Quantitative Structure−Property Relationship (QSPR) Correlation of Glass Transition Temperatures of High Molecular Weight Polymers

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A new quantitative structure−property relationship (QSPR) five-parameter correlation ($R^2 = 0.946$) of molar glass transition temperatures (T_g/M) for a diverse set of 88 polymers is developed with the Comprehensive Descriptors for Structural and Statistical Analysis (CODESSA) program. The descriptors are all calculated directly from the molecular structure, and the approach given is applicable, in principle, to all linear polymers of regular structure.

INTRODUCTION

The glass transition temperature, T_g, also known as the glass temperature or the glass−rubber transition temperature, is one of the most important properties of amorphous polymers. In the vicinity of T_g, a polymer experiences a sudden increase in the rate of molecular motions and, as a result, undergoes a series of conformational transformations. The torsional oscillations and/or rotations about most of the backbone bonds are activated, which causes a sharp increase in the free volume of the system as it is converted from the initial rigid (glassy) state to quasi-liquid state.[1] As a result of these processes, many physical properties of polymers change dramatically; for example, their coefficients of thermal expansion, heat capacities, and viscosities.

The T_g is difficult to determine experimentally and predict theoretically because the transition takes place over a comparatively wide temperature range and is dependent on conditions such as the method of measurement, duration of the experiment, and pressure during the measurement.[2,3] The T_g is also very dependent on the structural (cross-linking, chain stiffness), constitutional (additives, fillers, impurities), and conformational (tacticity) features of polymers.[3,4] For these reasons, the discrepancies between reported values of T_g in the literature can be quite high.

Over the past 20 years, there have been numerous attempts to predict T_gs for polymers by various approaches. Empirical methods were based on the correlational relationships with other physical or chemical properties of polymers; weighting factors were frequently included in the framework of group-counting models.[5−8] Thus, Van Krevelen used a group additive property (GAP) theory for predicting T_g.[9] In the GAP theory, the property under consideration is assumed to be the scalar sum of the corresponding properties of component chemical groups. GAP approaches can sometimes give relatively good predictive correlations, but a serious limitation is that these methods are only applicable for polymers containing chemical structural groups previously investigated. Bicerano[3] used a similar approach,

calculating structural parameters and adding increments based on the monomer structure. He obtained a good correlation with R^2 of 0.95, which related T_g with the solubility parameter and the weighted sum of 13 structural parameters for the data set of 320 polymers.

Koehler and Hopfinger[10,11] extended the GAP approach and combined GAP with molecular modeling, which allows the theoretical estimation of unknown parameters. They related T_g by multiple linear regression of seven structural parameters to intramolecular flexibility represented by linear contributions of conformational entropies of the repeating units computed from torsional rotation barrier about the backbone and side-chain bonds, and to intermolecular interactions represented by the dispersion and positive and negative electrostatic intermolecular energies. The Koehler-Hopfinger model has been simplified using the Tripos 5.2 force field method and a four-parameter correlation with R^2 of 0.902 was obtained for 12 alkyl acrylates.[12]

Recently, some alternative approaches have been developed that are not based on the group-counting or the GAP theory. Camelio et al.[13] correlated the T_g values of some 50 acrylates and methacrylates with their "backbone flexibility" as represented by the ratio of the total energy of repeating units inside the cylinder relative to the volume of this cylinder. All necessary parameters were calculated with molecular mechanics. This method resulted in a relatively good correlation with R^2 of 0.83.[13] In our previous study,[14] we used the Comprehensive Descriptors for Structural and Statistical Analysis (CODESSA) program[15] to develop a four-parameter quantitative-structure−property relationship (QSPR) model with R^2 of 0.928 for a set of T_g values of 22 linear, medium molecular weight polymers and copolymers.

