolved, ie it is a wavelength scan, if it is not an error message is printed.

(E) This line collects the header information.

(F) These lines test the spectrum resolution, if it is already on minimum then an error message is printed and the programme returns to the main menu.

(G) These lines print the deresolution menu, figure A4.22, the required resolution is selected by pressing key 1-4.

(H) This line sets the new value of **PTS**, **PTS1**.

(I) This line sets the new array **S()** to store the deresolved spectra.

(J) These lines to 460 deresolve the spectrum storing the data in **S()**.

(K) These lines set the new values of **SP** and **PTS**.

(L) This line allows the new spectrum to be stored on disc.

(M) This line prints an error message if required , see (A).

5. Main menu programme.

The main menu programme is the means by which all the other programmes are accessed and controlled, see figure A4.1. All the options of this programme can be selected by a single key press. There are three pages of the main menu with upto 8 options which can be selected by pressing keys 1-8, and 3 options which can be found on all three pages which are accessed by pressing the P, D and H keys. Pressing the 'P' allows the page to be changed. pressing 'D' allows the disc utilities menu to be accessed and finally pressing 'H' gives access to the help file. The programme is detailed in listing 31.

```
     10   REM MAIN MENU PROGRAMME
     20   REM © I.R.SURRY 1987
     30   TEXT
     40   HOME
(A)  100  REM DISPLAY PAGE ONE
     110  PRINT TAB(1); "MENU OPTIONS."; TAB(35); "MAIN
```

```
        MENU."; TAB(73); "PAGE 1."
    120 PRINT "-----------------------------------
        ------------------------"
    130 PRINT : PRINT
    140 PRINT TAB(4); "(1)-VIEW FILE."
    150 PRINT
    160 PRINT TAB(4); "(2)-PRINT FILE."
    170 PRINT
    180 PRINT TAB(4); "(3)-PLOT FILE."
    190 PRINT
    200 PRINT TAB(4); "(4)-OVERLAY FILES."
    210 PRINT
    220 PRINT TAB(4); "(5)-COMPARE 2 FILES."
    230 PRINT
    240 PRINT TAB(4); "(6)-MAGNIFY FILE."
    250 PRINT
    252 PRINT TAB(4); "(7)-IDENTIFY FILE."
    254 PRINT
    256 PRINT TAB(4); "(8)-"
    258 PRINT
    260 PRINT TAB(4); "(P)-CHANGE PAGE."; TAB(25);
        "(H)-HELP."; TAB(40); "(D)-DISC UTILITIES."
(B) 270 GET A$
    280 IF A$="" THEN GOTO 270
(C) 290 IF A$="P" THEN GOTO 500
(D) 300 IF A$="1" THEN LOAD "VIEW",R
    310 IF A$="2" THEN LOAD "PRINT",R
    320 IF A$="3" THEN LOAD "PLOT",R
    330 IF A$="4" THEN LOAD "OVER",R
    340 IF A$="5" THEN LOAD "COMPARE",R
    350 REM 6
    360 IF A$="7" THEN LOAD "FIND",R
    370 REM 8
(E) 390 IF A$="H" THEN LOAD "HELP",R
(F) 395 IF A$="D" THEN LOAD "DISC",R
    400 GOTO 270
(G) 500 REM PAGE 2
    510 HOME
    520 PRINT TAB(1); :CALCULATION OPTIONS."; TAB(35);
        "MAIN MENU."; TAB(73); "PAGE 2."
    530 PRINT "-----------------------------------
        ------------------------------"
```

```
      540  PRINT : PRINT
      550  PRINT TAB(4); "(1)-DERIVATIVE."
      560  PRINT
      570  PRINT TAB(4); "(2)-LOG A."
      580  PRINT
      590  PRINT TAB(4); "(3)-NET A."
      600  PRINT
      610  PRINT TAB(4); "(4)-OVERLAP."
      620  PRINT
      630  PRINT TAB(4); "(5)-PEAK PICK."
      640  PRINT
      650  PRINT TAB(4); "(6)-NORMALISE SPECTRUM."
      660  PRINT
      670  PRINT TAB(4); "(7)-SMOOTH SPECTRUM."
      680  PRINT
      690  PRINT TAB(4); "(8)-ADD SPECTRA."
      700  PRINT
      710  PRINT TAB(4); "(P)-CHANGE PAGE."; TAB(25);
           "(H)-HELP."; TAB(40); "(D)-DISC UTILITIES."
      720  GET A$
      730  IF A$="" THEN GOTO 720
(C)   740  IF A$="P" THEN GOTO 1000
(D)   750  IF A$="1" THEN LOAD "DERV",A
      760  IF A$="2" THEN LOAD "LOGA",A
      770  REM 3
      780  REM 4
      790  REM 5
      800  IF A$="6" THEN LOAD "NORM",A
      810  IF A$="7" THEN LOAD "SMOOTH",A
      820  IF A$="8" THEN LOAD "ADD",A
(E)   830  IF A$="H" THEN LOAD "HELP",A
(F)   835  IF A$="D" THEN LOAD "DISC",A
      840  GOTO 720
(H)  1000  REM PAGE 3
     1010  HOME
     1020  PRINT TAB(35); "MAIN MENU."; TAB(73); "PAGE 3."
     1030  PRINT "----------------------------------
           ----------------------------"
     1040  PRINT : PRINT
     1050  PRINT TAB(4); "(1)-SUBTRACT SPECTRA."
     1060  PRINT
     1070  PRINT TAB(4); "(2)-AVERAGE SPECTRA."
```

```
1080 PRINT
1090 PRINT TAB(4); "(3)-CORRECT BASELINE."
1100 PRINT
1110 PRINT TAB(4); "(4)-DERESOLVE SPECTRUM."
1120 PRINT
1130 PRINT TAB(4); "(5)-"
1140 PRINT
1150 PRINT TAB(4); "(6)-"
1160 PRINT
1170 PRINT TAB(4); "(7)-"
1180 PRINT
1190 PRINT TAB(4); "(8)-"
1200 PRINT
1210 PRINT TAB(4); "(P)-CHANGE PAGE."; TAB(25);
     "(H)-HELP."; TAB(40); "(D)-DISC UTILITIES."
1220 GET A$
1225 IF A$="P" THEN GOTO 10
1230 IF A$="" THEN GOTO 1220
1240 IF A$="1" THEN LOAD "SUB",8
1250 IF A$="2" THEN LOAD "AVERAGE",8
1260 IF A$="3" THEN LOAD "BASE",8
1270 IF A$="4" THEN LOAD "DER",8
1280 REM 5
1290 REM 6
1300 REM 7
1310 REM 8
1320 IF A$="H" THEN LOAD "HELP",8
1325 IF A$="D" THEN LOAD "DISC",8
1330 GOTO 1220
```

Listing 31. main menu programme.

(A) These lines to 260 print the main menu page 1, figure A4.22.

(B) This line collects the key press, 1-8, P, H or D.

(C) This line causes the menu page to be changed.

(D) These lines accept the key press 1-8 and load the required routine programme.

(E) This line loads the help programme.

(F) This line loads the disc utilities programme.

(G) These lines to 710 print page 2 of the main menu, figure A4.23.

(H) These lines print a page 3 for the main menu.

