AFML-TR-78-25-Part I
ADA060361

PREDICTING GLASS TRANSITION TEMPERATURES (T_g) OF POLYMERS FROM THEIR MOLECULAR STRUCTURE. PART I. INDIVIDUAL ATOM CONTRIBUTIONS

Polymer Branch
Nonmetallic Materials Division

April 1978

TECHNICAL REPORT AFML-TR-78-25-Part I

Final Report for Period December 1976 to December 1977

Approved for public release; distribution unlimited.

AIR FORCE MATERIALS LABORATORY
AIR FORCE WRIGHT AERONAUTICAL LABORATORIES
AIR FORCE SYSTEMS COMMAND
WRIGHT-PATTERSON AIR FORCE BASE, OHIO 45433

NOTICE

When Government drawings, specifications, or other data are used for any purpose other than in connection with a definitely related Government procurement operation, the United States Government thereby incurs no responsibility nor any obligation whatsoever; and the fact that the government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data, is not to be regarded by implication or otherwise as in any manner licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use, or sell any patented invention that may in any way be related thereto.

This report has been reviewed by the Information Office (ASD/OIP) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be releasable to the general public, including foreign nations.

F. E. Arnold
Project Engineer

R. L. Van Deusen, Chief
Polymer Branch
Nonmetallic Materials Division

FOR THE DIRECTOR

J. M. Kelble, Chief
Nonmetallic Materials Division

Copies of this report should not be returned unless return is required by security considerations, contractual obligations, or notice on a specific document.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE *(When Data Entered)*

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFML-TR-78-25-Part I	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE *(and Subtitle)* Predicting Glass Transition Temperatures (T_g) of Polymers from Their Molecular Structure. Part I. Individual Atom Contributions		5. TYPE OF REPORT & PERIOD COVERED Final Technical Report December 1976 - December 1977 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Dr. D. R. Wiff Dr. I. J. Goldfarb		8. CONTRACT OR GRANT NUMBER(s) F33615-75-C-5095
9. PERFORMING ORGANIZATION NAME AND ADDRESS See Block 18		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 24190415
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Materials Laboratory Air Force Systems Command Wright-Patterson Air Force Base, OH 45433		12. REPORT DATE April 1978 13. NUMBER OF PAGES 67
14. MONITORING AGENCY NAME & ADDRESS*(if different from Controlling Office)*		15. SECURITY CLASS. *(of this report)* Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT *(of this Report)*

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT *(of the abstract entered in Block 20, if different from Report)*

18. SUPPLEMENTARY NOTES

Air Force Materials Laboratory
Air Force Systems Command
Wright-Patterson Air Force Base, Ohio 45433

University of Dayton Research Institute
300 College Park Avenue
Dayton, Ohio 45469

19. KEY WORDS *(Continue on reverse side if necessary and identify by block number)*

Glass Transition Temperature
Free Volume
Van der Waals Radii
Van der Waals Volume
Close Packing

20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)* The present investigation is an extension of the method of Askadskii and Slonimskii to predict the glass transition temperature of amorphous polymers. The glassy volume of each polymer structure at a reference temperature is calculated using the Van der Waals radii of the individual atoms, the bonding distances, and the procedure of Kitaigorodskii. The volume of the repeat unit at T_g is approximated as the sum of the product of a weighting factor and a determined incremental volume contribution. Results using the L_1 error approximation and representing over 175 chemically or sterically different polymer structures are presented.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE *(When Data Entered)*

FOREWORD

This report was prepared by the Polymer Branch, Nonmetallic Materials Division. The work was initiated under Project No. 2419, "Nonmetallic and Composite Materials", Task No. 241904, Work Unit Directive 24190415, "Structural Resins". It was administered under the direction of Air Force Materials Laboratory, Air Force Wright Aeronautical Laboratories, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio, with Dr. F. E. Arnold as the AFML Project Scientist. Co-authors were Dr. D. R. Wiff, University of Dayton Research Institute (Contract Number F33615-75-C-5095) and Dr. I. J. Goldfarb, Air Force Materials Laboratory, (AFML/MBP).

This report covers research conducted from December 1976 to December 1977.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF ILLUSTRATIONS

SECTION I

INTRODUCTION

It is well recognized that amorphous polymeric materials exhibit three somewhat distinct material regions; glassy, rubbery, and liquid. There are kinetic restrictions in each of these regions on the rate at which molecules or segments of molecules rearrange themselves from one equilibrium configuration to another. Thus, when an external parameter such as temperature or pressure is varied, time is required for molecular segments to regain their equilibrium configuration. When temperature is lowered sufficiently so that the time necessary for molecular level rearrangement to occur is of the same order as the time scale of the experimental observation, the material will exhibit glassy region properties. Therefore, certain thermodynamic quantities such as the specific heat, expansion coefficient, or compressibility will show abrupt changes at the demarcation between the regions of rubbery and glassy behavior, namely T_g. In addition, because of the material response time to external mechanical forces, i.e., times associated with the molecular level configuration relaxations, the glass transition temperature can be determined from dynamic mechanical measurements. Whereas the main glass transition occurs when large segments of the polymer backbone chain become free to move, secondary transitions occur at lower temperatures where subgroups or side-chains become free to move or oscillate. At present, we are concerned only with the primary (glass) transition temperature.

Since a material's physical properties depend upon the intra- and inter-molecular interactions, scientists have been able to correlate physical properties by choosing a reference state of the individual material and relating other properties relative to this state. In the theory of polymer solutions, one relates measured properties to those at the θ - temperature of Flory (Reference 1). In the study of mechanical properties of polymers, data are correlatable by reference to the T_g of the material. The best known example of this is the WLF equation (References 2, 3) where the reference temperature isn't necessarily T_g, but T_g is a good choice. In all of these situations, the reference is a unique property of the material which identifies its intra- and inter-molecular interactions from those of other materials.

The question at hand is, how can one a priori to synthesizing a new polymer know it's T_g?

Trying to solve the T_g transition predictability problem from the rubbery region side does not seem very fruitful. There are theories such as the Rouse theory (Reference 4), Zimm theory (Reference 5) or Bueche theory (Reference 6) which correlate normal modes of polymer chain kinetics, intermolecular interactions, or accessible volume changes with physical properties. However, it is the glassy region where the chemical structure of the polymer molecule has profound effects.

The molecular and supermolecular structure of the material determines the value of T_g. Knowing the T_g associated with a given molecular and supermolecular structure, it can in turn be used as a reference in estimating the material's properties.

Of the many different methods for predicting T_g (References 7-14), the present investigation is directed toward use of the method by Askadskii (Reference 14). This method is based upon the experimental findings of Rogers and Mandelkern (Reference 15). They measured the specific volumes of a series of poly-(n-alkyl methacrylates) as a function of temperature and determined the respective glass transition temperatures. Some of their results are shown in Table 1. They mentioned that the specific volume-temperature data in the glassy state can be represented by a gradual curving line. As a result, a plot of log (T_g) versus the specific volume ($\bar{v}_g$) at T_g, relative to the specific volume ($\bar{v}_{25}$) at T_{25} = 25°C, i.e., ($\bar{v}_g/\bar{v}_{25}$) yielded a linear plot (Figure 1). It is with this information and studies correlating T_g with densities of polymers (Reference 16) that Askadskii postulates the semi-empirical relationship

$$\log T_g = \frac{\bar{v}_g}{\bar{v}_R} + A \qquad (1)$$

where $\bar{v}_g$ is the specific volume at T_g, $\bar{v}_R$ is the specific volume at the reference temperature T_R (°K), and A is the logarithm of this reference temperature minus unity, i.e., A = log (T_R) -1. Through studies by Bondi (References 17, 18) and Slonimskii, et. al. (Reference 19), a linear relationship exists between the specific volume of polymers in the glassy and rubbery regions and their corresponding van der Waals volume (Reference 20). The van der Waals volume is assumed to be bounded by the outer surface of a number of interpenetrating spheres. The radii of the spheres are assumed to be (constant) atomic radii for the elements involved and the distances between the centers are the (constant) bond distances.

In the following section, the procedure used to compute the van der Waals volume of any polymer structure is presented. Also, the volume at the glass transition temperature is approximated as the sum of the product of a weighting factor (number of times an incremental volume contribution occurs in a polymer) and a least square determined incremental volume contribution K_j. These incremental volume contributions will consist of individual types of atoms, bonding which affects the volume, unique steric effects in the polymer structure, etc. This is followed by application of Equation 1 to about 170 different polymer structures which consists of about five classes of polymers. Each class is composed of polymers differing from each other by addition and deletion of chemical units which affect the basic polymer backbone flexibility and in some cases these chemical units are pendant groups affecting the molecular packing. Some polymers listed will have the same van der Waals volume, but different T_g's. This is due to steric effects affecting the accessible polymer conformation volumes.

SECTION II

THEORY

1. VAN DER WAALS VOLUME

In Equation 1 the referenced specific volume and specific volume at the glass transition temperature are herein treated as per repeat unit of the polymer. Therefore, instead of specific volumes we can talk about the molar volumes of the repeat units since the molecular weights will cancel. That is

$$\frac{\bar{v}_g}{\bar{v}_R} = \frac{V_g/M}{V_R/M} = \frac{V_g}{V_R} \tag{2}$$

where V_g and V_R are now the molar volumes of the repeat unit at T_g and at a reference temperature T_R, and M is the molecular weight of the repeat unit. In essence, we are assuming that we are on the plateau region of a T_g versus molecular weight of polymer graphical plot, i.e., the molecular weight of the polymer is high enough so that there is no dependence of T_g upon molecular weight.

Now the repeat unit molar volume V_R can be replaced by

$$V_R = N_A \sum_{\ell} \Delta V_\ell \tag{3}$$

where N_A is Avogadro's number and ΔV_ℓ's are the intrinsic volumes of the atoms and atomic groups making up the molecule, i.e., repeat unit. The calculation of ΔV_ℓ is based on detailed studies of close packing of organic molecules made by Kitaigrodskii (References 19, 21, 22). According to these ideas, the volume of an atom can be represented by a radius ρ (Van der Waals radii). If the atom is chemically bound to other atoms,

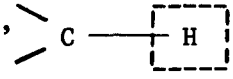
the adjacent atoms share part of the sphere of the first atom because the sum of the atomic radii of two valence-bonded atoms is always greater than the distance between their centers, i.e., the corresponding bond length d_j (Figure 2).

Then the volume increment ΔV_ℓ for the ℓth atom is the van der Waals radii spherical volume minus the volumes of the spherical segments cut off from this sphere by adjacent valence-bonded atoms.

$$\Delta V_\ell = \frac{4}{3}\pi \rho_\ell^3 - \sum_j \pi \frac{h_j^2}{3} (3\rho_\ell - h_j) \tag{4}$$

where

$$h_j = \rho_\ell - \frac{\rho_\ell^2 + d_j^2 - \rho_j^2}{2d_j} \tag{5}$$

The van der Waals radii for various atoms are listed in Table 2. The bond lengths used for the present computation are listed in Table 3. As an example of this, let us compute the van der Waals volume of a hydrogen atom bonded to an aromatic carbon, i.e., 

From Tables 2 and 3, $\rho_c = 1.80A$, $\rho_H = 1.17A$ and $d_{C-H} = 1.08A$. Using Equation 5, we get

$$h_1 = 1.17 - \frac{(1.17)^2 + (1.08)^2 - (1.80)^2}{2(1.08)} = 1.50A$$

and from Equation 4

$$\Delta V_H = \frac{4}{3}\pi\ (1.17)^3 - \frac{\pi(1.50)^2}{3}\ \left[3\ (1.17) - 1.50\right] = 1.99A^3$$

Thus, the contribution of a single hydrogen atom bonded with an aromatic carbon contributes to the volume of a molecule or polymer repeat unit, $1.99A^3$. The total volume of a repeat unit will be $\sum_\ell \Delta V_\ell$ where $\ell = 1, 2, ----$, L; L being the maximum number of incremental volumes in the repeat unit

(Table 4). Multiplying this repeat unit volume by Avogadro's number then yields the molar van der Waals volume $N_A \Sigma_\ell \Delta V_\ell$. The temperature corresponding to this reference volume can be taken as 25°C (298°K) if the van der Waals volume is multiplied by a constant. Askadskii (Reference 19) found this constant to be 1.45, but incorporated it into the least square determined K_j's.

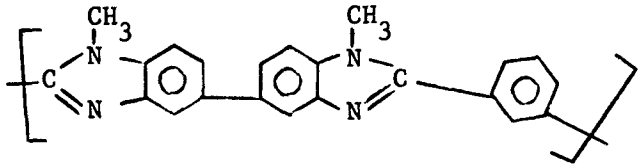
2. WEIGHT FACTORS AND INCREMENTAL VOLUMES

Next, consider the evaluation of the molar volume V_g in Equation 2. Here the subscript, g, is used to emphasize that this is the molar volume at the glass transition temperature T_g. The various chemical groups, types of atoms, unique intra- and interaction bonding, steric isomers, etc., contributions to the volumes at T_g are evaluated by a minimization technique. The individual polymer repeat units are differentiated from each other by having occupation numbers or weighting factors associated with those volume factors, K_j present in the repeat unit. That is

$$(V_g)_i = \sum_j d_{ij} K_j \qquad (6)$$

where d_{ij} is the jth weighting factor or occupation number associated with the volume factor K_j, and $(V_g)_i$ is the molar volume for the ith polymer having a glass transition temperature $(T_g)_i$. Typical volume factor contributions are those associated with the hydrogen, carbon, nitrogen, oxygen, sulfur, fluorine, and chlorine atoms. The steric effects involved with the bonding to a benzene ring whether the bonds are ortho-, meta-, or para are accounted for through separate volume factors. A listing of the T_g's and weighting factors for all of the polymers used in the present analysis is given in Table 5. Here the polymer number is in correspondence with the

sequenced chemical structures presented in Table 6. This cataloging procedure is best exemplified by considering the chemical structure #2, Table 6,



Here there are 16 hydrogen atoms, 22 carbon atoms, and 4 nitrogen atoms. There are two CH_3-groups through which dipole-dipole interaction can occur; one backbone benzene ring where the adjacent bonding is meta; two partially condensed rings, two double bonds, three benzene rings in total, two amine groups, and two (C = N) bonds. Looking at Table 5, one can see that the chosen weighting factors for polymer #2 are 16, 22, 4, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 1, 0, 2, 0, 0, 0, 6, 2, 3, 0, 0, 0, 0, 2, 2, 0, 0 for a total of 33 weights coefficients.

SECTION III

COMPUTATION AND RESULTS

One of the first problems encountered in determining the K_j's, given the α_{ij} and $(T_g)_i$ values, is the possibility of computational round-off error accumulation when considering about 50 K_j's and 200 T_g's. Because of the simplicity and computational accuracy associated with the simplex algorithm used in linear and quadratic programming (References 23, 24), a linear programming computational scheme was chosen for the present calculation. In this scheme, the K_j's are chosen so as to minimize the absolute value of the errors in the T_g's, i.e., the error minimized is

$$\sum_i | \varepsilon_i | = \sum_i | \text{ Calculated } T_g)_i - \text{Experimental } T_g)_i | \qquad (7)$$

This is mathematically the L_1 norm for error evaluation.