Despite this progress, it would be of significant theoretical and practical utility to perform a QSPR analysis of the T_g values for a large set of polymers with diverse chemical structures. Provided that the QSPR projections of T_g into the large array of theoretical molecular descriptors is successful, the resulting equation should cast light on the most important physical interactions contributing to this property. Furthermore, because only theoretical descriptors derived solely from the molecular structure would be

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Table 1. Polymers Used in the Study with Observed and Calculated T_g (K) Values

name	exp. T_g	calc. T_g	$\Delta T_g{}^a$	name	exp. T_g	calc. T_g	$\Delta T_g{}^a$
poly(ethylene)	195	192	3	poly(vinyl *n*-octyl ether)	194	204	−10
poly(ethylethylene)	228	234	−6	poly(vinyl *n*-decyl ether)	197	179	18
poly(butylethylene)	220	247	−27	poly(oxyoctamethylene)	203	185	18
poly(cyclopentylethylene)	348	345	3	poly(oxyhexamethylene)	204	198	6
poly(cyclohexylethylene)	363	325	38	poly(vinyl *n*-pentyl ether)	207	237	−30
poly(acrylic acid)	379	395	−16	poly(vinyl 2-ethylhexyl ether)	207	236	−29
poly(methylacrylate)	281	250	31	poly(*n*-octyl acrylate)	208	197	11
poly(ethylacrylate)	251	288	−37	poly(*n*-octyl methacrylate)	253	261	−8
poly(*sec*-butylacrylate)	253	266	−13	poly(*n*-heptyl acrylate)	213	208	5
poly(vinyl alcohol)	358	325	33	poly(*n*-nonyl acrylate)	216	172	44
poly(vinyl chloride)	348	262	86	poly(*n*-hexyl acrylate)	216	223	−7
poly(acrylonitrile)	378	378	0	poly(1-heptene)	220	240	−20
poly(vinyl acetate)	301	279	22	poly(vinyl *n*-butyl ether)	221	235	−14
poly(styrene)	373	352	21	poly(*n*-propyl acrylate)	229	249	−20
poly(2-chlorostyrene)	392	400	−8	poly(vinyl isobutyl ether)	251	274	−23
poly(3-chlorostyrene)	363	364	−1	poly(vinyl *sec*-butyl ether)	253	263	−10
poly(4-chlorostyrene)	389	392	−3	poly(pentafluoroethyl ethylene)	314	306	8
poly(2-methylstyrene)	409	361	48	poly(2,3,3,3-tetrafluoropropylene)	315	293	22
poly(3-methylstyrene)	374	359	15	poly(3,3-dimethylbuthyl methacrylate)	318	328	−10
poly(4-methylstyrene)	374	352	22	poly(*N*-butyl acrylamide)	319	376	−57
poly(4-fluorostyrene)	379	350	29	poly(vinyl trifluoroacetate)	319	262	57
poly(propylene)	233	227	6	poly(3-methyl-1-butene)	323	279	44
poly(1-pentene)	220	253	−33	poly(*n*-butyl α-chloroacrylate)	330	327	3
poly(ethoxyethylene)	254	251	3	poly(*sec*-butyl methacrylate)	330	318	12
poly(*tert*-butylacrylate)	315	318	−3	poly(heptafluoropropyl ethylene)	331	328	3
poly(*n*-butyl acrylate)	219	244	−25	poly(3-pentyl acrylate)	257	280	−23
poly(vinyl hexylether)	209	227	−18	poly(5-methyl-1-hexene)	259	264	−5
poly(l,l-dimethylethylene)	199	257	−58	poly(oxy-2,2-dichloromethyltrimethylene)	265	334	−69
poly(l,l-dichloroethylene)	256	336	−80	poly(*n*-hexyl methacrylate)	268	266	2
poly(l,l-difluoroethylene)	233	271	−38	poly(vinyl isopropyl ether)	270	296	−26
poly(α-methylstyrene)	409	382	27	poly[*p*-(*n*-butyl)styrene]	279	390	−111
poly(methyl methacrylate)	378	298	80	poly(*n*-butyl methacrylate)	293	281	12
poly(ethyl methacrylate)	324	305	19	poly(2-methoxyethyl methacrylate)	293	271	22
poly(isopropyl methacrylate)	327	312	15	poly(3,3,3-trifluoropropylene)	300	307	−7
poly(ethyl chloroacrylate)	366	341	25	poly(4-methyl-1-pentene)	302	296	6
poly(2-chloroethyl methacrylate)	365	304	61	poly(vinyl chloroacetate)	304	341	−37
poly(*tert*-butyl methacrylate)	380	339	41	poly(*n*-propyl methacrylate)	306	347	−41
poly(phenyl methacrylate)	393	350	43	poly(3-cyclopentyl-1-propene)	333	357	−24
poly(chlorotrifluoroethylene)	373	337	36	poly(3-phenyl-1-propene)	333	376	−43
poly(oxymethylene)	218	219	−1	poly(*n*-propyl α-chloroacrylate)	344	328	16
poly(oxyethylene)	206	191	15	poly(*sec*-butyl α-chloroacrylate)	347	301	46
poly(oxytrimethylene)	195	201	−6	poly(3-cyclohexyl-1-propene)	348	372	−24
poly(oxytetramethylene)	190	200	−10	poly(vinyl acetal)	355	385	−30
poly(ethylene terephthalate)	345	306	39	poly(vinyl formal)	378	367	11