6.0 Disc utilities.

The disc utilities menu allows common disc organisation functions to be carried out within the UVDMP. The functions which can be carried out are, catalogue disc, rename file, erase file, copy file and convert file for printing. The catalogue disc utility prints on the monitor a list of all the data files on a chosen disc. The rename file utility allows a data file to be renamed with another name upto 8 characters long. The erase file utility allows a data file to be removed from the disc. The copy file utility allows a copy of a data file to be made on a new disc. The final function allows the file header of a spectrum to be changed in such a way that it can be relayed to the DU7 and printed on its dedicated printer. The convert spectrum programme should be used with care as altered files will cause errors if used with the UVDMP and it is recommended that converted files are saved on a separate disc.

```
      10    REM DISC UTILITIES
      20    REM THIS PROGRAMME WILL WORK WITH DATA FILES
            ONLY.
(A)   30    ON ERROR GOTO 6000
(B)   40    LET P$="DISC"
      50    LET OFFSET=12233
      60    RESET
      100   HOME
(C)   110   PRINT TAB(33); "DISC UTILITIES MENU."
      120   PRINT "------------------------------------
            --------------------"
      130   PRINT
      140   PRINT TAB(4); "(1)-CATALOGUE DISC."
      150   PRINT
      160   PRINT TAB(4); "(2)-RENAME FILE."
      170   PRINT
      180   PRINT TAB(4); "(3)-ERASE FILE."
      190   PRINT
      200   PRINT TAB(4); "(4)-COPY FILE."
      210   PRINT
      220   PRINT TAB(4); "(5)-CONVERT SPECTRUM FOR PRINTING."
      230   PRINT
      233   PRINT TAB(4); "(6)-RETURN TO MAIN MENU.:
      240   GET A$
```

```
      250  IF A$="" THEN GOTO 240
(D)   260  IF A$="1" THEN GOTO 1000 : REM catalogue DISC
      270  IF A$="2" THEN GOTO 2000 : REM RENAME DISC
      280  IF A$="3" THEN GOTO 3000 : REM ERASE DISC
      290  IF A$="4" THEN GOTO 4000 : REM COPY FILE
      300  IF A$="5" THEN GOTO 5000 : REM CONVERT SPECTRUM
      305  IF A$="6" THEN LOAD "MENU",R
      310  GOTO 240

(E)   1000 REM catalogue DISC
      1010 HOME
      1020 FILES "B:*.DAT"
      1025 PRINT "------------------------------------
           --------------------"
      1030 PRINT : PRINT
      1040 PRINT "PRESS ANY KEY TO CONTINUE."
      1050 GET A$
      1060 GOTO 10

(F)   2000 REM RENAME FILE
      2010 HOME
      2020 FILES "B:*.DAT"
      2030 PRINT "------------------------------------
           ---------------"
      2040 PRINT : PRINT
      2050 PRINT "RENAME WHICH FILE?"
      2060 INPUT N$
      2070 PRINT "RENAME FILE AS?"
      2080 INPUT M$
      2090 IF N$="" OR M$="" THEN PRINT "ERROR NO FILE NAME
           GIVEN."  : PRINT : PRINT "PRESS ANY KEY TO
           CONTINUE." : GET A$ : GOTO 10
      2100 LET N$="B:"+N$+".DAT"
      2110 LET M$="B:"+M$+".DAT"
      2120 NAME N$ AS M$
      2130 PRINT
      2140 PRINT "PRESS ANY KEY TO CONTINUE."
      2150 GET A$
      2160 GOTO 10

(G)   3000 REM ERASE FILE
      3005 RESET
```

```
3010 HOME
3020 FILES "B:*.DAT"
3025 PRINT "--------------------------------
     ------------------"
2030 PRINT : PRINT
3040 PRINT "ERASE WHICH FILE?"
3050 INPUT N$
3060 IF N$="" THEN PRINT "ERROR NO FILE NAME GIVEN." :
     PRINT : PRINT "PRESS ANY KEY TO CONTINUE." : GET A$ :
     GOTO 10
3070 PRINT
3080 PRINT "ERASE"; N$; "ARE YOU SURE (Y/N) ?"
3090 GET A$
3100 IF A$="" THEN GOTO 3090
3110 IF A$="N" THEN PRINT "FILE NOT ERASED" : PRINT "
     PRINT "PRESS ANY KEY TO CONTINUE." : GET A$ : GOTO
     10
3120 IF A$="Y" THEN GOTO 3140
3130 GOTO 3090
3140 LET N$="B:"+N$".DAT"
3150 KILL N$
3160 PRINT
3170 PRINT "FILE ERASED."
3180 PRINT
3190 PRINT "PRESS ANY KEY TO CONTINUE."
3200 GET A$
3210 GOTO 10
```

(H)

```
4000 REM COPY FILE
4001 HOME
4002 FILES "B:*.DAT"
4003 PRINT "--------------------------------
     --------------------"
4004 PRINT : PRINT
4005 PRINT "COPY WHICH FILE?"
4006 INPUT N$
4009 IF LEN(N$)>8 THEN PRINT : PRINT "FILE NAME TOO
     LONG, MAXIMUM OF 8 CHARACTERS." : PRINT : PRINT
     "PRESS ANY KEY TO CONTINUE." : GET K$ : GOTO 10
4010 IF N$="" THEN PRINT "NO FILE NAME GIVEN." : PRINT :
     PRINT "PRESS ANY KEY TO CONTINUE." : GET K$ : GOTO
     10
```

```
4011 LET N$="B:"+N$+".DAT"
4015 HOME : PRINT TAB(35); "COPYING FILE."
4020 LI=4030 : CHAIN "A:TYPE",10,ALL
4030 LI=4040 : CHAIN "A:IDENT",10,ALL
4040 LI=4050 : CHAIN "A:HEADER",10,ALL
4050 LI=4055 : CHAIN "A:ARRAY',10,ALL
4055 LI=4060 : CHAIN "A:STORE",100,ALL
4060 PRINT
4070 PRINT "COPY COMPLETE."
4080 PRINT
4090 PRINT "PRESS ANY KEY TO CONTINUE."
4100 GET K$
4110 LOAD "A:DISC",R

(I)  5000 REM CONVERT SPECTRUM FOR PRINTING
5010 HOME
5020 FILES "B:*.DAT"
5030 PRINT
5040 PRINT "------------------------------
     ----------------------"
5050 PRINT : PRINT
5060 PRINT "CONVERT WHICH FILE?";
5070 INPUT N$
5080 IF LEN(N$)>8 OR LEN(N$)=0 THEN PRINT "UNSUITABLE
     FILE NAME." : PRINT : PRINT "PRESS ANY KEY TO
     CONTINUE." : GET K$ : GOTO 5000
5090 LET N$="B:"+N$+".DAT"
5095 HOME
5100 LI=5110 : CHAIN "A:TYPE",10,ALL
5110 LI=5120 : CHAIN "A:IDENT",10,ALL
5120 IF SCAN=1 OR SCAN=2 OR SCAN=3 OR SCAN=4 OR
     SCAN=5 OR SCAN=6 OR SCAN=7 THEN PRINT : PRINT
     "FILE IS ALREADY SUITABLE FOR PRINTING" : PRINT :
     PRINT "PRESS ANY KEY TO CONTINUE." : GET K$ : GOTO
     10
5130 LI=5140 : CHAIN "A:HEADER",10,ALL
5140 LI=5150 : CHAIN "A:ARRAY",10,ALL
5150 LI=5160 : CHAIN "A:MAXMIN",10,ALL
5160 IF YMAX<=4.5 AND YMIN>=-4.5 THEN SCAN=1 : GOTO
     5180
5170 LET SCAN=2
5180 HOME
```

```
5190 PRINT : PRINT
5200 INVERSE
5210 PRINT "WARNING CONVERTING A FILE WILL MAKE IT
     INCOMPATIBLE WITH MANY ROUTINES IN THIS" : PRINT
     "COMPUTER PROGRAMME, YOU ARE ADVISED TO STORE
     ALL SUCH FILES ON A SEPARATE DISC."
5220 NORMAL
5230 PRINT : PRINT "PRESS ANY KEY TO CONTINUE."
5240 GET K$
5250 LI=5260 : CHAIN "A:STORE",100,ALL
5260 LOAD "DISC",R

(J)  6000 REM ERROR
     6010 HOME
     6020 TEXT
     6030 PRINT
     6040 PRINT "AN ERROR HAS OCCURRED DURING THE EXECUTION
          OF THIS ROUTINE, CHECK ALL DISCS AND" PRINT "FILE
          NAMES USED."
     6050 PRINT
     6060 PRINT "PRESS ANY KEY TO CONTINUE."
     6070 GET K$
     6080 IF K$="" THEN GOTO 6080
     6090 LOAD "MENU",R
```

Listing 32. Disc utilities programme.