Choosing the K_j's (Table 7) to be used for a given system of polymers does involve some experience. Mathematically we are treating them as a linearly independent set of variables. Therefore, most scientists would feel uneasy as to which K_j's to keep and which ones to leave out of a given analysis. An advantage for using the linear programming technique is it's ability to restrict all K_j's ≥ 0. In the present study this was used so that those K_j's which are not relevant will be determined to be zero. Thus, all volume contributions will be positive. If a priori one knows that a certain bonding will be such as to give a negative K_j, the appropriate weighting factor can easily be made negative.

Combining Equations 1, 2, 3, and 6, we have

$$\log T_g)_i = \frac{\sum d_{ij} K_j}{N_A \sum_\ell \Delta V_\ell} + A \qquad (8)$$

which is the form given by Askadskii (Reference 19). The computation was performed by evaluating the K_j's which minimized the error criterion, namely the L_1 norm, for a given A. Then stepwise A was changed and another set $\{K_j, j = 1, \ldots J\}$ was determined which was in correspondence with a minimum error analysis. Finally, the chosen $\{K_j^*\}$ and A^* was the inferior of these minima. To show that this was a reliable procedure, initial values for K_j, the volumes and weighting factors for real polymers and a single value for A were assumed (Table 8). These values were then used to compute analogous experimental data. Using these computed experimental T_g data, the volumes and weighting factors for the real polymers used in this test and a variety of values for A, the set $\{K_j^*\}$ was found which was in correspondence with the inferior minimum associated with the sequence of A's used. This set $\{K_i^*\}$ can be seen to be the same as the initially assumed $\{K_j\}_{initial}$ (Table 7). Closer examination of the assumed and computed $\{K_j\}$ reveals that $K^*_{13} = K^*_{14} = K^*_{15} = K^*_{17} = 0$. The reason for this is that all of the weighting factors in columns 13, 14, 15, and 17 are zero. There is also a small discrepancy between K_{10}, K_{11}, K_{12}, and K^*_{10}, K^*_{11}, K^*_{12}. The only reason for this is that due to the very large repeat unit volumes for polymers 9-13 and the uniform weighting factors in these rows and columns, the information was lost in the matrix inversion process. Possibly if the pivot tolerances were made smaller these starting numbers could be recovered.

In order to conserve on computer time, a series of imide polymers (numbers 34-82 in Tables 5 and 6) totaling 49 different chemical structures were used in the present preliminary studies. Three experiments were performed: first, using all 33 weighting factors (Table 5) and assuming all $K_j \geq 0$, vary A so as to find the inferior of the error criterion of Equation 7. Secondly, eliminating those weighting factors which are zero, approximate a standard least square procedure by allowing positive and negative K_j's while also scanning the parameter A so as to obtain the inferior error criterion. Thirdly, in order to have a comparison of the present volume factors with those of Askadskii (Reference 19), set A = 1.435 and admitting only solutions $K_j \geq 0$ find the volume factors which minimize the error criterion of Equation 7.

The first of these experiments yielded the results presented in Tables 9 and 10. The inferior error analysis was in correspondence with A = 1.140. The problem arising here is that the volume contribution for sulfur atoms is zero even though sulfur appears in polymers numbered 70-81. The second of these experiments yielded (Tables 9 and 10) which show that now sulfur will have a negative volume contribution. The third experiment again yielded the volume contribution for sulfur as zero. It should be noted that in all three cases the analysis (coefficient of variation) was 0.4538%, 0.4535%, and 0.4544% respectively.

SECTION IV

CONCLUSIONS

The present analysis shows promise for this approach at predicting glass transition temperatures. Modifications can easily be made so that only K_j's ≥ 0 for atom volumes and positive and negative volume contributions for bonding effects will be admissible. The choice of the parameter A will definitely affect the magnitude of the volume factors K_j. Therefore, this parameter A should be fixed at a value associated with a reference temperature of 25°C or 298K. Then other class of polymer parameters C_k may be included so that Equation 8 will become

$$\log T_{g_i} = \frac{\sum_j \alpha_{ij} K_j}{N_A \sum_1 \Delta V_1} + \sum_{k=1}^{\text{number of classes}} C_k + A \qquad (9)$$

where $C_k = 1$ if polymer i belongs to class k and zero otherwise. Once a large enough set of polymers from various classes is used to establish atom and certain frequently occurring bonding volume factors an iterative self refinement scheme might be used in order to include new T_g data as it becomes available. To determine the necessity of using C_k's one should measure the specific volumes of other classes of polymers in a Rogers-Mandelkern fashion (Reference 15) to see whether each gives a straight line plot only shifted relative to each other (Figure 2).

REFERENCES

1. P. J. Flory, Principles of Polymer Chemistry, Cornell University Press, Ithaca, N. Y., 1953.

2. I. M. Ward, Mechanical Properties of Solid Polymers, Wiley-Interscience, New York, N. Y. 1971.

3. J. D. Ferry, Viscoelastic Properties of Polymers, John Wiley & Sons, Inc., New York, N. Y., 1961.

4. P. E. Rouse, J. Chem. Phys. 21, 1272 (1953).

5. B. H. Zimm, J. Chem Phys., 24, 269 (1956).

6. F. Bueche, J. Chem. Phys., 22, 603 (1953).

7. R. F. Boyer, (ed)., Transitions and Relaxations in Polymers, Interscience, New York, N. Y., 1967.

8. M. C. Shen and A. Eisenberg, "Glass Transitions in Polymers", Rubber Chem. Technol., 43, 95 (1970).

9. R. A. Hayes, J. Appl. Polymer Sci., 5, 318 (1961).

10. J. M. Barton and W. A. Lee, Polymer 9, 602 (1968).

11. W. A. Lee and G. J. Knight, Brit. Polymer J. 2, 73 (1970).

12. W. A. Lee, J. Polymer Sci, A-2, 8, 555 (1970).

13. H. G. Weyland, P. J. Hoftyzer, and D. W. Van Krevelen, Polymer, 11, 79 (1970).

14. A. A. Askadskii and G. A. Sloimskii, Polymer Sci. USSR, 13, (8), 2158 (1971).

15. S. S. Rogers and L. Mandelkern, J. Phys. Chem., 61, 985 (1957).

16. A. A. Askadskii, Polymer Sci, USSR, 9 (2), 471 (1967).

17. A. J. Bondi, J. Phys. Chem. 68, 441 (1964).

18. A. J. Bondi, Physical Properties of Molecular Crystals, Liquids and Glasses, John Wiley & Sons, Inc., New York, N. Y. 1968.

19. G. E. Slonimskii, A. A. Askadskii, and A. I. Kitaigorodskii, Polymer Sci., USSR 12 (3), 556 (1970).

20. D. W. Van Krevelen, Properties of Polymers, Correlations with Chemical Structure, Elsevier Publishing Company, New York, N. Y., p. 51, 1972.

21. B. Wunderlich, Macromolecular Physics, Academic Press, New York, N. Y., 1973.

22. A. I. Kitaigorodskii, Organic Chemical Crystallography, Consultants Bureau, New York, N. Y., 1961

23. S. I. Gass, Linear Programming, Methods and Applications, McGraw-Hill Company, 4th Ed., 1975.

24. J. C. G. Boot, Quadratic Programming, North-Holland Publishing Company, 1964.

TABLE 1

SPECIFIC VOLUME - TEMPERATURE DATA ACCORDING TO ROGERS AND MANDELKERN (REFERENCE 15)

Polymer	T_g(°C)	Specific Volumes (cm^3/g) $\bar{v}_{25°C}$	$\bar{v}_g$	$\bar{v}_{120°C}$	T_g(°K)	log T_g	v_g/v_{25}
Poly-(methyl methacrylate)	105	0.855	0.870	0.877_5	378.2	2.578	1.0175
Poly-(ethyl methacrylate)	65	0.889	.900	.928	338.2	2.529	1.0124
Poly-(n-propyl methacrylate)	35	$.928_5$	$.931_5$	$.981_5$	308.2	2.489	1.0032
Poly-(n-butyl methacrylate)	20	.950	$.947_5$	1.007_5	293.2	2.467	0.9974
Poly-(n-hexyl methacrylate)	-5	$.992_5$	.972	1.055	268.2	2.428	0.9793
Poly-(n-octyl methacrylate)	-20	1.030	1.002	1.089	253.2	2.403	0.9728
Poly-(n-dodecyl methacrylate)	-65	1.076	1.015_5	1.141	208.2	2.318	0.9491

25°C = 298.2°K, log 298.2 = 2.475

log 298.2 = 2.475

TABLE 2

VAN DER WAALS RADII FOR ATOMS USED IN THIS INVESTIGATION

Atom	ρ(A)	Atom	ρ(A)
C	1.80	Cl	1.78
H	1.17	F	1.50
O	1.36	S	1.85
N	1.57		

TABLE 3

BOND LENGTHS USED IN THE PRESENT INVESTIGATION

Bond	d_i(A)	Bond	d_i(A)
C - C	1.54; 1.48*	C - N	1.37; 1.40+
C = C	1.40	C - Cl	1.77
C = C	1.34	C - F	1.34
C - H	1.08	C = O	1.28
C - O	1.50; 1.36*	C ≡ N	1.16
C ≡ C	1.20		
N ≡ N	1.09		

* The first figure is the bond length with an aliphatic carbon, the second with an aromatic carbon

+ The first figure is the C-N bond length in most compounds, the second is the bond length in aliphatic polyamides

TABLE 4

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

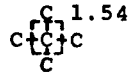
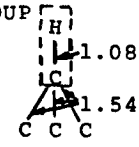
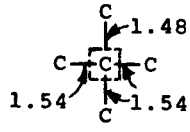
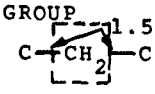
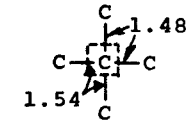
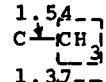
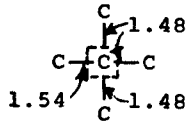
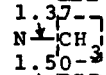
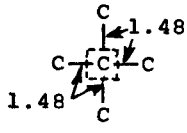
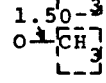
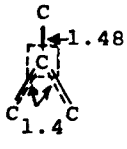
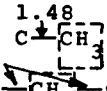
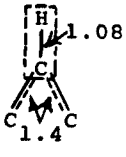
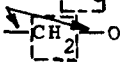
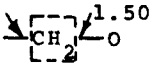
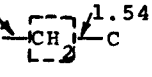
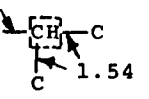
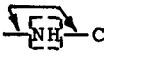
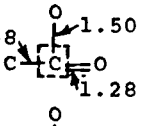
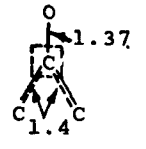
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
QUATERNARY CARBON ATOM 	5.0	ALIPHATIC CH GROUP 	11.1
ALIPHATIC CARBON ATOMS COMBINED WITH AROMATIC CARBON ATOMS 	4.7	ALIPHATIC CH_2 GROUP 	17.1
	4.5	ALIPHATIC CH_3 GROUPS 	23.5
	4.2		25.06
	4.0		24.6
AROMATIC CARBON ATOM 	8.4	AROMATIC CH_3 GROUP 	23.3
AROMATIC CH GROUP 	14.7		19.3
			20.2
			20.2
			15.3
			8.3
			15.7
			11.65

TABLE 4 (CONTINUED)

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

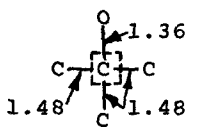
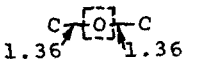
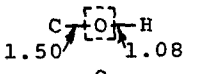
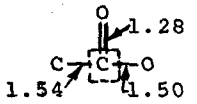
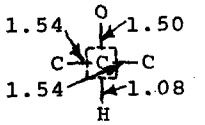
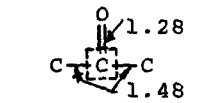
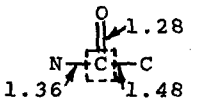
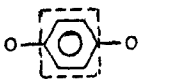
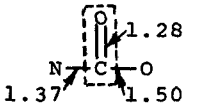
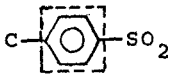
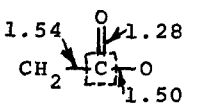
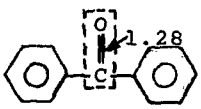
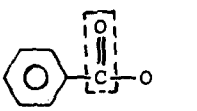
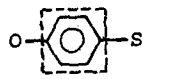
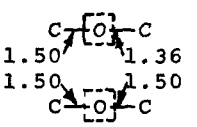
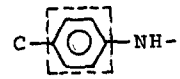
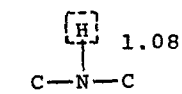
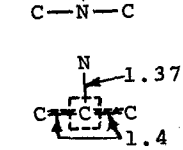
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	7.25		2.1
	5.85		5.6
	15.9		12.2
	12.3		78.85
	14.1		82.10
	23.3		76.2
	21.75		83.7
	18.15		79.2
	21.55		79.45
	2.7		75.6
	3.4		76.2
			77.4
			81.9
			3.5
			10.2

TABLE 4 (CONTINUED)

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

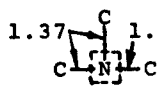
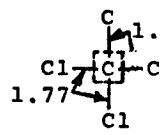
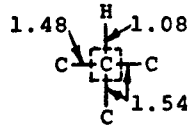
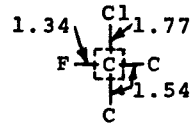
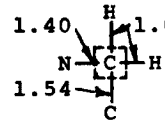
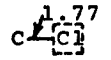
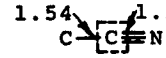
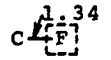
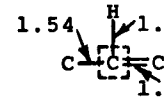
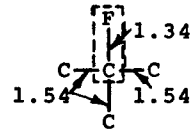
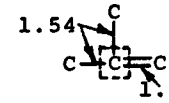
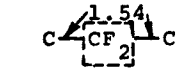
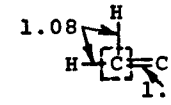
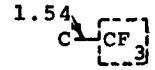
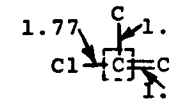
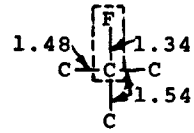
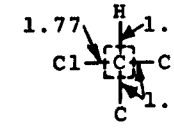
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	0.9		7.1
	8.6		9.48
	4.7		8.05
	14.7		19.85
	15.9		9.2
	10.0		9.1
	13.1		16.3
	9.0		27.5
	17.1		38.8
	10.0		16.0
	10.1		

TABLE 4 (CONTINUED)