^{a} $\Delta T_g = T_g(exp) - T_g(calc)$.

involved, the equation should, in principle, be applicable to any chemical structure. In the present paper we introduce a new QSPR model developed with CODESSA for a diverse set of 88 polymers.

DATA PREPARATION AND ANALYSIS

The T_g data for 88 uncross-linked homopolymers in their most common atactic forms were taken from a published compilation (Table 1).[3] The polymers chosen for the data set cover a relatively wide range of T_gs transition temperatures and represent an extensive variety of chemical groups. The majority of the polymers fall into the classes of homochain polymers (only carbon atoms in the main chain) and polyoxides, but several polyamides and polycarbonates were also included. The data set contained large subsets of polyethylenes, polyacrylates, polymethacrylates, polystyrenes, polyethers, and polyoxides. The entire set was characterized by a high degree of structural variety, with the functionalities represented in the side chains including halides, cyanides, carboxylates, acetates, amides, ethers, alcohols, hydrocarbon chains, and aromatic and nonaromatic rings. The T_g values ranged from 190 to 417.5 K.
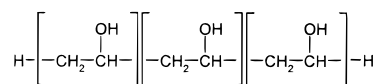
Figure 1. Sample of trimeric repeating units for poly(vinyl alcohol).

It was impossible to calculate descriptors directly for the entire molecules because all the polymers possessed high molecular weights. Therefore, models consisting of repeating units, end-capped by hydrogen, were chosen as small, yet representative structures, to calculate the descriptors (Figure 1). The final molecular descriptors were calculated only for the middle repeating unit of the trimeric structure; however, by this procedure, the influence from adjacent repeating units was also taken into account. The terminal groups were not considered separately because all polymer chains were assumed to be terminated by a hydrogen atom. According to this approach, the descriptors are independent of the polymer molecular weight. This assumption is justified given the fact that, in most cases, T_g remains almost constant with molecular weights above ∼25 000, and all the polymers in the set considered here have molecular weights of

Table 2. Descriptors Involved in the Best Five Parameter QSPR Model Derived for T_g/M ($R^2 = 0.9460$, $R_{cv}^2 = 0.9376$, $F = 287.45$, $s^2 = 0.119$)

descriptor	X	ΔX	t test	$R^{2\ a}$
intercept	3.31	0.18	18.05	
moment of inertia I_C	72.37	6.82	10.60	0.464
HASA−2/TFSA [semi-MO PC]	38.91	2.94	13.22	0.324
log (Kier shape index (2nd order) + 1)	−1.40	0.11	−12.30	0.696
most negative atomic charge	1.95	0.57	3.39	0.043
FPSA-3 fractional PPSA (PPSA-3/TFSA) [semi-MO PC]	14.28	2.10	6.81	0.021

[a] Correlation coefficient of the descriptor with the molecular weight.