(A) This line sets the error message at line 6000, see (J).

(B) This line sets the value of P$ to 'DISC'.

(C) These lines to 233 print the disc utilities menu, figure A4.24.

(D) These line direct the programme to the required subroutine of the disc utilities programme.

(E) This subroutine catalogues the data disc.

(F) This subroutine allows a data file to be renamed.

(G) This subroutine allows a data file to be erased.

(H) This subroutine allows a data file to be copied to another disc.

(I) This subroutine allows a data file to be converted and saved in such a way that it can be downloaded to the DU7 and printed on its dedicated printer.

(J) This line prints the error message if required see (A).

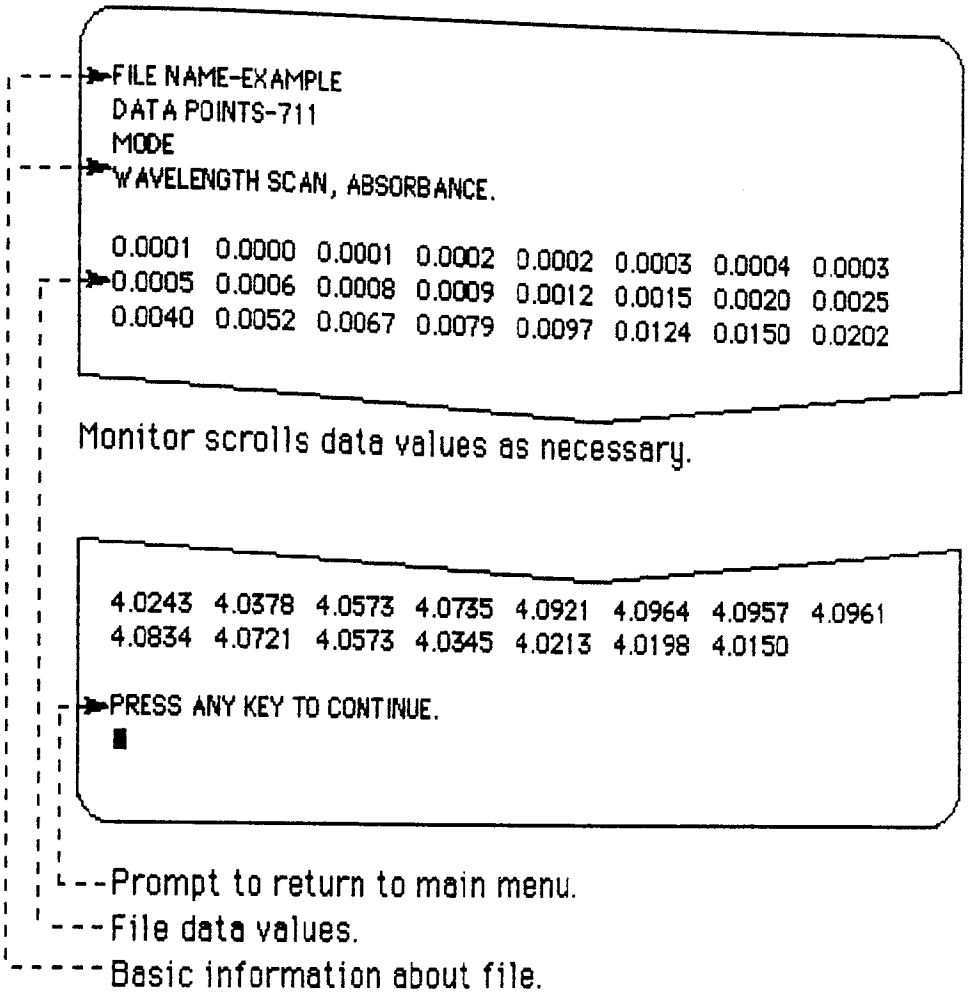


Figure A4.9. Monitor display from the view file programme.

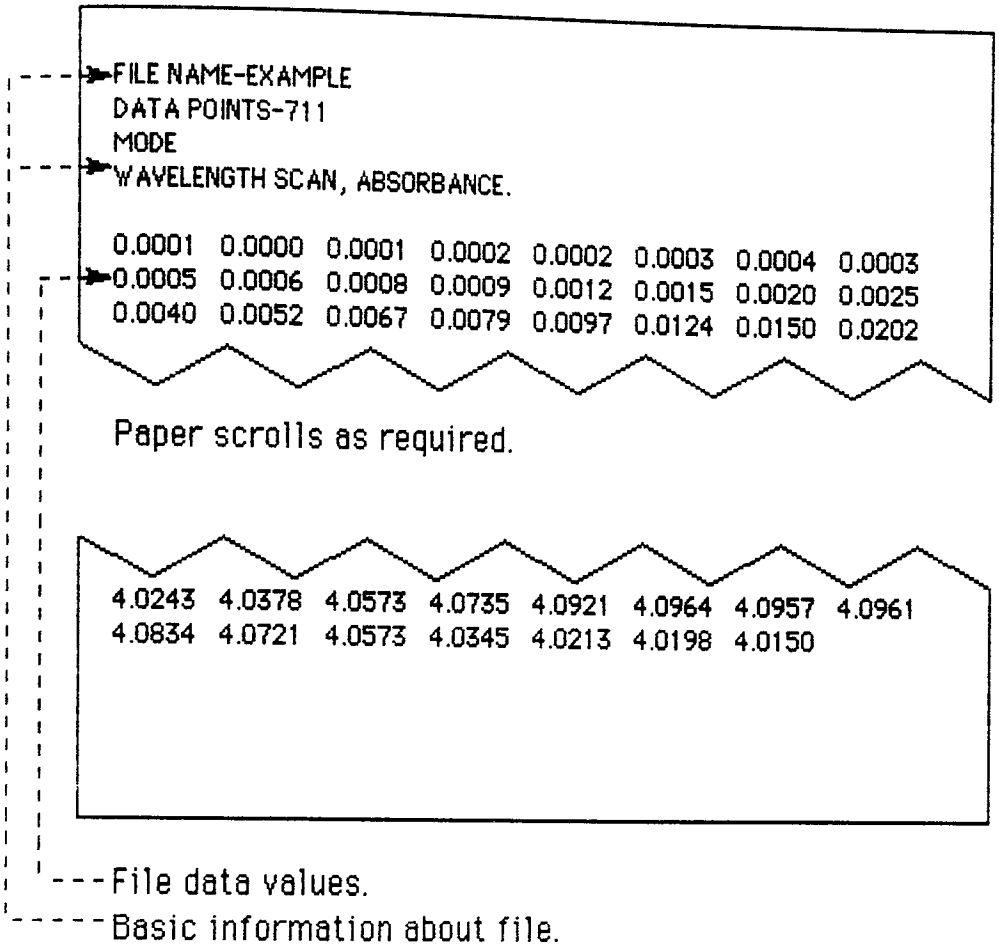


Figure A4.10. Example of printer output from the print file programme.