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

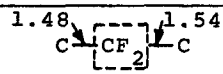
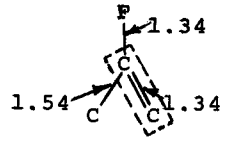
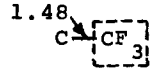
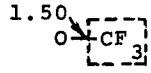
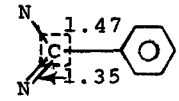
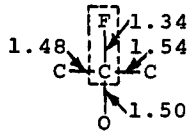
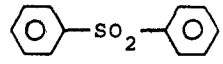
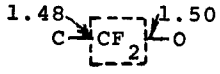
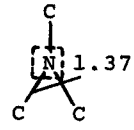
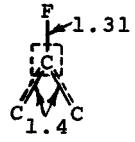
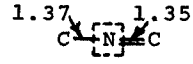
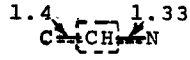
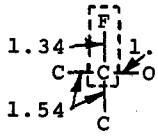
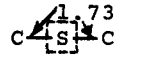
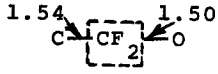
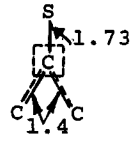
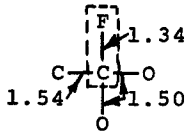
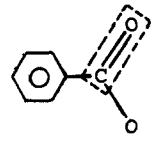
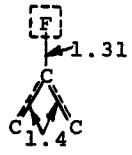
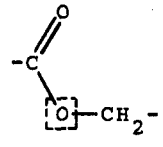
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	27.3		20.3
	38.5		
	41.9		12.9
	19.0		27.0
	30.3		0.9
	10.65		5.99
			14.81
	19.3		2.58
	30.65		9.02
	22.3		21.55
	9.0		3.4

TABLE 4 (CONTINUED)

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

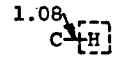
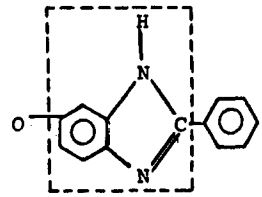
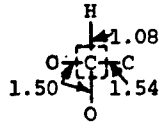
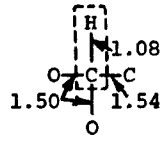
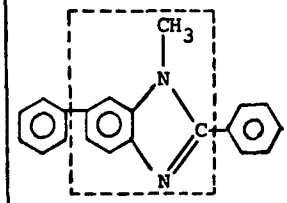
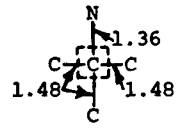
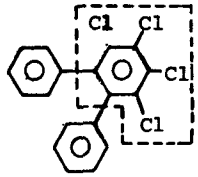
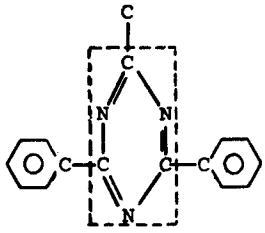
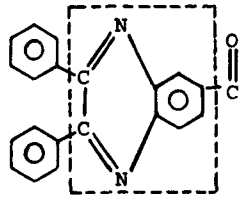
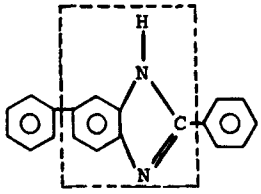
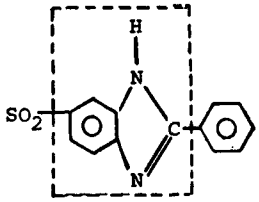
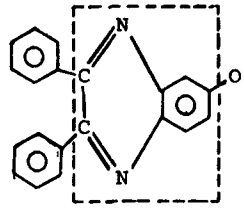
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	1.99		103.4
	13.3		
	15.3		117.8
	5.8		
			54.7
	54.7		
			105.3
	100.1		
	100.72		108.55

TABLE 4 (CONTINUED)

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

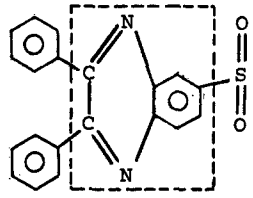
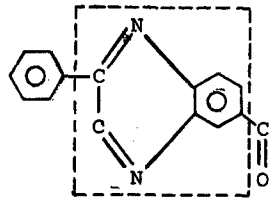
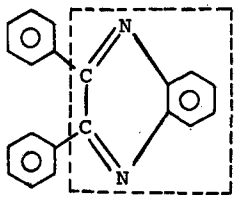
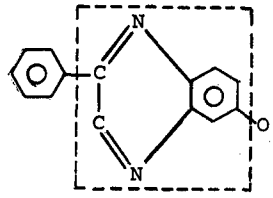
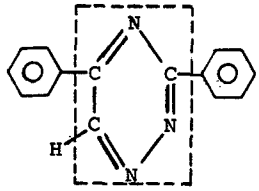
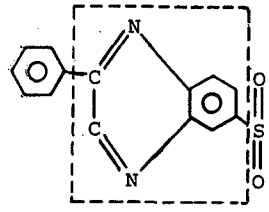
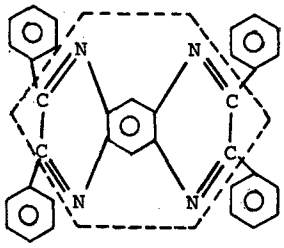
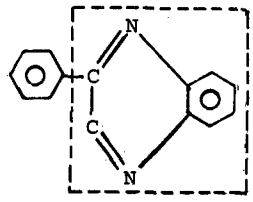
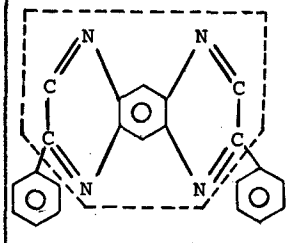
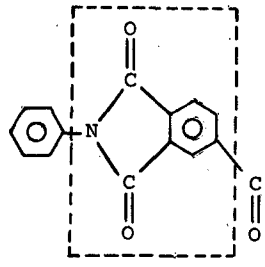
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	105.92		109.91
	105.3		113.16
	58.77		110.53
	135.0		109.91
	144.2		108.0

TABLE 4 (CONTINUED)
INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

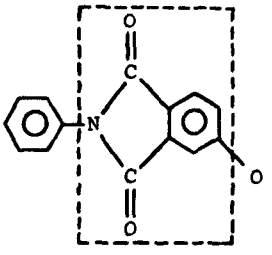
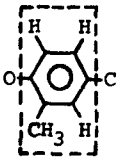
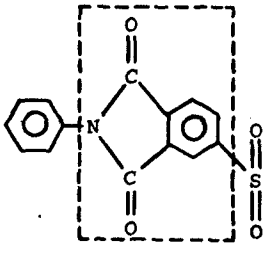
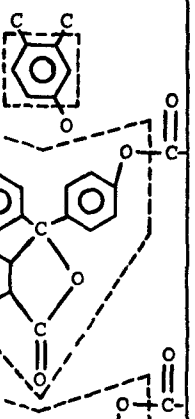
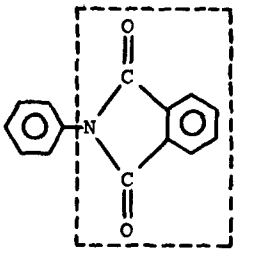
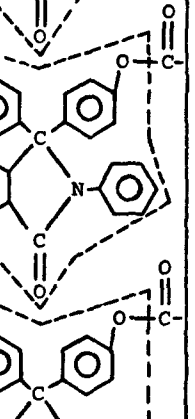
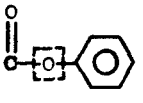
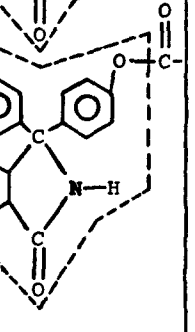
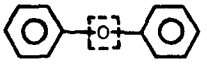
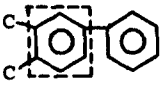
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	111.25		95.85
	108.62		72.55 270.9
	108.0		349.05
	2.7		272.75
	2.1		
	69.3		
	80.65		

TABLE 4 (CONCLUDED)

INCREMENTAL VOLUMES ARE INDICATED BY DASHED LINE ENCLOSURES

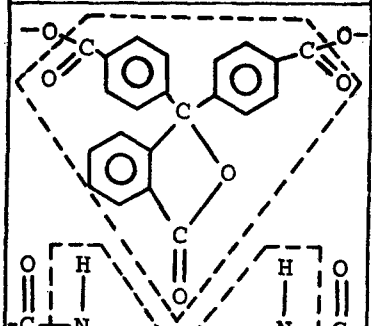
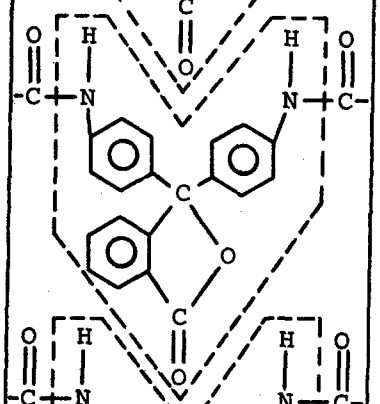
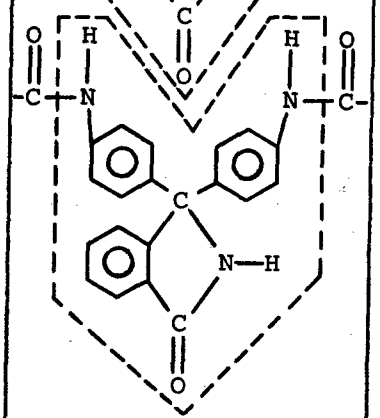
ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3	ATOM/ATOMIC GROUP	VOLUME INCREMENT A^3
	302.1		
	279.2		
	281.05		

TABLE 5

GLASS TRANSITION TEMPERATURES, VOLUMES, AND WEIGHTING FACTORS OF POLYMERS USED IN THIS INVESTIGATION. THE POLYMER NUMBER IS IN CORRESPONDENCE WITH THE CHEMICAL STRUCTURES GIVEN IN TABLE 6.

No.	Vol(A^3)	Tg(K)	Weighting Factors																													
1	393.00	359.6	16	27	4	1	0	0	0	2	0	0	0	0	0	0	0	0	2	2	0	1	0	0	3	4	0	0	0	0	2	2	0	0
2	708.00	311.2	16	22	4	0	0	0	0	0	0	0	2	0	0	0	0	0	1	0	2	0	0	0	0	2	3	0	0	0	0	2	2	0	0
3	543.00	278.0	8	20	4	0	0	0	4	2	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	2	3	0	0	0	0	2	2	0	0
4	773.00	351.4	16	26	4	0	0	0	0	2	0	0	0	0	0	0	0	2	0	0	2	0	0	0	0	2	4	0	0	0	0	2	2	0	0
5	723.00	304.0	12	20	4	2	1	0	0	2	0	0	0	0	0	0	0	1	0	2	0	0	1	0	4	3	0	0	0	0	2	2	0	0
6	673.00	388.3	16	26	4	3	1	0	0	2	0	0	0	0	0	0	1	0	0	2	2	0	0	1	0	4	4	0	1	0	0	2	2	0	0
7	590.00	450.0	20	34	4	0	0	0	0	0	1	0	0	0	0	0	0	0	1	2	2	0	0	0	4	5	0	0	0	0	0	4	0	0	
8	526.00	453.2	20	34	4	1	0	0	0	0	0	0	0	0	0	0	1	0	1	0	2	2	0	0	0	4	5	0	1	0	0	0	4	0	0
9	571.00	453.2	20	34	4	1	0	0	0	0	1	0	0	0	0	0	1	0	0	1	2	2	0	0	0	4	5	0	1	0	0	0	4	0	0
10	593.00	450.0	20	34	4	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	2	0	0	0	4	5	0	0	0	0	0	4	0	0	
11	543.00	388.2	16	28	4	2	0	0	0	0	0	0	0	0	0	0	2	0	0	2	2	0	0	0	0	4	4	0	2	0	0	0	4	0	0
12	553.00	379.6	16	28	4	1	0	0	0	0	0	0	0	0	0	0	1	0	0	2	2	0	0	0	0	4	4	0	1	0	0	0	4	0	0
13	541.00	537.4	24	40	4	2	0	0	0	0	0	0	0	0	0	0	2	0	0	2	2	2	0	0	0	4	6	0	2	0	0	0	4	0	0
14	496.00	344.2	13	23	7	1	0	0	0	0	5	0	0	0	0	0	1	0	0	2	0	0	0	0	0	9	2	0	1	0	0	0	7	0	0
15	668.00	374.4	16	28	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	0	1	4	4	0	0	0	0	0	4	0	0
16	665.00	219.8	8	16	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	4	2	0	0	0	0	0	4	0	0
17	638.00	374.4	16	28	4	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	2	0	0	1	4	4	0	0	0	0	0	4	0	0	
18	626.00	304.0	12	22	4	1	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	1	4	3	0	1	0	0	0	4	0	0		
19	645.00	450.0	20	34	4	0	0	0	0	0	0	0	0	0	0	0	0	1	2	2	0	0	0	4	5	0	0	0	0	0	4	0	0		
20	649.00	295.4	12	22	4	0	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0	0	4	3	0	0	0	0	0	4	0	0		
21	618.00	478.2	20	34	4	2	1	0	0	0	0	0	0	0	0	0	0	0	1	2	2	0	1	0	6	5	0	0	0	0	0	4	0	0	
22	615.00	323.7	12	22	4	2	1	0	0	0	0	0	0	0	0	0	0	1	2	0	0	1	0	6	3	0	0	0	0	0	4	0	0		
23	598.00	468.2	20	35	4	1	0	0	0	0	0	0	0	0	0	0	0	1	2	2	1	0	0	5	5	0	0	0	0	0	4	0	0		
24	591.00	313.6	12	23	4	1	0	0	0	0	0	0	0	0	0	0	0	1	2	0	1	0	0	5	3	0	0	0	0	0	4	0	0		
25	577.00	456.5	20	34	4	1	0	0	0	0	0	0	0	0	0	1	0	0	1	2	2	0	0	0	4	5	0	1	0	0	0	4	0	0	
26	579.00	304.0	12	22	4	1	0	0	0	0	0	0	0	0	1	0	0	0	1	2	0	0	0	0	4	3	0	1	0	0	0	4	0	0	
27	573.00	534.2	24	40	4	1	0	0	0	0	0	0	0	0	1	0	0	0	2	2	2	0	0	0	4	6	0	1	0	0	0	4	0	0	
28	563.00	562.4	24	40	4	3	1	0	0	0	0	0	0	0	1	0	0	0	2	2	2	0	1	0	6	5	0	1	0	0	0	4	0	0	
29	544.00	552.4	24	41	4	2	0	0	0	0	0	0	0	0	0	1	0	0	2	2	2	1	0	0	5	6	0	1	0	0	0	4	0	0	
30	561.00	529.4	24	40	4	2	1	0	0	0	0	0	0	0	0	0	0	0	2	2	2	0	1	0	4	6	0	0	0	0	0	4	0	0	
31	508.00	381.7	20	34	4	2	0	0	0	0	0	0	0	0	0	2	0	0	3	2	0	0	0	0	4	5	0	2	0	0	0	4	0	0	
32	578.00	446.6	20	34	4	0	0	0	0	0	0	0	0	0	0	0	0	0	3	2	0	0	0	0	4	5	0	0	0	0	0	4	0	0	
33	489.00	548.0	24	40	4	3	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	4	2	0	0	0	0	4	6	0	3	0	0	0	4	0	0
34	521.00	397.6	14	29	2	6	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	2	0	5	0	0	5	4	0	1	0	0	0	0	0	2
35	538.00	397.6	14	29	2	5	0	0	0	0	0	0	0	0	0	0	1	1	0	1	2	0	5	0	0	5	4	0	1	0	0	0	0	0	2
36	536.00	397.6	14	29	2	6	0	0	0	0	0	0	0	0	0	1	0	1	1	2	0	5	0	0	5	4	0	1	0	0	0	0	0	0	2
37	553.00	397.6	14	29	2	6	0	0	0	0	0	0	0	0	0	1	0	0	2	2	0	5	0	0	5	4	0	1	0	0	0	0	0	0	2
38	531.00	396.5	16	29	2	5	0	0	0	0	0	1	0	0	0	0	1	0	2	0	2	0	4	0	0	4	4	0	1	0	0	0	0	0	2
39	552.00	396.5	16	29	2	5	0	0	0	0	0	1	0	0	0	0	1	1	0	1	2	0	4	0	0	4	4	0	1	0	0	0	0	0	2
40	547.00	396.5	16	29	2	5	0	0	0	0	0	1	0	0	0	0	1	0	1	1	2	0	4	0	0	4	4	0	1	0	0	0	0	0	2

TABLE 5 CONTINUED

GLASS TRANSITION TEMPERATURES, VOLUMES, AND WEIGHTING FACTORS OF POLYMERS USED IN THIS INVESTIGATION. THE POLYMER NUMBER IS IN CORRESPONDENCE WITH THE CHEMICAL STRUCTURES GIVEN IN TABLE 6.