$>50\,000$.[16] As the T_g is itself an intensive property,[3] it was divided by the molecular weight of the repeating unit (M), and T_g/M was used as an extensive property for the correlation analysis.

The structure of the trimer of the repeating units for each polymer was drawn and preoptimized with the PCMODEL program.[17] The preoptimized structures were then optimized with a semiempirical AM1 method[18] using the MOPAC 6.0 program[19] to obtain the necessary quantum-chemical descriptors for the further calculations. Over 400 constitutional, topological, geometrical, and quantum chemical[20] descriptors were calculated for the middle fragment of the trimeric system from the results of the semiempirical calculations using the CODESSA[15] program.

The correlation analysis to find the best QSPR model was carried out using the best multilinear regression analysis method in the framework of the CODESSA program. Initially, 218 descriptors were preselected by removing (i) descriptors that could not be calculated for every structure in the data set and (ii) descriptors with an essentially constant value for all structures. Thereafter, the intercorrelations between all these 218 descriptors were calculated, and orthogonal pairs of descriptors i and j (with $R_{ij}^2 < 0.1$) were selected. From this set of orthogonal pairs, the best 400 descriptor pairs (defined as those with the highest two-parameter regression correlation coefficients) were selected for further development to higher order regressions. Next, for each of the 400 descriptor pairs selected, a noncollinear descriptor scale, k (with $R_{ik}^2 < 0.5$ and $R_{kj}^2 < 0.5$) was added, and the three-parameter regression was calculated. This procedure was repeated with all descriptor scales noncollinear to a given pair of descriptors, and the best 400 triplets (defined as those with highest correlation coefficients) were selected for the next higher order regression analysis. In this way, the number of noncollinear descriptor scales in the model was incrementally increased up to the optimum as determined by the Fisher criterion at the given probability level and the cross-validated correlation coefficient.[21] The cross-validated regression correlation coefficient also describes the stability of each regression model obtained by focusing on the sensitivity of the model to the elimination of any single data point.