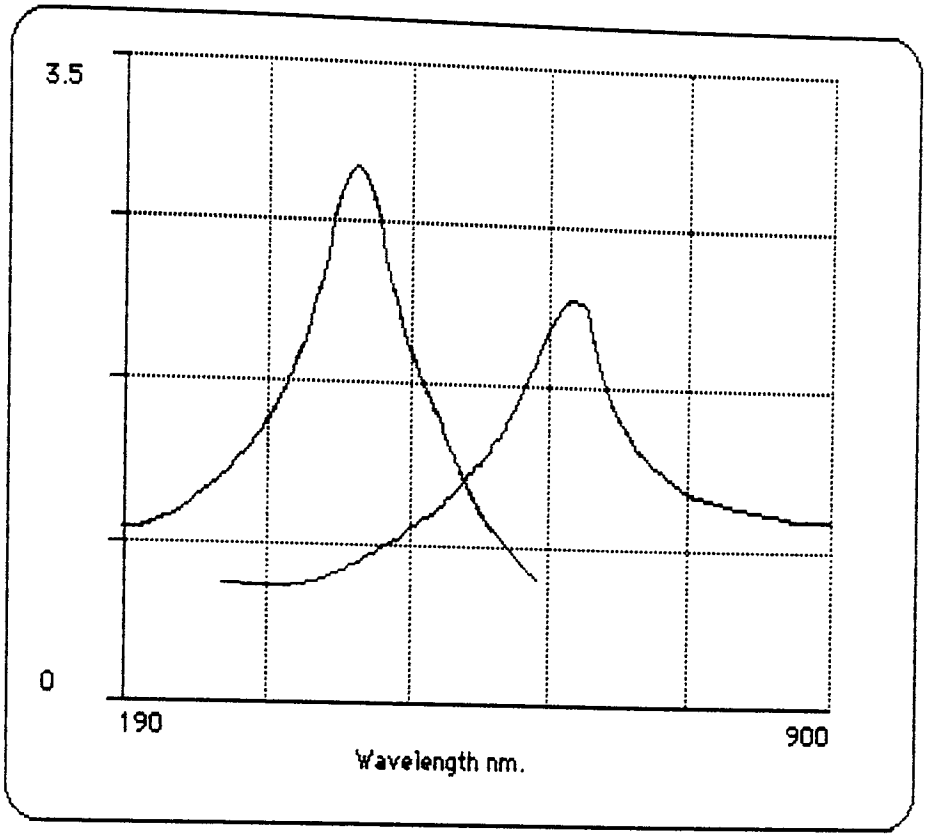


Figure A4.11. Example of monitor display from the overlay spectra programme.

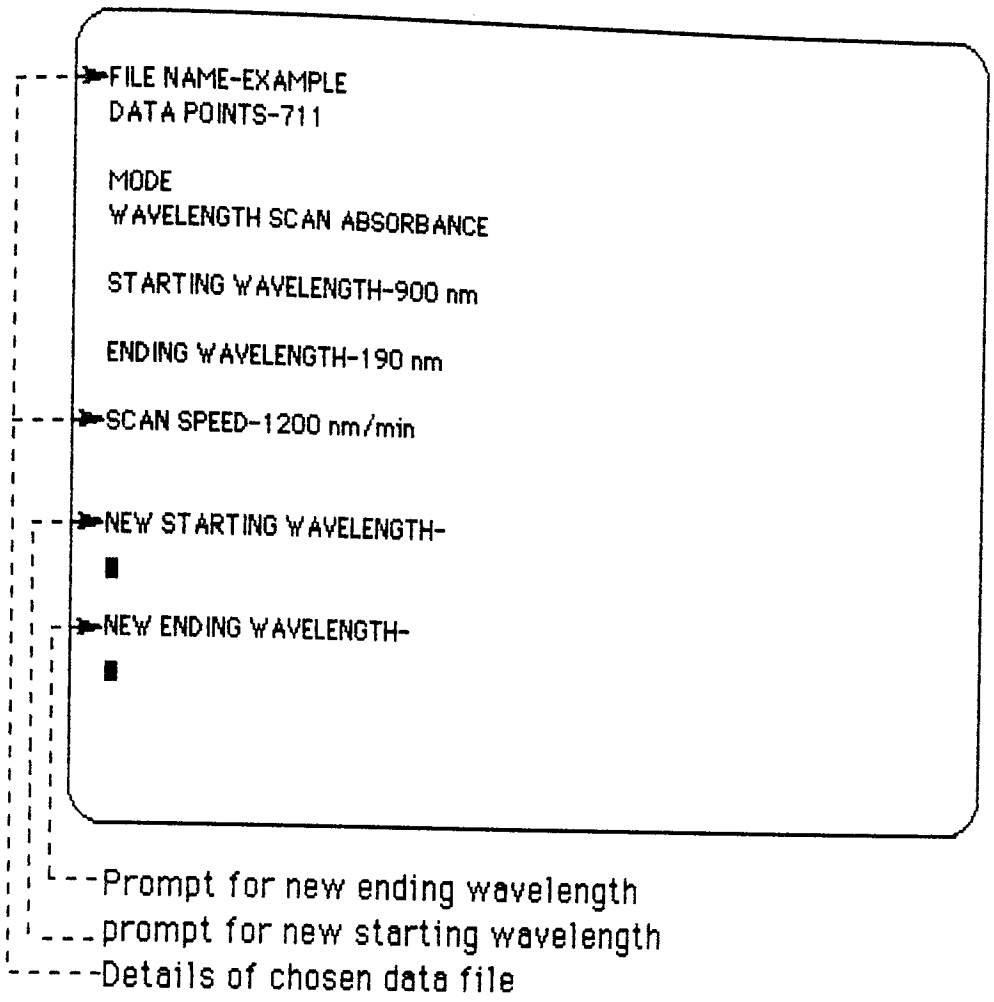


Figure A4.12. Example of monitor display from the magnify spectra programme.

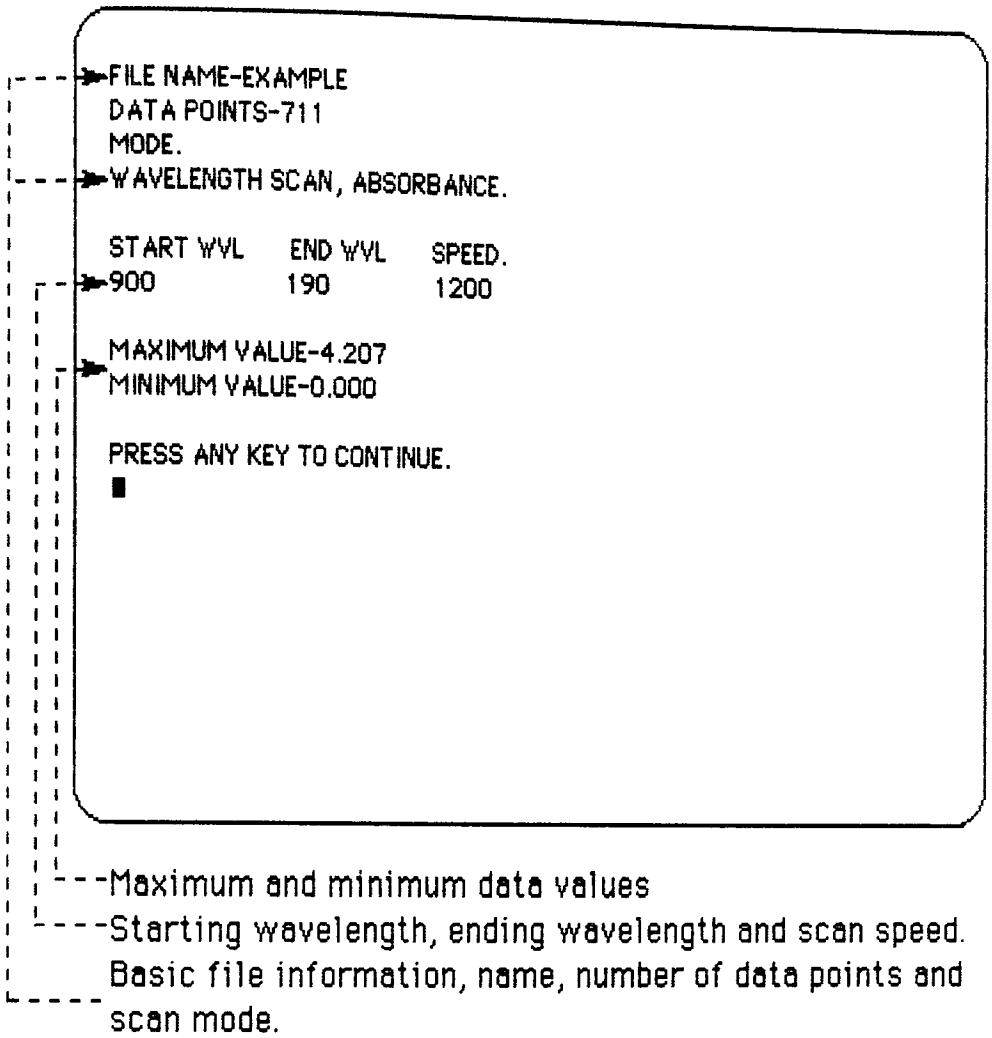
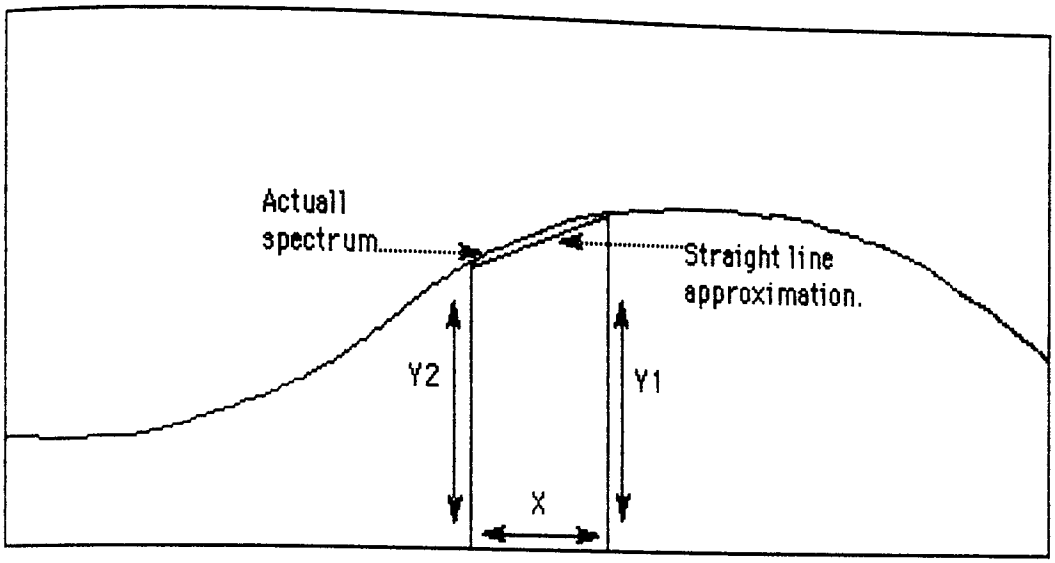