41	567.00	396.5	16	29	2	5	0	0	0	0	0	1	0	0	0	0	1	0	0	2	2	0	4	0	0	4	4	0	1	0	0	0	0	0	2
42	537.00	388.0	14	28	2	6	0	0	0	0	0	0	0	0	0	0	2	1	0	1	2	0	4	0	0	4	4	0	2	0	0	0	0	0	2
43	543.00	388.0	14	28	2	6	0	0	0	0	0	0	0	0	0	0	2	0	0	2	2	0	4	0	0	4	4	0	2	0	0	0	0	0	2
44	586.00	303.8	10	22	2	5	0	0	0	0	0	0	0	0	0	0	1	0	1	0	2	0	4	0	0	4	3	0	1	0	0	0	0	0	2
45	723.00	303.8	10	22	2	5	0	0	0	0	0	0	0	0	0	0	1	0	0	1	2	0	4	0	0	4	3	0	1	0	0	0	0	0	2
46	533.00	470.6	14	32	2	5	0	6	0	0	0	0	0	0	0	2	0	0	2	0	2	0	5	0	0	5	4	0	0	0	0	0	0	0	2
47	562.00	470.6	14	32	2	5	0	6	0	0	0	0	0	0	0	2	0	1	0	1	2	0	5	0	0	5	4	0	0	0	0	0	0	0	2
48	561.00	470.6	14	32	2	5	0	6	0	0	0	0	0	0	0	2	0	0	1	1	2	0	5	0	0	5	4	0	0	0	0	0	0	0	2
49	584.00	470.6	14	32	2	5	0	6	0	0	0	0	0	0	0	2	0	0	0	2	2	0	5	0	0	5	4	0	0	0	0	0	0	0	2
50	521.00	469.5	16	32	2	4	0	6	0	0	1	0	0	0	0	2	0	0	2	0	2	0	4	0	0	4	4	0	0	0	0	0	0	0	2
51	518.00	469.5	16	32	2	4	0	6	0	0	1	0	0	0	0	2	0	1	0	1	2	0	4	0	0	4	4	0	0	0	0	0	0	0	2
52	545.00	469.5	16	32	2	4	0	6	0	0	0	0	0	0	0	2	0	0	1	1	2	0	4	0	0	4	4	0	0	0	0	0	0	0	2
53	563.00	469.5	16	32	2	4	0	6	0	0	0	0	0	0	0	2	0	0	0	2	2	0	4	0	0	4	4	0	0	0	0	0	0	0	2
54	549.00	461.0	14	31	2	5	0	6	0	0	0	0	0	0	0	2	1	1	0	1	2	0	4	0	0	4	4	0	1	0	0	0	0	0	2
55	580.00	461.0	14	31	2	5	0	6	0	0	0	0	0	0	0	2	1	0	0	2	2	0	4	0	0	4	4	0	1	0	0	0	0	0	2
56	576.00	376.8	10	25	2	4	0	6	0	0	0	0	0	0	0	2	0	0	1	0	2	0	4	0	0	4	3	0	0	0	0	0	0	0	2
57	612.00	376.8	10	25	2	4	0	6	0	0	0	0	0	0	0	2	0	0	0	1	2	0	4	0	0	4	3	0	0	0	0	0	0	0	2
58	493.00	634.8	22	44	2	7	0	6	0	0	0	0	0	0	0	2	2	0	2	2	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
59	507.00	634.8	22	44	2	7	0	6	0	0	0	0	0	0	0	2	2	1	0	3	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
60	510.00	634.8	22	44	2	7	0	6	0	0	0	0	0	0	0	2	2	0	1	3	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
61	521.00	634.8	22	44	2	7	0	6	0	0	0	0	0	0	0	2	2	0	0	4	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
62	489.00	633.7	22	44	2	6	0	6	0	0	0	1	0	0	0	2	2	0	2	2	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
63	497.00	633.7	22	44	2	6	0	6	0	0	0	1	0	0	0	2	2	1	0	3	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
64	504.00	633.7	24	44	2	6	0	6	0	0	0	1	0	0	0	2	2	0	1	3	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
65	511.00	633.7	24	44	2	6	0	6	0	0	0	1	0	0	0	2	2	0	0	4	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
66	508.00	625.2	22	43	2	7	0	6	0	0	0	0	0	0	0	2	2	0	0	4	2	0	4	0	0	4	5	0	2	0	0	0	0	0	2
67	510.00	625.2	18	37	2	6	0	6	0	0	0	0	0	0	0	2	2	0	0	3	2	0	4	0	0	4	5	0	2	0	0	0	0	0	2
68	513.00	541.0	18	37	2	6	0	6	0	0	0	0	0	0	0	2	2	0	1	2	2	0	4	0	0	4	5	0	2	0	0	0	0	0	2
69	527.00	541.0	18	37	2	6	0	6	0	0	0	0	0	0	0	2	2	0	0	3	2	0	4	0	0	4	5	0	2	0	0	0	0	0	2
70	473.00	556.9	22	41	2	7	1	0	0	0	0	0	0	0	0	0	2	0	2	2	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
71	485.00	556.9	22	41	2	7	1	0	0	0	0	0	0	0	0	0	2	1	0	3	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
72	486.00	556.9	22	41	2	7	1	0	0	0	0	0	0	0	0	0	2	0	1	3	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
73	494.00	556.9	22	41	2	7	1	0	0	0	0	0	0	0	0	0	2	0	0	4	2	0	5	0	0	5	6	0	2	0	0	0	0	0	2
74	520.00	535.9	24	41	2	6	1	0	0	0	0	1	0	0	0	0	2	0	2	2	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
75	513.00	535.9	24	41	2	6	1	0	0	0	0	1	0	0	0	0	2	1	0	3	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
76	527.00	535.9	24	41	2	6	1	0	0	0	0	1	0	0	0	0	2	0	1	3	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
77	540.00	535.9	24	41	2	6	1	0	0	0	0	1	0	0	0	0	2	0	0	4	2	0	4	0	0	4	6	0	2	0	0	0	0	0	2
78	489.00	547.4	22	40	2	7	1	0	0	0	0	0	0	0	0	0	3	1	0	3	2	0	4	0	0	4	6	0	3	0	0	0	0	0	2
79	494.00	547.4	22	40	2	7	1	0	0	0	0	0	0	0	0	0	3	0	0	4	2	0	4	0	0	4	6	0	3	0	0	0	0	0	2
80	497.00	463.2	18	34	2	6	1	0	0	0	0	0	0	0	0	0	2	0	1	2	2	0	4	0	0	4	5	0	2	0	0	0	0	0	2
81	499.00	463.2	18	34	2	6	1	0	0	0	0	0	0	0	0	0	2	0	0	3	2	0	4	0	0	4	5	0	2	0	0	0	0	0	2
82	537.00	439.8	20	37	2	6	0	0	0	0	0	1	0	0	0	0	0	0	0	3	2	0	6	0	0	6	5	0	0	0	0	0	0	0	2
83	507.00	439.8	20	37	2	6	0	0	0	0	0	1	0	0	0	0	0	0	2	1	2	0	6	0	0	6	5	0	0	0	0	0	0	0	2
84	489.00	498.8	22	37	2	5	0	0	0	0	0	2	0	0	0	0	0	0	2	1	2	0	5	0	0	5	5	0	0	0	0	0	0	0	2

TABLE 5 CONTINUED

GLASS TRANSITION TEMPERATURES, VOLUMES, AND WEIGHTING FACTORS OF POLYMERS USED IN THIS INVESTIGATION. THE POLYMER NUMBER IS IN CORRESPONDENCE WITH THE CHEMICAL STRUCTURES GIVEN IN TABLE 6

85	519.00	593.6	24	44	2	7	0	0	0	0	0	1	0	0	0	0	0	0	0	4	2	0	7	0	0	7	6	0	0	0	0	0	0	2
86	489.00	518.0	24	44	2	7	0	0	0	0	0	1	0	0	0	0	0	0	2	2	2	0	7	0	0	7	6	0	0	0	0	0	0	2
87	543.00	389.6	16	28	0	6	0	0	0	0	0	0	0	0	0	0	2	0	1	2	0	1	3	0	0	3	4	0	0	3	0	0	0	0
88	543.00	389.6	16	28	0	6	0	0	0	0	0	0	0	0	0	2	0	1	2	0	1	3	0	0	3	4	0	0	3	0	0	0	0	0
89	543.00	389.6	16	28	0	6	0	0	0	0	0	0	0	0	0	2	0	0	3	0	1	3	0	0	3	4	0	0	3	0	0	0	0	0
90	583.00	389.6	16	28	0	6	0	0	0	0	0	0	0	0	0	2	0	0	3	0	1	3	0	0	3	4	0	0	3	0	0	0	0	0
91	363.00	451.2	28	30	0	6	0	0	0	0	0	0	0	0	0	2	0	0	2	0	1	3	0	0	3	3	0	0	3	0	0	0	0	0
92	563.00	467.8	21	34	1	5	0	0	0	0	0	0	0	0	0	2	0	0	3	0	2	3	0	0	3	5	0	0	2	0	0	0	0	1
93	563.00	467.8	21	34	1	5	0	0	0	0	0	0	0	0	0	2	0	1	2	0	2	3	0	0	3	5	0	0	2	0	0	0	0	1
94	583.00	573.0	24	42	0	8	0	0	0	0	0	0	0	0	0	2	0	0	4	0	2	4	0	0	4	5	0	0	4	0	0	0	0	0
95	483.00	391.3	20	28	0	4	0	0	0	0	0	0	1	0	0	0	2	0	0	3	0	1	2	0	0	2	4	0	0	2	0	0	0	0
96	588.00	394.7	18	28	2	4	0	0	0	2	0	0	0	0	0	0	0	0	1	2	0	1	3	0	0	3	4	0	0	1	0	0	0	2
97	563.00	465.2	22	43	2	7	0	6	0	0	0	0	0	0	0	2	2	1	0	3	2	0	4	0	0	4	5	0	2	0	0	0	0	2
98	618.00	396.6	19	28	3	3	0	0	0	3	0	0	0	0	0	0	0	0	0	3	0	1	3	0	0	3	4	0	0	0	0	0	0	3
99	608.00	394.7	18	28	2	4	0	0	0	2	0	0	0	0	0	0	0	0	0	3	0	1	3	0	0	3	4	0	0	1	0	0	0	2
100	587.00	512.6	24	39	0	4	0	0	0	0	0	0	0	0	0	2	0	0	4	0	2	2	0	0	2	6	0	0	0	0	0	0	0	0
101	483.00	387.5	22	26	2	4	0	0	0	2	0	4	0	0	0	0	0	0	0	2	0	1	3	0	0	3	3	0	0	1	0	0	0	2
102	453.00	435.9	30	30	2	4	0	0	0	2	0	0	0	0	0	0	0	0	0	2	0	1	3	0	0	3	3	0	0	0	0	0	0	2
103	607.00	470.3	22	34	2	4	0	0	0	2	0	0	0	0	0	0	0	0	0	4	0	1	3	0	0	3	5	0	0	1	0	0	0	2
104	458.00	457.8	31	30	3	3	0	0	0	3	0	0	0	0	0	0	0	0	0	2	0	1	3	0	0	3	3	0	0	0	0	0	0	3
105	543.00	437.0	20	33	0	4	0	0	0	0	0	0	0	0	0	2	0	1	2	0	2	3	0	0	2	5	0	0	2	0	0	0	0	0
106	585.00	465.2	20	34	0	6	0	0	0	0	0	0	0	0	0	2	0	0	4	0	1	3	0	0	3	5	0	0	3	0	0	0	0	0
107	513.00	389.6	16	28	0	6	0	0	0	0	0	0	0	0	0	2	0	1	2	0	1	3	0	0	3	4	0	0	3	0	0	0	0	0
108	600.00	478.9	22	34	2	5	0	0	0	2	0	0	0	0	0	1	0	0	4	0	1	3	0	0	3	5	0	1	1	0	0	0	0	2
109	518.00	473.8	20	34	0	7	0	0	0	0	0	0	0	0	0	3	0	0	4	0	1	3	0	0	3	5	0	1	3	0	0	0	0	0
110	423.00	367.3	22	25	0	4	0	0	0	0	0	0	4	0	0	0	2	0	0	3	0	0	2	0	0	2	3	0	0	2	0	0	0	0
115	378.00	95.4	8	5	0	2	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
116	338.00	112.9	10	6	0	2	0	0	0	0	0	2	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
117	308.00	130.0	12	7	0	2	0	0	0	0	0	3	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
118	293.00	147.1	14	8	0	2	0	0	0	0	0	4	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
119	268.00	181.3	18	10	0	2	0	0	0	0	0	6	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
120	253.00	215.5	22	12	0	2	0	0	0	0	0	8	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
121	193.00	283.9	30	16	0	2	0	0	0	0	0	12	2	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
122	300.00	67.0	3	3	0	0	0	3	0	0	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
123	315.00	72.2	2	3	0	0	0	4	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
124	425.00	82.6	0	3	0	0	0	5	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
125	378.00	134.9	3	8	0	0	0	5	0	0	1	1	0	5	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0
126	467.00	150.2	0	8	0	0	0	8	0	0	0	0	0	6	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0
127	476.00	125.4	3	8	0	0	0	3	0	0	0	0	0	1	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0
128	314.00	94.5	3	4	0	0	0	5	0	0	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
129	331.00	122.0	3	5	0	0	0	7	0	0	1	1	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
130	268.00	1041.3	12	39	211	056	0	2	0	2	1	028	0	9	0	0	1	0	0	2	0	0	2	1	0	7	2	0	0	0	0	2		