Figure A4.13. Example of monitor display from the identify file programme.



The slope of the curve y1, y2 is approximately equal to the slope of the straight line y1,y2.

The slope is therefore equal to (Y1-Y2)/X.

Figure A4.14. Method of slope approximation in derivative programme.

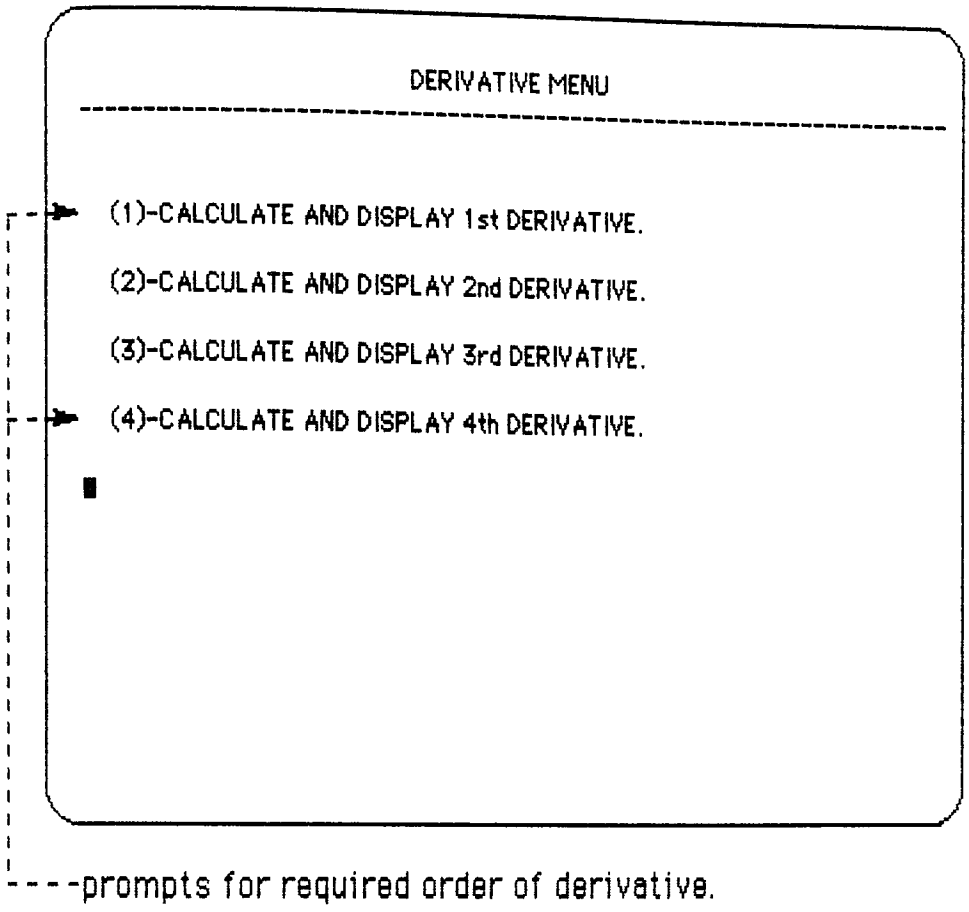
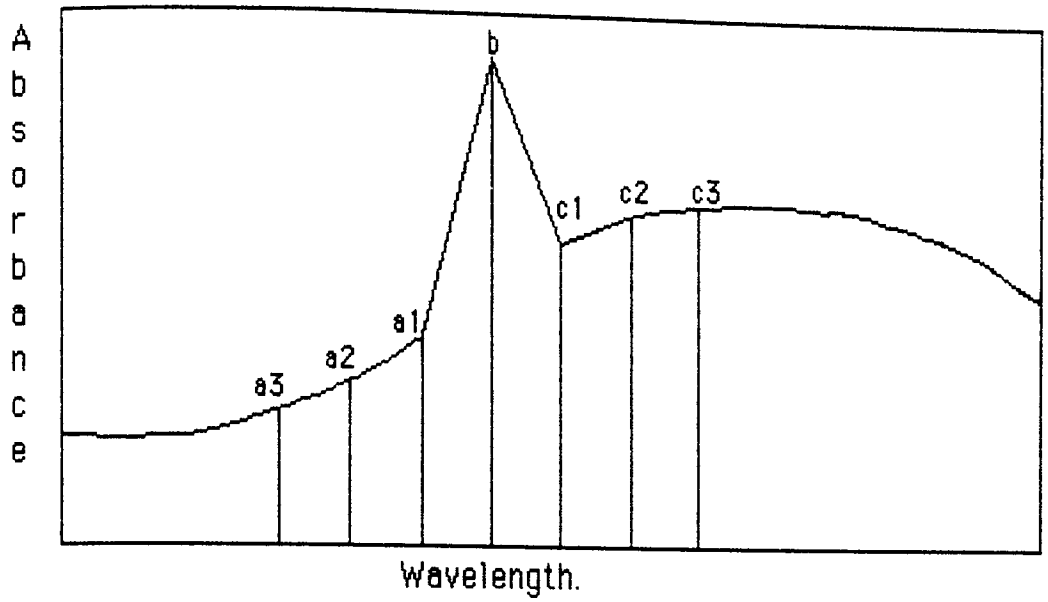


Figure A4.15. Menu display produced by the derivative programme.



Smoothing over 3 points.

$$\frac{a1 + a2 + a3}{3} \equiv a2$$

b^*= smoothed value of b

$$\therefore b^* \equiv \frac{a1 + b + c1}{3}$$

Smoothing over 5 points.

$$b^* \equiv \frac{a2 + a1 + b + c1 + c2}{5}$$

Figure A4.16. Smoothing algorithm used in smooth spectrum programme.

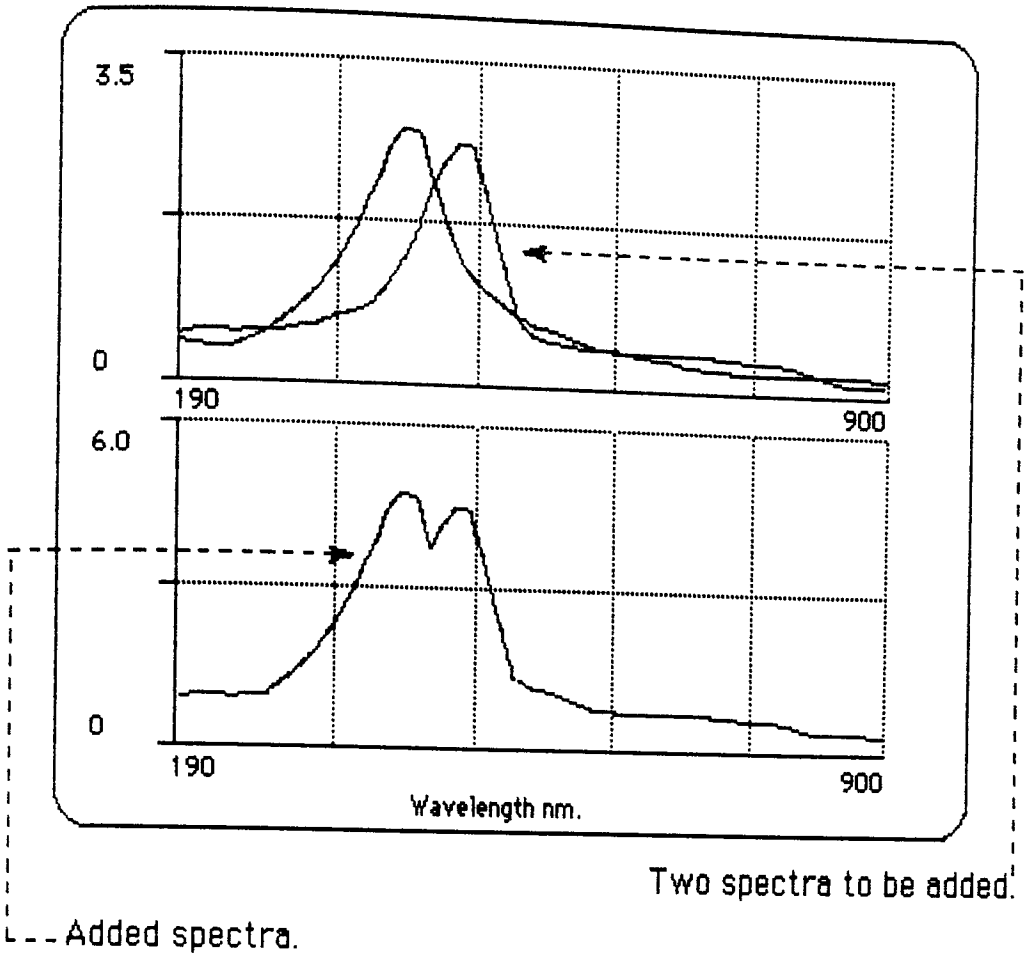


Figure A4.17. Display from add two spectra programme.

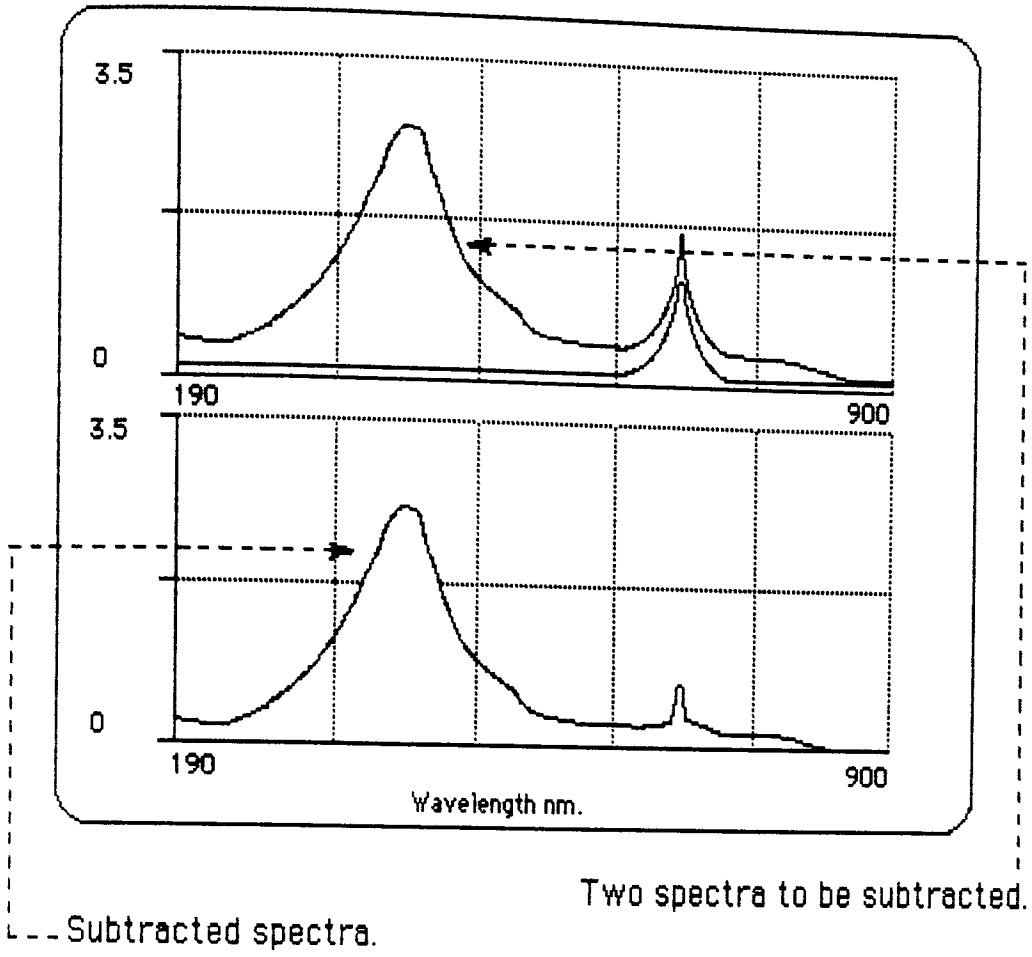


Figure A4.18. Display from subtract two spectra programme.