TABLE 5
GLASS TRANSITION TEMPERATURES, VOLUMES AND WEIGHTING FACTORS OF POLYMERS USED IN THIS INVESTIGATION. THE POLYMER NUMBER IS IN CORRESPONDENCE WITH THE CHEMICAL STRUCTURES GIVEN IN TABLE 6

131	221.00	1053.9	18	38	211	056	0	2	0	8	0	028	0	9	0	0	0	0	0	2	0	0	2	0	0	7	2	0	0	0	0	2
132	249.00	1105.2	10	38	212	064	0	2	0	4	0	032	010		0	0	0	0	0	2	0	0	2	0	0	8	2	0	0	0	0	2
133	223.00	1026.1	14	36	212	056	0	0	0	6	0	028	010		0	0	0	0	0	2	0	0	2	0	0	8	2	0	0	0	0	2
134	255.00	1055.8	6	38	211	060	0	2	0	2	0	428	0	9	0	0	0	0	0	2	0	0	2	1	0	7	2	0	0	0	0	2
135	263.00	322.5	0	12	3	1	019	0	0	0	0	0	1	6	2	1	0	0	0	0	0	0	0	0	3	0	0	1	0	0	0	3	0	0
136	260.00	386.9	0	14	3	2	023	0	0	0	0	0	2	6	3	2	0	0	0	0	0	0	0	0	3	0	0	2	0	0	0	3	0	0
137	259.00	414.5	0	15	3	2	025	0	0	0	0	0	2	7	3	2	0	0	0	0	0	0	0	0	3	0	0	2	0	0	0	3	0	0
138	257.00	442.0	0	16	3	2	027	0	0	0	0	0	2	8	3	2	0	0	0	0	0	0	0	0	3	0	0	2	0	0	0	3	0	0
139	255.00	267.8	0	10	3	1	015	0	0	0	0	0	0	6	1	0	0	0	0	0	0	0	0	0	3	0	0	1	0	0	0	3	0	0
140	148.00	34.2	4	2	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
141	258.00	51.7	6	3	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
142	213.00	69.1	8	4	0	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
143	223.00	22.7	2	1	0	1	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
144	243.00	49.1	3	2	0	0	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
145	254.00	63.9	2	2	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
146	378.00	54.1	3	3	1	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0
147	183.00	64.4	6	4	0	0	0	0	0	0	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
148	200.00	81.9	8	5	0	0	0	0	0	0	1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
149	225.00	79.2	5	4	0	0	0	0	1	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
150	160.00	35.0	0	2	0	0	0	4	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
151	318.00	64.6	0	2	0	0	0	3	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
152	301.00	80.0	6	4	0	2	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0
153	358.00	41.6	4	2	0	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
154	373.00	110.1	8	8	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0
155	325.00	230.7	22	12	2	2	0	0	0	2	010		0	0	0	0	0	0	0	0	0	0	2	0	0	2	0	0	0	0	0	0	0	2
156	335.00	132.5	13	7	1	1	0	0	0	1	0	6	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
157	323.00	149.6	15	8	1	1	0	0	0	1	0	7	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
158	323.00	166.7	17	9	1	1	0	0	0	1	0	8	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
159	315.00	183.8	19	10	1	1	0	0	0	1	0	9	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
160	319.00	200.9	21	11	1	1	0	0	0	1	010		0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
161	310.00	218.0	23	12	1	1	0	0	0	1	011		0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
162	314.00	235.1	25	13	1	1	0	0	0	1	012		0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1
164	342.00	165.9	8	10	0	4	0	0	0	0	0	2	0	0	0	0	2	0	0	1	0	0	2	0	0	2	1	0	0	2	0	0	0	0
165	263.00	236.2	14	16	0	3	0	0	0	0	0	0	2	0	0	0	2	0	0	2	0	0	1	0	0	1	2	0	0	2	0	0	0	0
170	653.00	394.7	18	28	2	4	0	0	0	2	0	0	0	0	0	0	0	0	0	3	0	1	3	0	0	3	4	0	0	1	0	0	0	2
171	658.00	470.3	22	34	2	4	0	0	0	2	0	0	0	0	0	0	0	0	0	4	0	1	3	0	0	3	5	0	0	1	0	0	0	2
172	658.00	578.1	26	42	2	6	0	0	0	2	0	0	0	0	0	0	0	0	0	4	0	2	4	0	0	4	6	0	0	2	0	0	0	2
173	673.00	580.0	27	42	3	5	0	0	0	3	0	0	0	0	0	0	0	0	0	4	0	2	4	0	0	4	6	0	0	1	0	0	0	3
174	593.00	478.9	22	34	2	5	0	0	0	2	0	0	0	0	0	0	1	0	0	4	0	1	3	0	0	3	5	0	1	1	0	0	0	2

TABLE 6

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

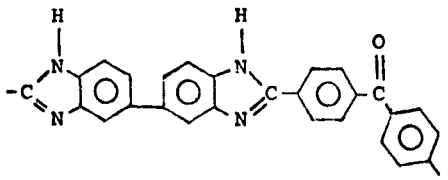
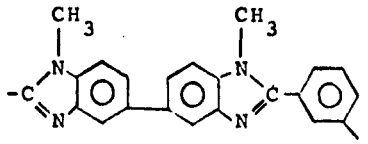
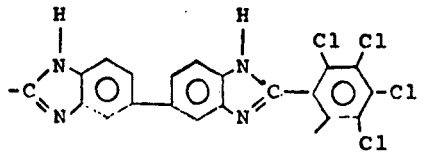
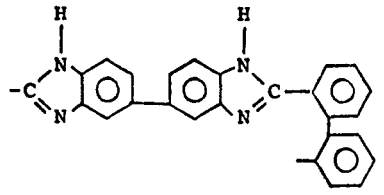
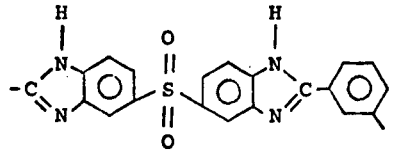
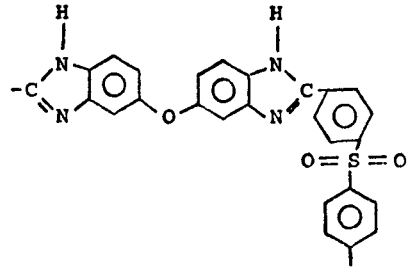
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT*	Tg (K) EXP.	CALC.
1		412	369.55	393	
2		336	311.2	708	521.2
3		446	278.0	543	514.5
4		384	351.4	773	742.5
5		372	304.0	723	711.8
6		464	388.3	673	654.4

TABLE 6 (CONTINUED)
CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

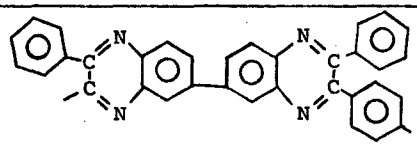
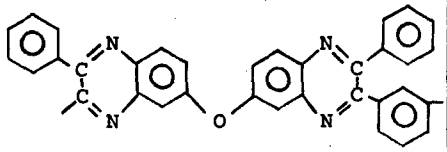
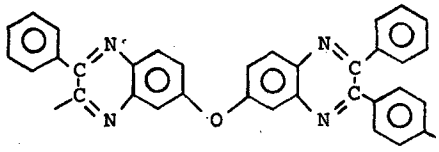
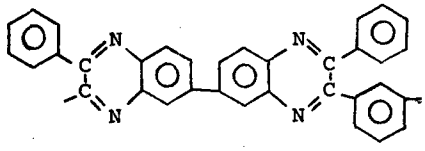
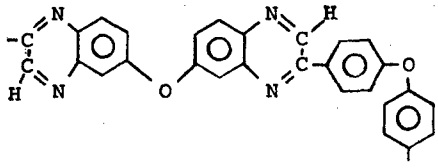
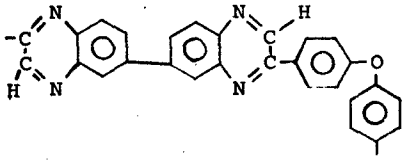
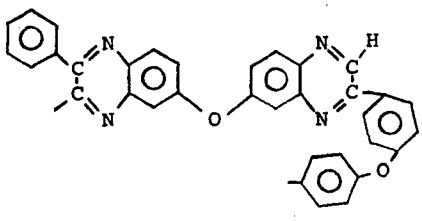
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
7		484	450.0	590	
8		500	453.2	526	547.5
9		500	453.2	571	
10		484	450.0	593	558.0
11		440	388.22	543	544.2
12		424	379.62	553	580.7
13		592	537.40	541	537.2

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

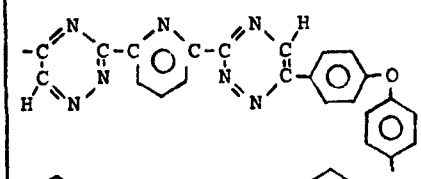
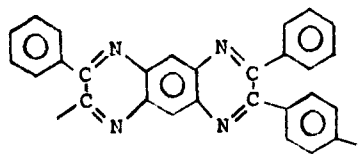
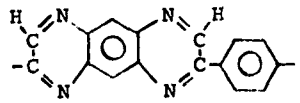
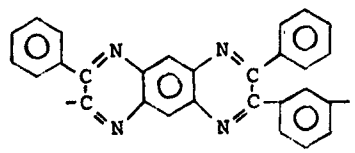
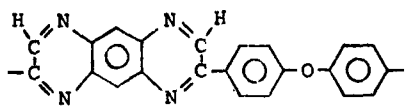
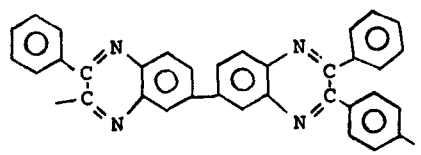
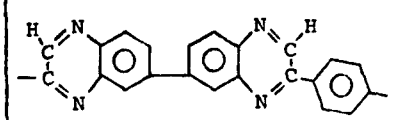
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
14		403	344.23	496	428.5
15		408	374.4	668	591.7
16		256	219.8	665	716.3
17		408	374.4	638	638.7
18		348	304.0	626	622.7
19		484	450.0	645	570.2
20		332	295.42	649	644.6

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

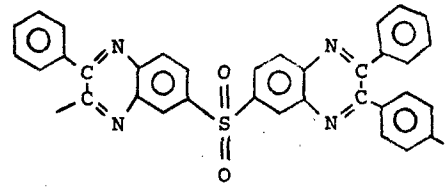
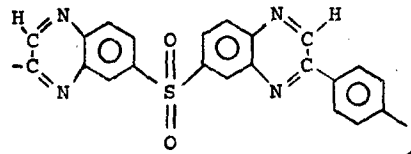
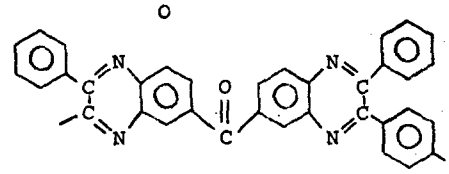
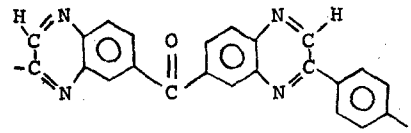
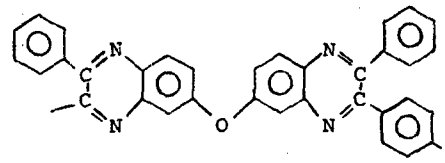
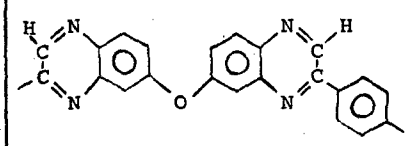
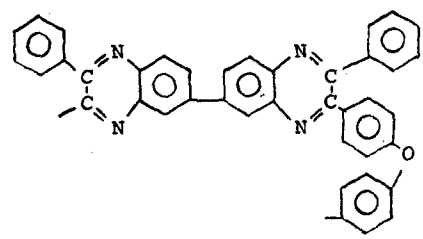
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
21		548	478.2	618	587.7
22		396	323.66	615	664.8
23		512	468.15	598	565.7
24		360	313.57	591	632.5
25		500	456.5	577	547.4
26		348	304.02	579	591.6
27		576	534.2	573	545.8

TABLE 6 (CONTINUED)
CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

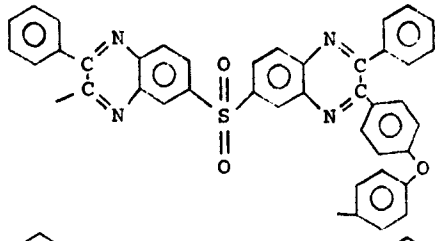
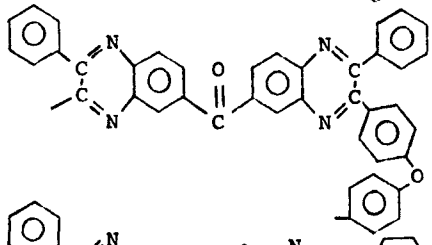
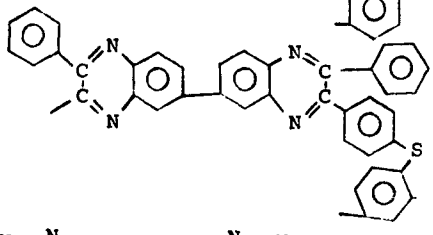
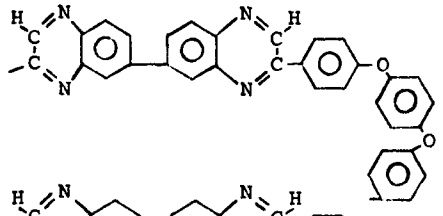
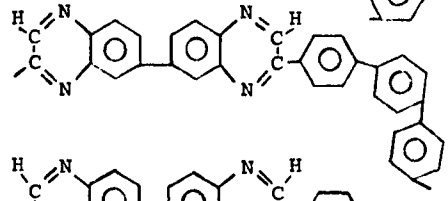
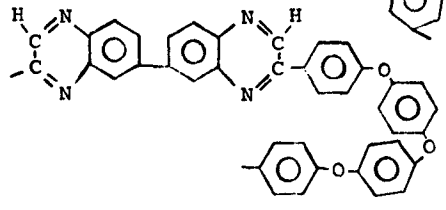
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	Tg (K) CALC.
28		640	562.4	563	560.4
29		604	552.35	544	542.9
30		592	529.38	561	522.3
31		516	381.72	508	557.4
32		484	446.62	578	623.1
33		608	548.02	489	541.8