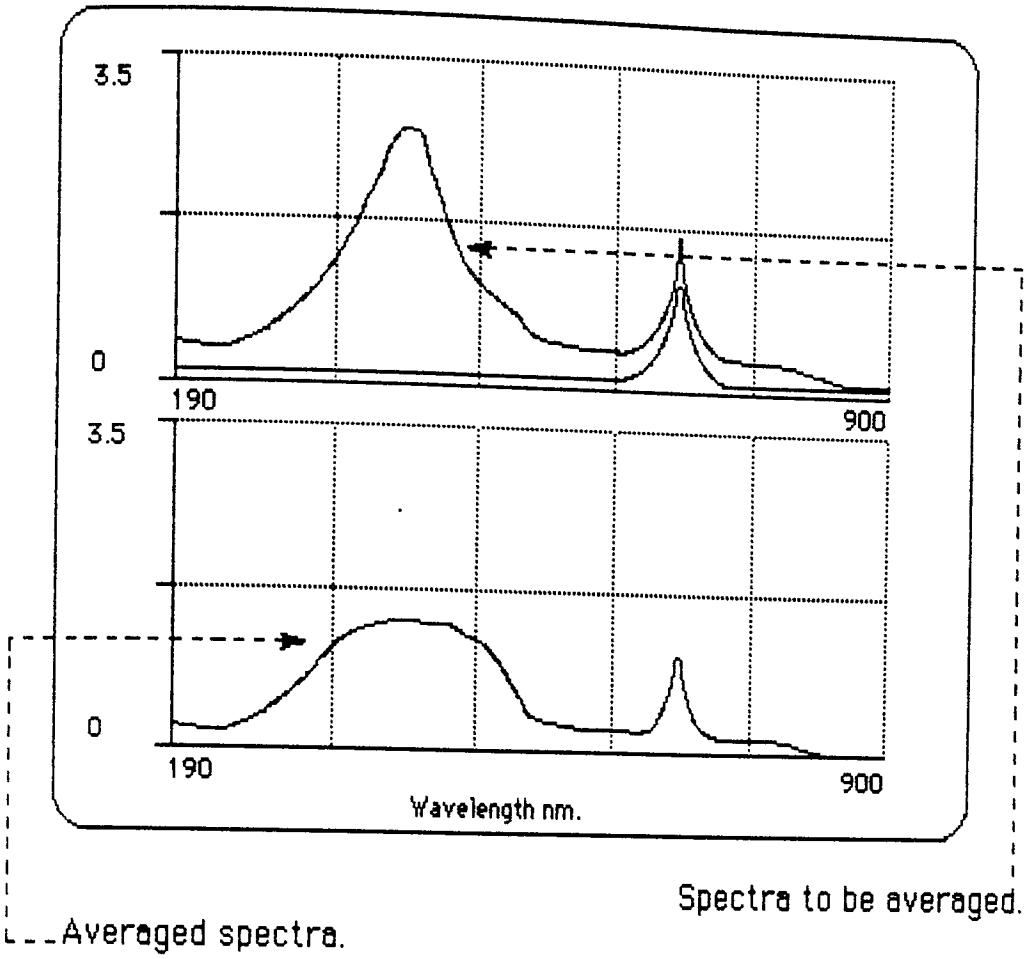


Figure A4.19. Display from average spectra programme.

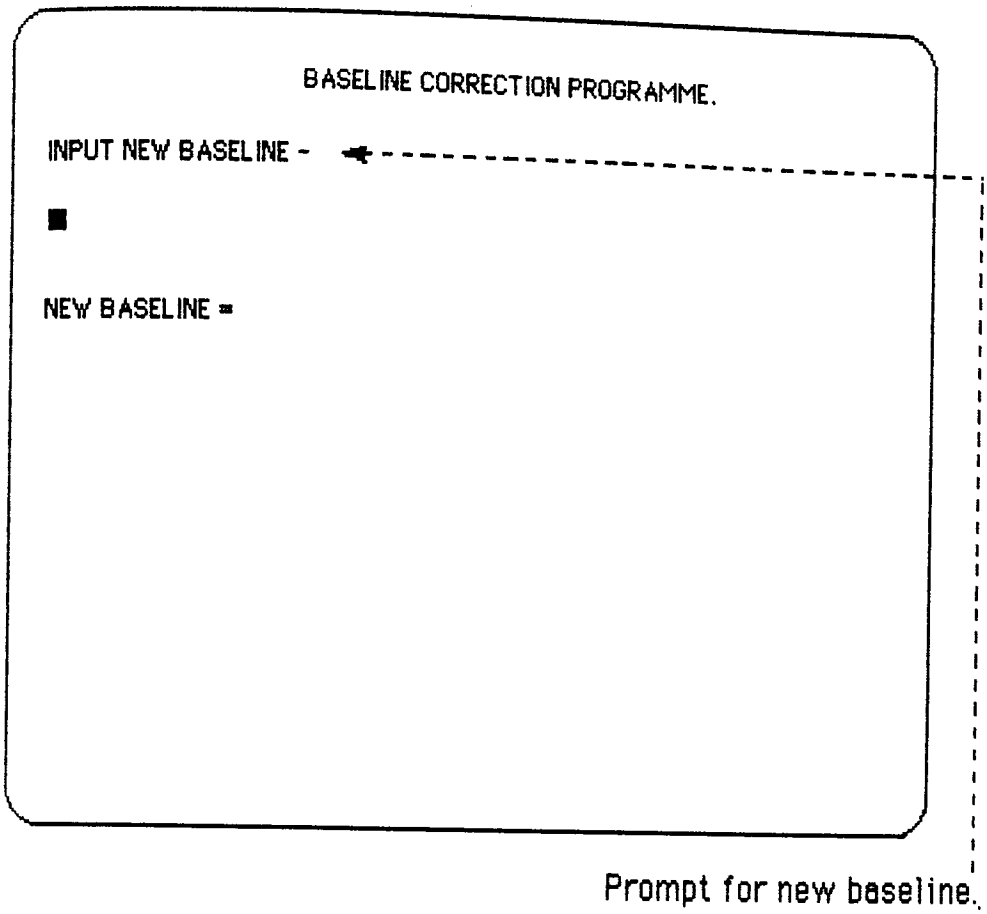


Figure A4.20. Display from correct baseline programme.

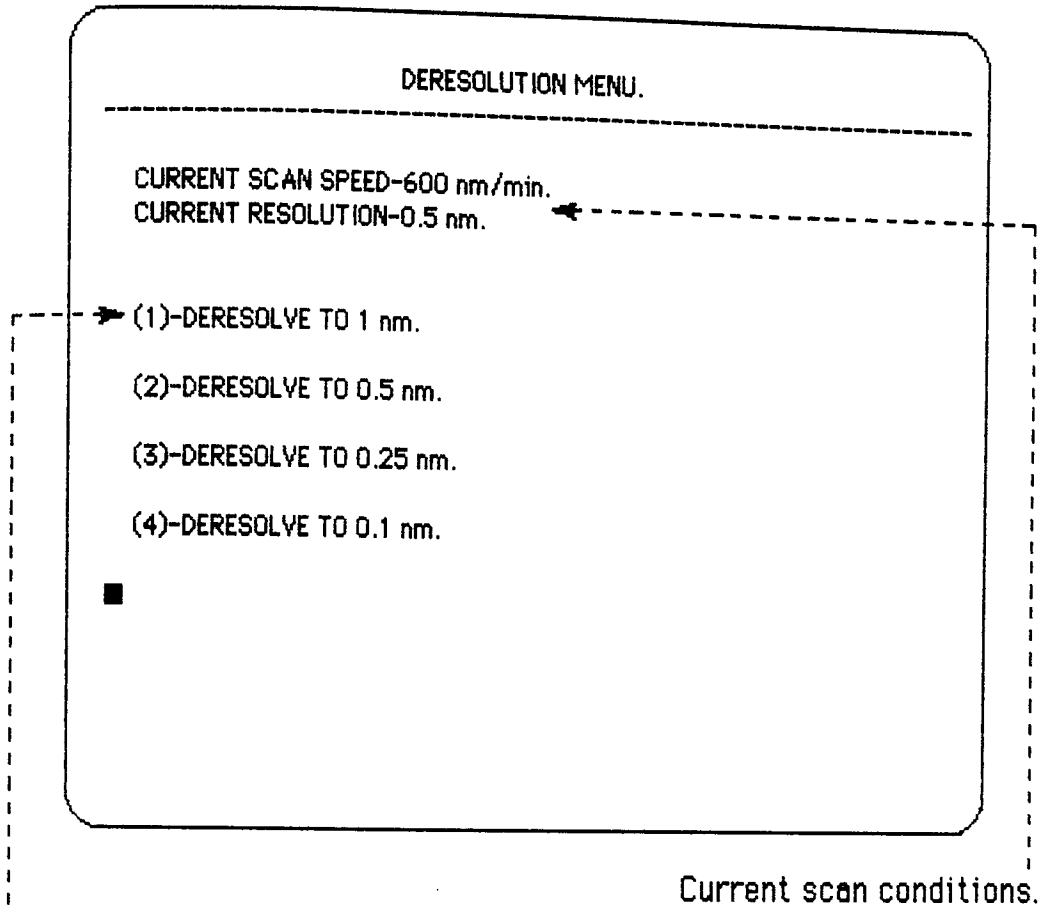


Figure A4.21. Display from the deresolve spectrum programme.