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

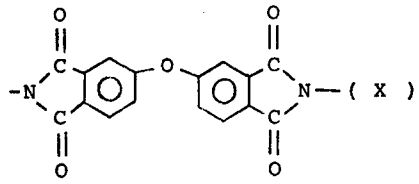
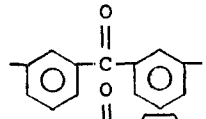
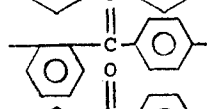
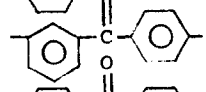
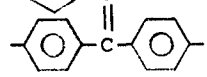
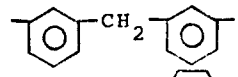
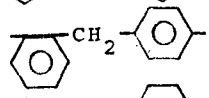
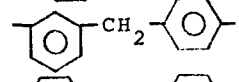
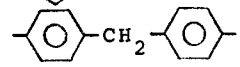
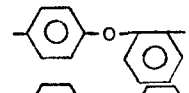
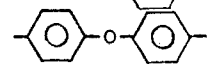
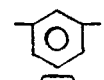
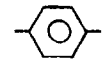
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
					
34	(X) = 	486	397.55	521	543.1
35	(X) = 	486	397.55	538	590.5
36	(X) = 	486	397.55	536	556.6
37	(X) = 	486	397.55	553	570.4
38	(X) = 	472	396.50	531	595.1
39	(X) = 	472	396.50	552	647.2
40	(X) = 	472	396.50	547	610.0
41	(X) = 	472	396.50	567	625.2
42	(X) = 	474	388.00	537	559.4
43	(X) = 	474	388.00	543	539.9
44	(X) = 	382	303.80	586	556.2
45	(X) = 	382	303.80	723	574.4

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

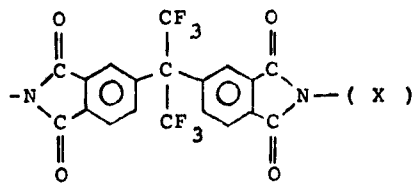
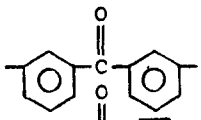
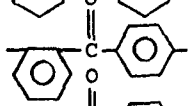
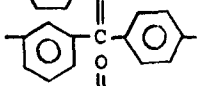
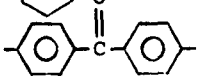
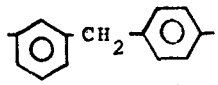
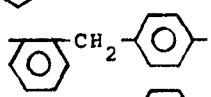
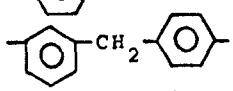
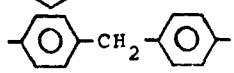
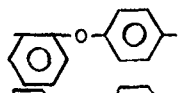
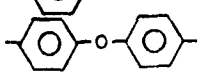
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
					
46	(X) = 	620	470.55	533	525.8
47	(X) = 	620	470.55	562	564.3
48	(X) = 	620	470.55	561	536.8
49	(X) = 	620	470.55	584	548.1
50	(X) = 	606	469.5	521	512.7
51	(X) = 	606	469.5	518	550.4
52	(X) = 	606	469.5	545	523.5
53	(X) = 	606	469.5	563	534.5
54	(X) = 	608	461.00	549	538.7
55	(X) = 	608	461.00	580	522.9
56	(X) = 	516	376.8	576	533.2
57	(X) = 	516	376.8	612	547.2

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

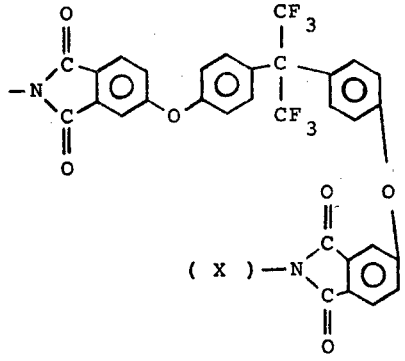
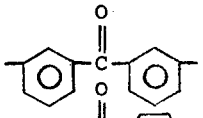
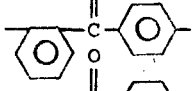
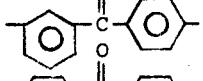
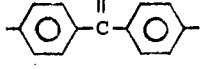
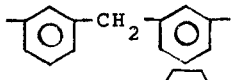
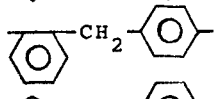
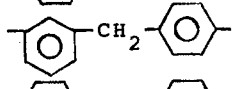
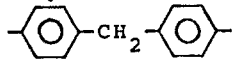
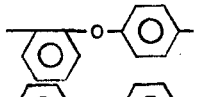
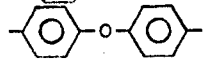
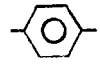
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
					
58	(X) = 	804	634.75	493	508.9
59	(X) = 	804	634.75	507	536.3
60	(X) = 	804	634.75	510	516.8
61	(X) = 	804	634.75	521	524.8
62	(X) = 	790	633.7	489	499.5
63	(X) = 	790	633.7	497	526.4
64	(X) = 	790	633.7	504	507.2
65	(X) = 	790	633.7	511	515.1
66	(X) = 	792	625.20	508	517.9
67	(X) = 	792	625.20	510	506.6
68	(X) = 	700	541.0	513	504.5
69	(X) = 	700	541.0	527	513.7

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

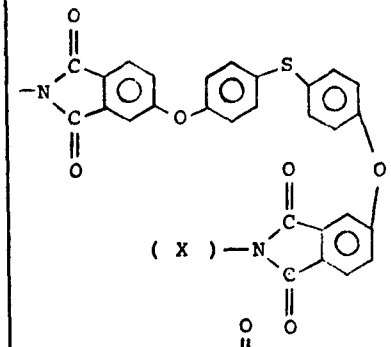
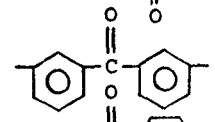
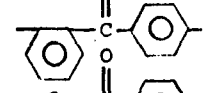
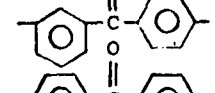
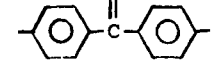
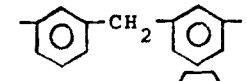
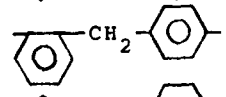
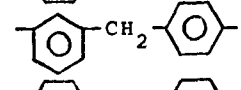
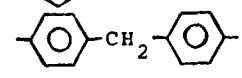
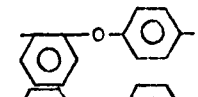
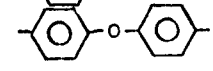
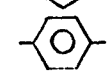
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
					
70	(X) = 	686	556.93	473	497.0
71	(X) = 	686	556.93	485	527.6
72	(X) = 	686	556.93	486	505.8
73	(X) = 	686	556.93	494	514.8
74	(X) = 	672	555.88	520	486.5
75	(X) = 	672	555.88	513	516.5
76	(X) = 	672	555.88	527	495.1
77	(X) = 	672	555.88	540	503.9
78	(X) = 	674	547.38	489	506.8
79	(X) = 	674	547.38	494	494.2
80	(X) = 	582	463.18	497	495.9
81	(X) = 	582	463.18	499	506.5

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

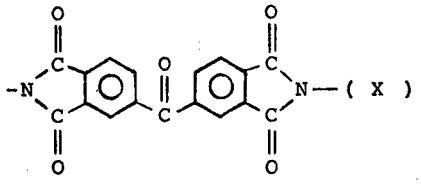
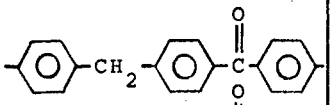
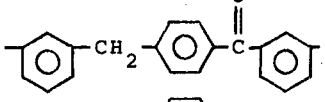
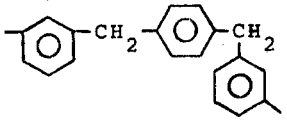
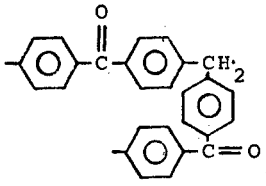
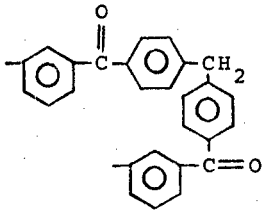
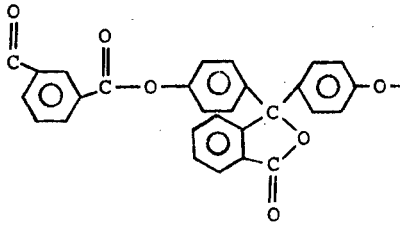
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
					
82	(X) = 	588	499.8	537	579.0
83	(X) = 	588	499.8	507	556.8
84	(X) = 	574	498.75	489	543.8
85	(X) = 	692	593.55	519	575.6
86	(X) = 	692	593.55	489	557.0
87,88		448	389.6	543	486.0

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

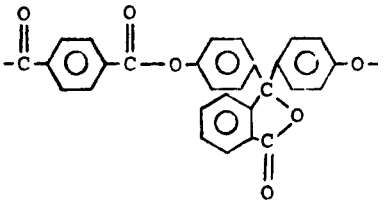
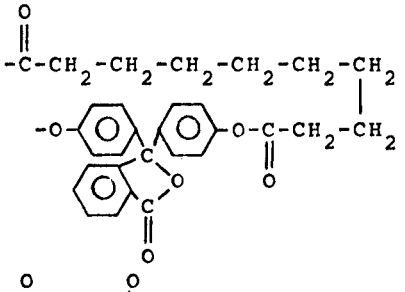
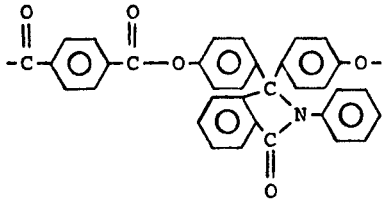
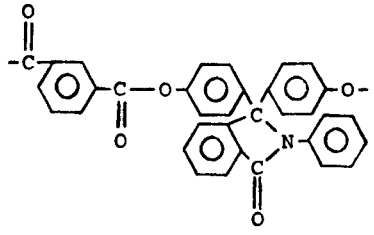
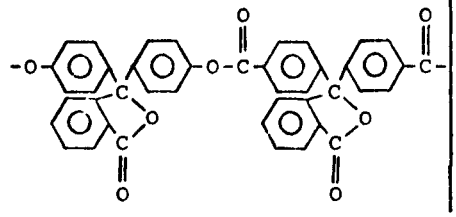
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
89		448	389.6	543	
90	SAME AS #89	448	389.6	583	498.3
91		484	451.2	363	411.0
92		523	467.75	563 593	531.2
93		523	467.75	563	520.2
94		656	573.0	583	517.5

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

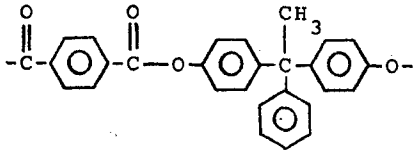
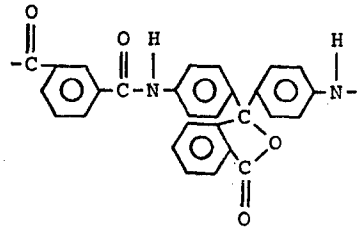
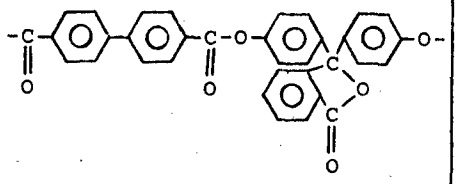
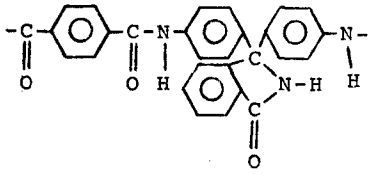
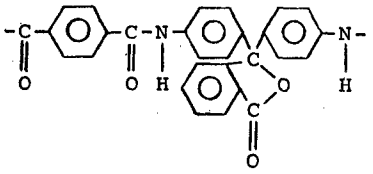
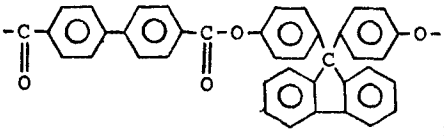
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
95		420	391.3	483	486.2
96		446	394.7	588	650.0
97		524	465.2	563	511.2
98		445	396.55	618	645.2
99		446	394.7	608	666.2
100		556	512.6	587	557.4

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

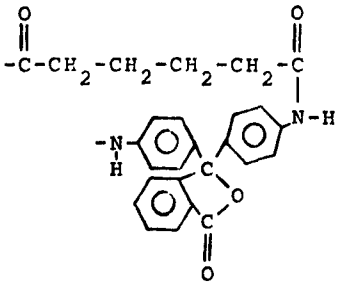
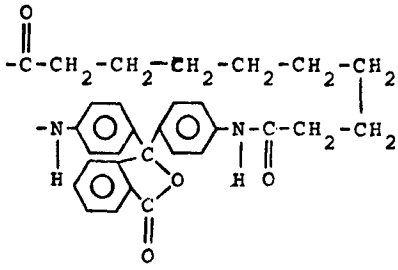
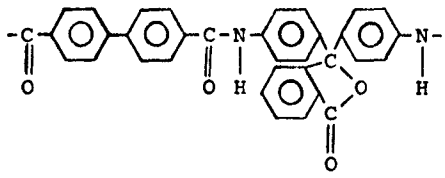
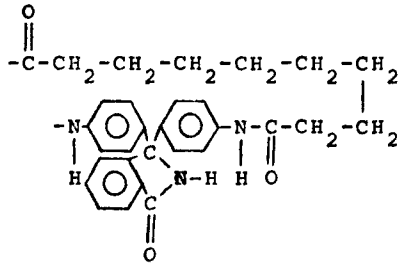
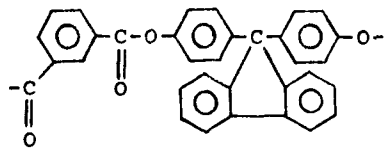
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
101		426	387.5	483	555.3
102		482	455.9	453	405.5
103		522	470.3	607	652.1
104		481	457.75	458	535.1
105		480	437.0	543	540.9

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

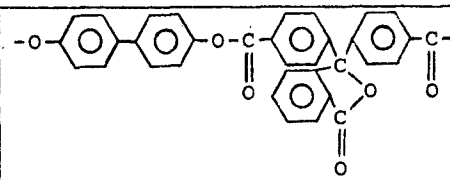
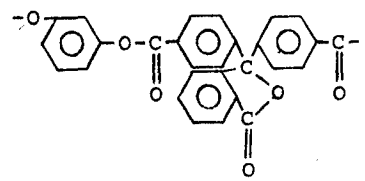
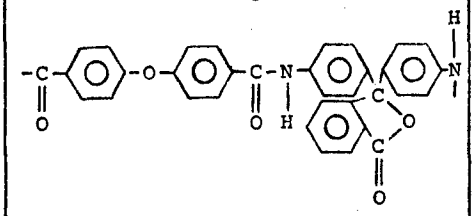
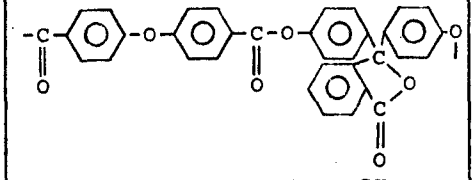
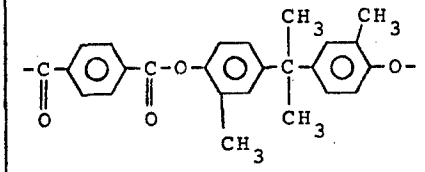
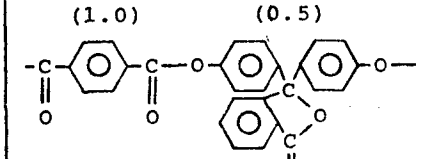
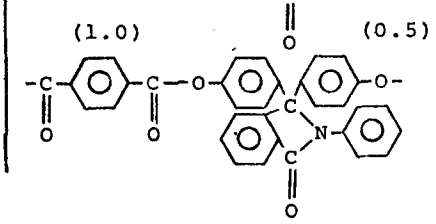
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
106		524	465.2	585	512.3
107		448	389.6	513	486.0
108		538	478.9	600	617.4
109		540	473.8	518	485.8
110		386	367.3	423	376.2
111	(1.0) (0.5)  (1.0) (0.5) 	485.5	428.68	563	

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

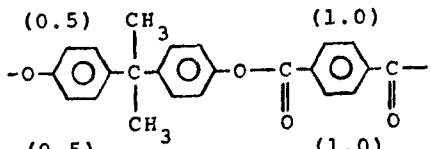
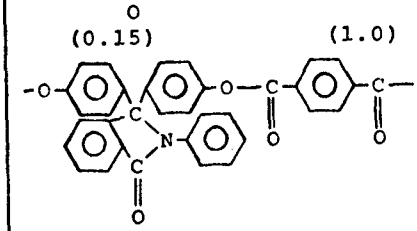
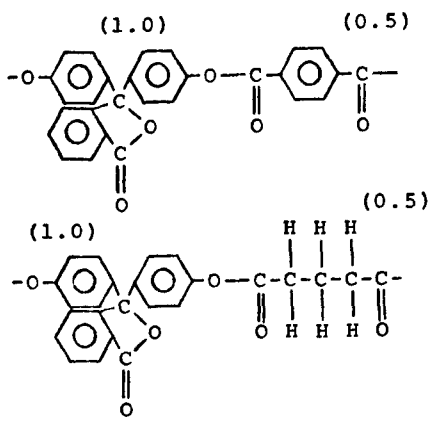
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
112		440.5	400.53	510	
113		382.75	353.48	481	
114		431	377.65	433	

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

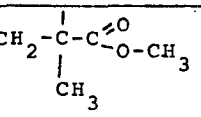
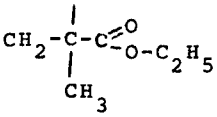
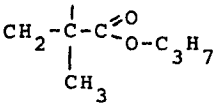
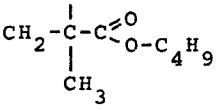
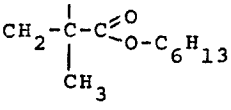
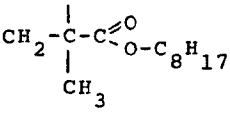
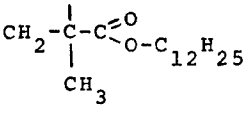
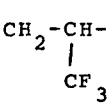
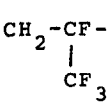
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
115		100	95.35	378	289.6
116		114	112.85	338	288.2
117		128	129.95	308	289.4
118		142	147.05	293	290.2
119		170	181.25	268	291.5
120		198	215.45	253	292.3
121		254	283.85	193	293.4
122		96	67.0	300	270.2
123		114	72.2	315	279.4

TABLE 6 (CONTINUED)
CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

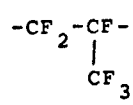
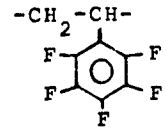
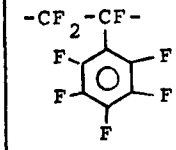
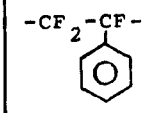
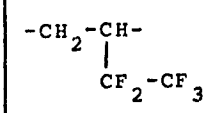
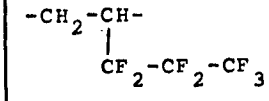
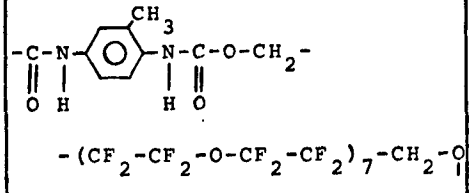
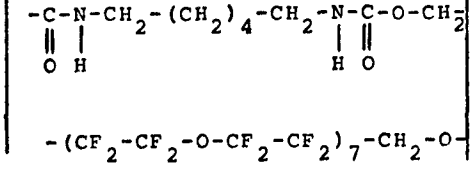
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
124		150	82.6	425	295.1
125		194	134.85	378	414.0
126		248	150.15	467	418.0
127		158	125.4	476	457.9
128		146	94.5	314	289.3
129		196	122.0	331	300.4
130		1748	1041.3	268	285.8
131		1742	1053.9	221	270.7

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

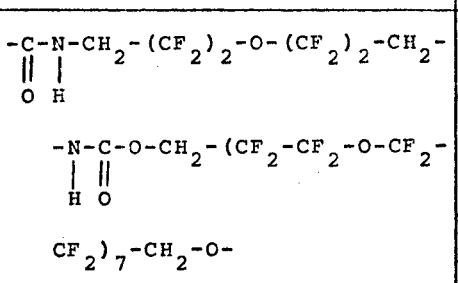
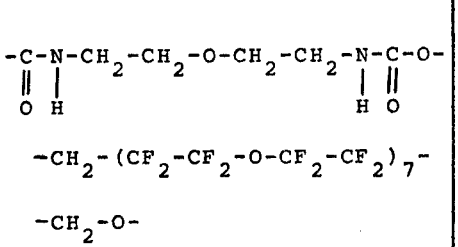
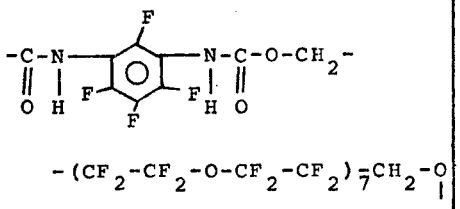
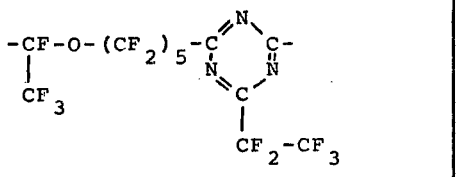
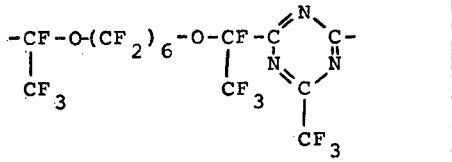
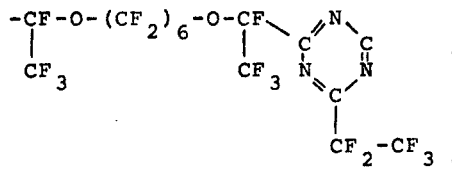
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
132		1902	1105.2	249	268.5
133		1730	1026.1	223	265.0
134		1806	1055.8	255	277.6
135		563	322.45	263	286.4
136		679	386.9	260	277.5
137		729	414.5	259	281.2

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

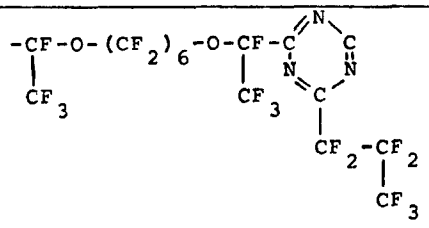
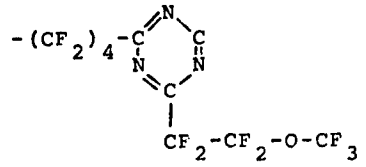
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
138		779	442.0	257	284.6
139		463	267.75	255	294.5
140	$-CH_2-CH_2-$	28	34.2	148	209.8
141	$-CH_2-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-CH_3$	42	51.7	258	231.6
142	$-CH_2-\underset{\displaystyle CH_3}{\underset{\vert}{C}}-CH_3$	56	69.1	213	244.0
143	$-CH_2-O-$	30	22.7	223	216.6
144	$-CH_2-\underset{\displaystyle Cl}{\underset{\vert}{CH}}-$	62.5	49.05	243	252.2
145	$-CH_2-\underset{\displaystyle Cl}{\underset{\vert}{\overset{\displaystyle Cl}{\overset{\vert}{C}}}}-$	97	63.9	254	278.4
146	$-CH_2-\underset{\displaystyle C\equiv N}{\underset{\vert}{CH}}-$	53	54.1	378	378.0
147	$CH_2=CH-\underset{\displaystyle CH_2-}{\underset{\vert}{CH}}-$	54	64.4	183	207.5
148	$-CH_2-CH=\underset{\displaystyle CH_3}{\underset{\vert}{C}}-CH_2-$	68	81.9	200	191.5

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUTION

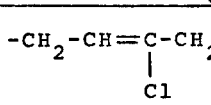
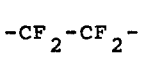
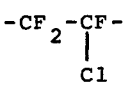
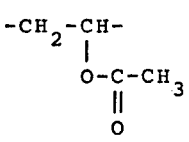
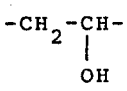
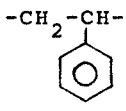
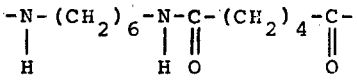
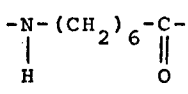
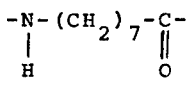
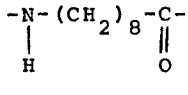
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
149		88.5	79.15	225	201.1
150		100	55.0	160	
151		116.5	64.6	318	287.5
152		86	79.95	301	273.9
153		44	41.6	358	358.0
154		104	110.1	373	458.4
155		226	230.7	325	345.5
156		127	132.45	335	320.7
157		141	149.55	323	305.5
158		155	166.65	323	294.0

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

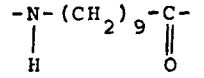
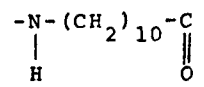
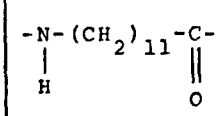
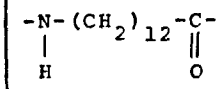
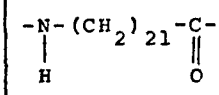
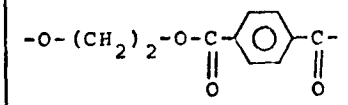
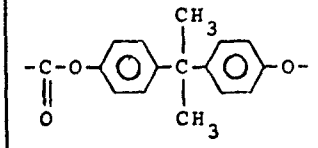
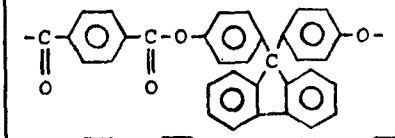
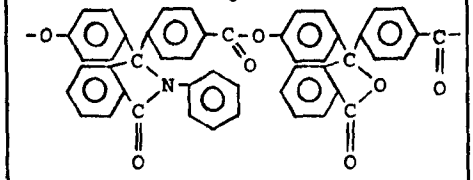
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
159		169	183.75	315	284.9
160		183	200.85	319	277.6
161		197	217.95	310	271.5
162		211	235.05	314	266.5
163		337	388.95		
164		192	165.9	342	351.7
165		254	236.15	263	
166		480	437.0		
167		731	651.15		

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

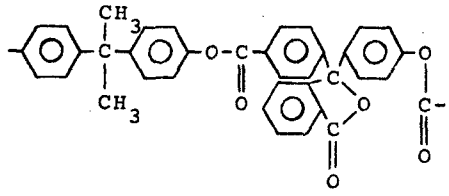
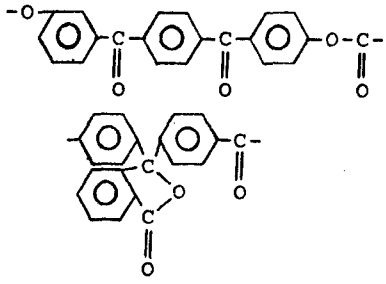
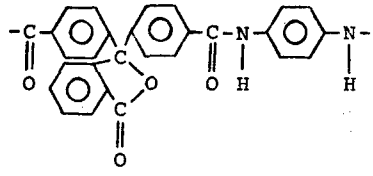
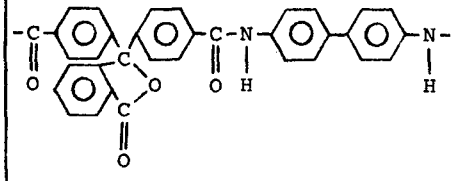
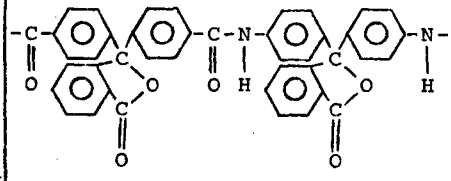
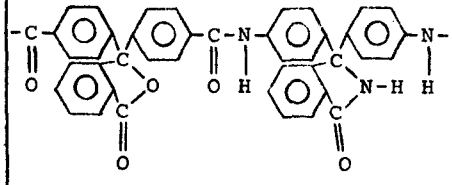
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
168		566	516.7		
169		656	577.1		
170		446	394.7	653	666.2
171		522	470.3	658	652.1
172		654	578.1	658	630.7
173		653	579.95	673	671.0

TABLE 6 (CONTINUED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

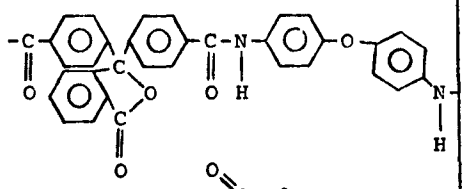
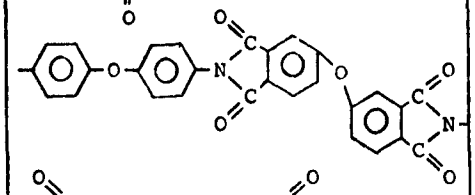
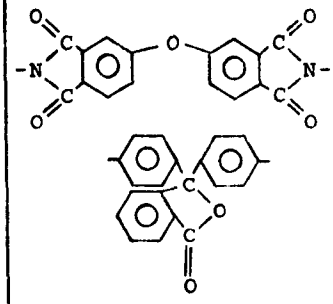
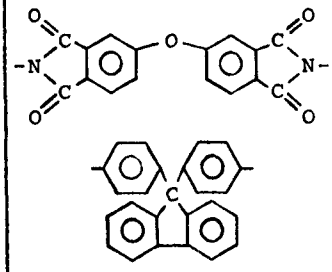
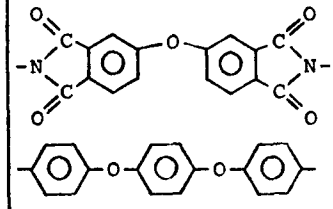
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
174		538	478.9	593	617.4
175		474	392.2		
176		590	491.4		
177		622	538.8		
178		566	476.4		

TABLE 6 (CONCLUDED)

CHEMICAL STRUCTURES OF POLYMERS USED IN THE PRESENT EVALUATION

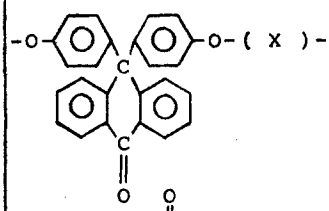
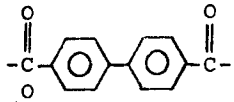
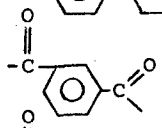
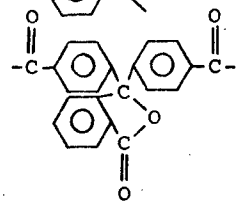
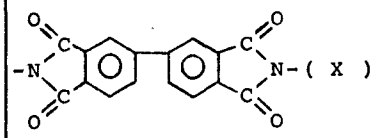
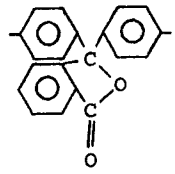
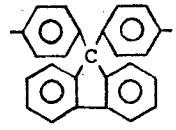
POLYMER NUMBER	STRUCTURAL FORMULA OF REPEAT UNIT	MOL.WT. OF UNIT	VOLUME OF UNIT	Tg (K) EXP.	CALC.
					