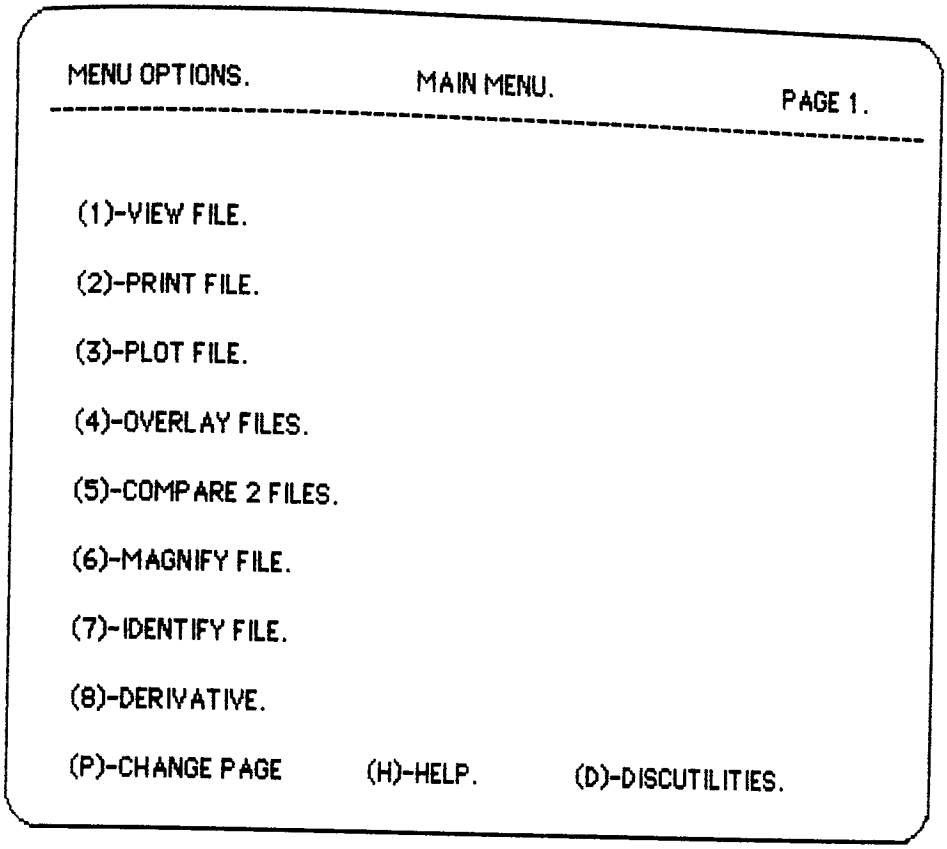


Figure A4.22. Main menu page 1.

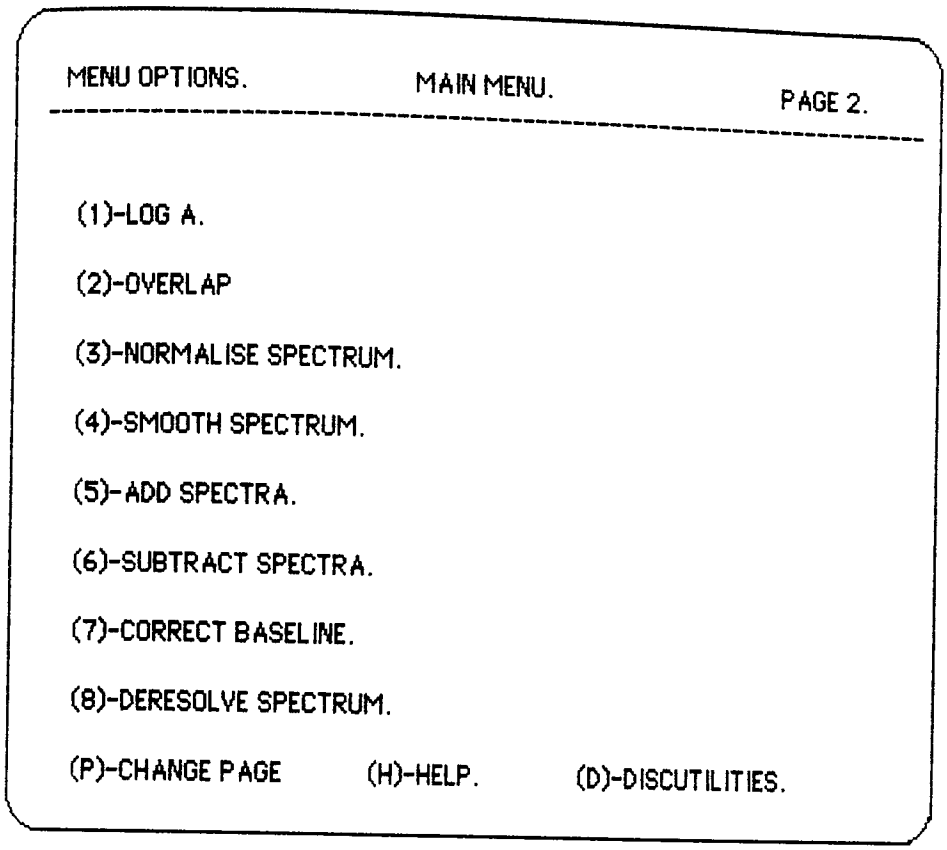


Figure A4.23. Main menu page 2.

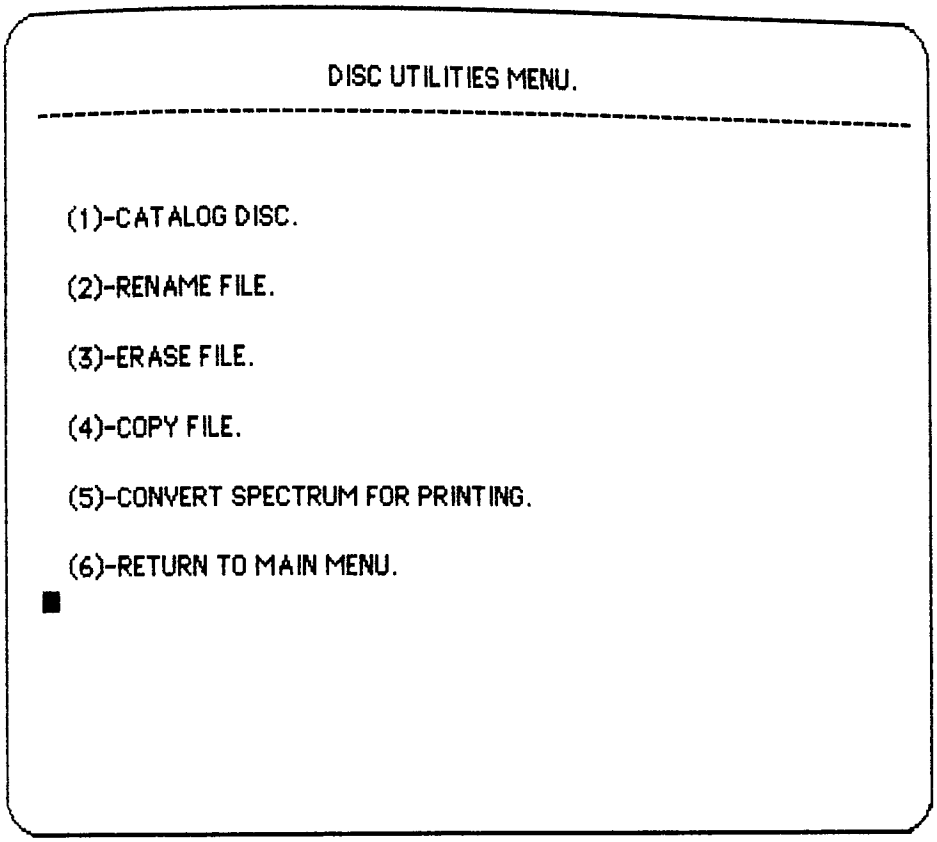


Figure A4.24. Disc utilities main menu.