179		584	530.75		
180		508	455.15		
181		716	638.55		
					
182		574	482.1		
183		606	530.2		

TABLE 7

IDENTIFICATION OF K_j'S USED IN THIS ANALYSIS

j	K_j, Nomenclature	j	K_j, Nomenclature
1	Hydrogen atom	18	Backbone phenyl bonding, Para
2	Carbon atom	19	Partially condensed ring 
3	Nitrogen atom	20	Pendant phenyl
4	Oxygen atom	21	-C- in backbone (O)
5	Sulfur atom	22	$-SO_2-$ in backbone
6	Fluorine atom	23	Fully condensed ring 
7	Chlorine atom	24	Double Bonds =
8	Hydrogen bonding	25	Benzene rings 
9	Dipole-dipole, CH group	26	Triple Bonds ≡
10	Dipole-dipole, CH_2 group	27	Ether oxygen in backbone
11	Dipole-dipole, CH_3 group	28	Ester oxygen in backbone
12	Dipole-dipole, CF group	29	Alcohol oxygen in polymer
13	Dipole-dipole, CF_2 group	30	Amine nitrogen in polymer
14	Dipole-dipole, CF_3 group	31	C=N bonds
15	Oxygen in chain backbone	32	C≡N bonds
16	Backbone phenyl bonding, Ortho	33	Amide nitrogen in polymer
17	Backbone phenyl bonding, Meta		

TABLE 8

TH THE BEST SET $\{K_j^*\}$ WAS USED IN CORRESPONDENCE WITH A=1.435, THE SAME AS THE INITIAL VALUE

Polymer No.	Volume A^3	Weighting Factors																	Analogous Experimental Tg(°K)	Computed Tg(°K)
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17		
1	67.00	3	3	0	0	3	0	1	1	0	0	0	1	0	0	0	0	0	108.8	108.8
2	72.20	2	3	0	0	4	0	0	1	0	1	0	1	0	0	0	0	0	76.8	76.8
3	82.60	0	3	0	0	6	0	0	0	0	1	1	1	0	0	0	0	0	69.5	69.5
4	134.85	3	8	0	0	5	0	1	1	0	5	0	0	0	0	0	0	0	100.4	100.4
5	150.15	0	8	0	0	8	0	0	0	0	6	1	0	0	0	0	0	0	79.3	79.3
6	125.40	3	8	0	0	3	0	0	0	0	1	1	0	0	0	0	0	0	75.6	75.6
7	94.50	3	4	0	0	5	0	1	1	0	0	1	1	0	0	0	0	0	90.8	90.8
8	122.00	3	5	0	0	7	0	1	1	0	0	2	1	0	0	0	0	0	82.2	82.2
9	1041.30	12	39	2	11	56	2	0	2	1	0	28	0	0	0	0	7	0	76.6	76.6
10	1053.90	18	38	2	11	56	2	0	8	0	0	28	0	0	0	0	7	0	75.8	75.8
11	1105.20	10	38	2	12	64	2	0	4	0	0	32	0	0	0	0	8	0	75.1	75.1
12	1026.10	14	36	2	12	56	0	0	6	0	0	28	0	0	0	0	8	0	73.1	73.1
13	1055.80	6	38	2	11	60	2	0	2	0	4	28	0	0	0	0	7	0	75.7	75.7
14	322.45	0	12	3	1	19	0	0	0	0	1	6	2	0	0	0	1	0	70.8	70.8
15	386.90	0	14	3	2	23	0	0	0	0	2	6	3	0	0	0	2	0	76.0	76.0
16	414.50	0	15	3	2	25	0	0	0	0	2	7	3	0	0	0	2	0	74.7	74.7
17	442.00	0	16	3	2	27	0	0	0	0	2	8	3	0	0	0	2	0	73.6	73.6
18	267.75	0	10	3	1	15	0	0	0	0	0	6	1	0	0	0	1	0	69.7	69.7
Assumed K_j		0.5	3.5	1.5	0.6	0.75	8.0	6.2	0.325	0.90	1.25	0.5	3.5	1.5	0.6	0.75	8.0	6.2		
Computed K_j^*		0.5	3.5	1.5	0.6	1.0	8.0	6.2	0.325	0.90	1.0	0.0	2.75	0.0	0.0	0.0	8.0	0.0		

TABLE 9

EXPERIMENTAL AND CALCULATED T_g'S

Polymer No. Table 6	Experimental Tg (K)	Calculated Tg (K)		
		I	II	III
34	521.0	518.8	519.5	518.8
35	538.0	542.5	543.5	543.4
36	536.0	536.0	536.0	536.0
37	553.0	553.8	553.0	553.8
38	531.0	531.0	531.0	531.0
39	552.0	555.3	555.6	556.3
40	547.0	548.7	547.9	548.7
41	567.0	566.9	565.3	567.0
42	537.0	534.6	534.1	536.3
43	543.0	546.0	543.6	546.8
44	586.0	586.0	586.0	585.0
45	723.0	611.6	610.4	610.6
46	533.0	533.0	533.8	533.0
47	562.0	553.5	554.5	554.3
48	561.0	547.9	548.0	547.9
49	584.0	563.2	562.7	563.3
50	521.0	522.9	521.0	524.2
51	518.0	543.0	541.3	545.2
52	545.0	537.5	545.0	538.9
53	563.0	552.5	559.6	554.0
54	549.0	547.0	546.7	548.5
55	580.0	556.7	554.9	557.5
56	576.0	592.0	592.2	591.2
57	612.0	612.7	612.0	612.0
58	493.0	493.0	492.9	492.5
59	507.0	507.0	507.0	507.0
60	510.0	503.2	502.6	502.7
61	521.0	513.6	512.5	513.1
62	489.0	489.0	483.1	489.0
63	497.0	502.9	497.0	503.5
64	504.0	510.5	509.5	510.0
65	511.0	521.1	519.6	520.6
66	508.0	508.5	511.9	508.4
67	510.0	501.9	506.3	502.3
68	513.0	523.3	522.5	522.1
69	527.0	535.9	534.7	534.8
70	473.0	474.8	475.3	474.8

TABLE 9 (Concluded)

EXPERIMENTAL AND CALCULATED T_g'S

Polymer No. Table 6	Experimental Tg (K)	Calculated Tg (K)		
		I	II	III
71	485.0	490.2	490.9	490.8
72	486.0	486.0	486.0	486.0
73	494.0	497.4	497.0	497.5
74	520.0	482.7	482.7	482.7
75	513.0	498.4	498.5	499.0
76	527.0	494.1	493.6	494.1
77	540.0	505.7	504.7	505.8
78	489.0	484.3	483.9	485.4
79	494.0	491.6	490.1	492.1
80	497.0	505.2	505.2	504.6
81	499.0	519.5	518.9	519.0
82	537.0	537.0	537.0	537.0

TABLE 10

COMPUTED VOLUME FACTORS K_j WHERE $A_I = 1.140$, $A_{II} = 1.000$, AND $A_{III} = 1.435$

Factor No. Table 7	Computed K_j's		
	I	II	III
1	1.87	2.78	1.79
2	9.24	10.04	7.02
3	20.91	20.61	20.54
4	5.69	7.35	4.65
5	0.00	-0.24	0.00
6	8.43	9.05	7.20
7	0.00		
8	0.00		
9	0.00	-2.28	0.00
10	4.78	2.96	4.48
11	0.00		
12	0.00		
13	0.00		
14	0.00	0.00	0.00
15	0.00	-1.71	0.00
16	1.26	0.00	1.43
17	0.00	-1.45	0.00
18	3.39	1.80	3.40
19	0.00		
20	0.00		
21	1.42	0.00	1.79
22	0.00		
23	0.00		
24	0.00	0.00	0.00
25	0.00	0.00	0.00
26	0.00		
27	0.00		
28	0.00	0.00	0.00
29	0.00		
30	0.00		
31	0.00		
32	0.00		
33	0.00		

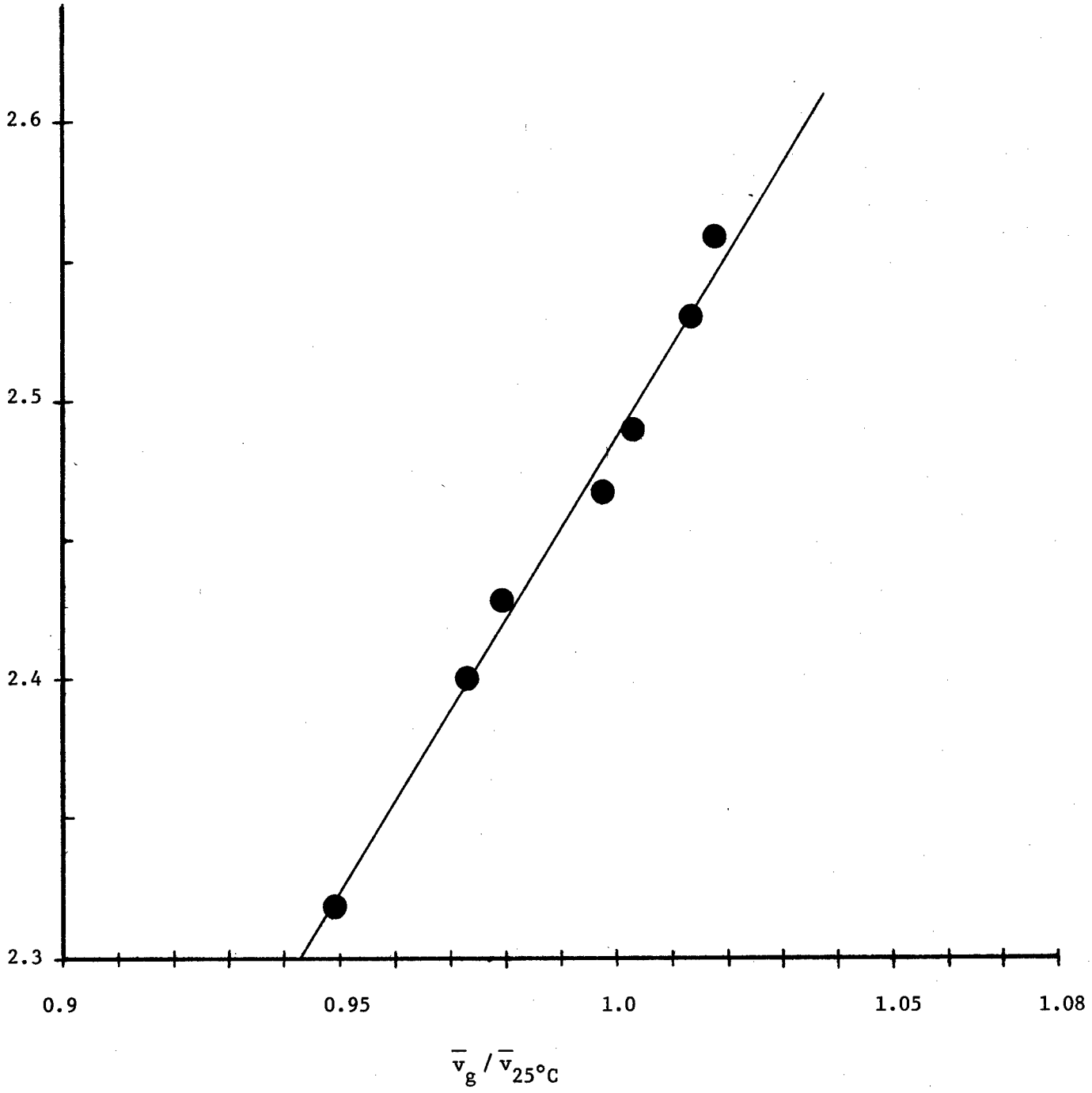


Figure 1. Linear Relationship Between Log T_g and $v_g/v_{25^\circ C}$. Data from Reference 15.

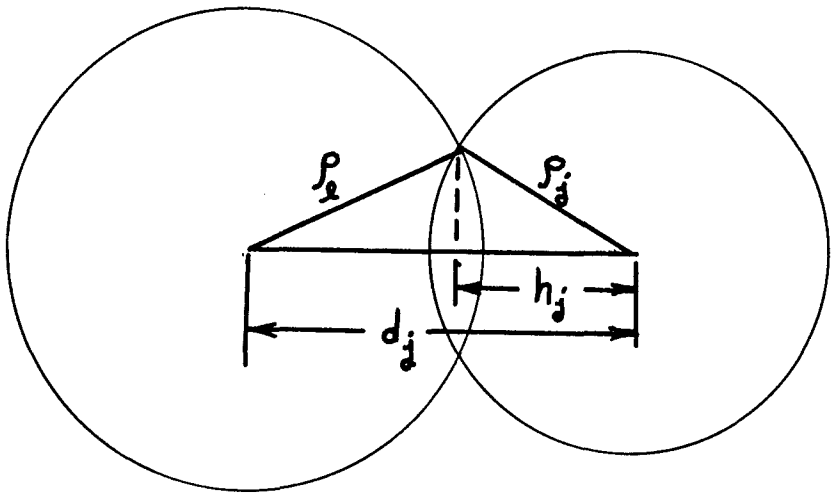


Figure 2. Schematic Diagram of the Chemical Combination of Two Atoms.

☆U.S.Government Printing Office: 1978 — 757-080/99