RESULTS AND DISCUSSION

The best five parameter correlation equation obtained for the entire data set of 88 polymers had the squared correlation coefficient $R^2 = 0.946$ and is presented in detail in Table 2 and Figure 2. Calculated T_g values are given in Table 1
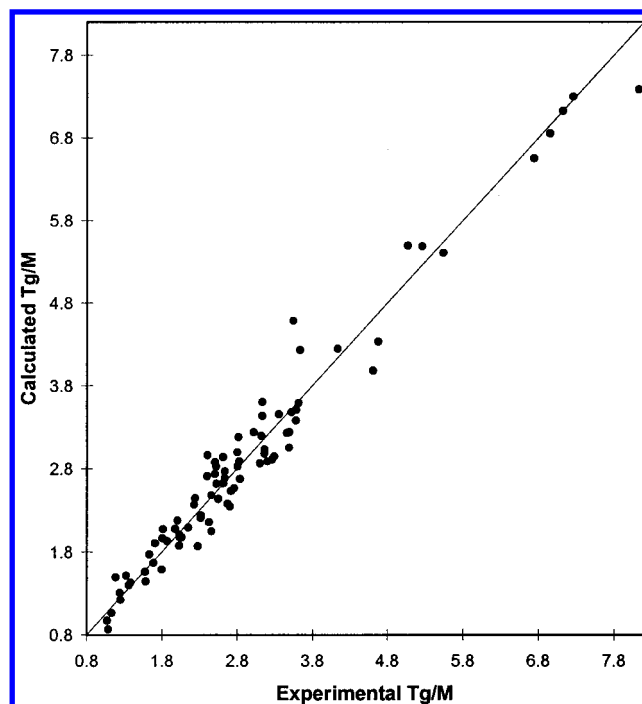
Figure 2. Plot of predicted versus experimental values of T_g/M obtained with descriptors calculated for the middle fragment of trimers ($R^2 = 0.946$).
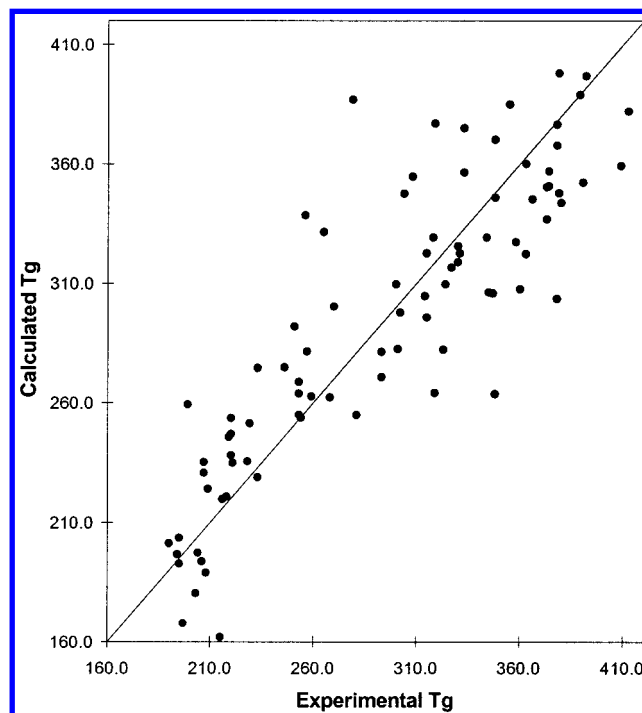
Figure 3. Plot of predicted T_g values (calculated from predicted T_g/M values) versus experimental values of T_g ($R^2 = 0.754$).

and Figure 3. The number of descriptors (five) in the final QSPR was determined on the basis of the data set size (88 structures) and on the basis of the analysis of Fisher criterion and cross-validated correlation coefficient as already discussed.

According to the t test, the most significant descriptor in the QSPR model is the *moment of inertia* I_C, which is the smallest of the three principal moments of inertia of the molecule. The *moment of inertia* I measures the mass distribution relative to the principal axis of rotation and is

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related to the rotational energy of the molecule. In eq 1, m_i is the atomic mass and r_{iz} is the distance of the ith atomic nucleus from the principal rotational axis of the molecule[22]:

$$I = \sum_i m_i r_{iz}^2 \qquad (1)$$

The *Kier shape index* (second order) is a topological descriptor that depends on the number of skeletal atoms, molecular branching, and a special parameter a_i, which is defined as the ratio between the atomic radius, r_i, and the radius of the carbon atom in the sp^3 hybridization state, r_o.[23] The second-order *Kier shape index* is calculated by eq 2, where N_{SA} is the number of skeleton atoms, ^2P is the number of paths of length 2 in the molecular skeleton, and α is the sum of the a_i parameters for all skeleton atoms minus 1:

$$^2\kappa = (N_{SA} + \alpha - 1)(N_{SA} + \alpha - 2)^2(^2P + \alpha)^2 \qquad (2)$$

The *most negative atomic charge* in the molecule is calculated by Mulliken population analysis according to eq 3, where AO is the number of atomic valence orbitals of the nth atom, Z_n is the core charge of this atom, and C_{ni}^2 is the element of density matrix:

$$Q_n = Z_n + \sum_i^{AO} c_{ni}^2 \qquad (3)$$

HASA-2/TFSA is defined as the sum of the square roots of the partial surface areas of the hydrogen acceptor atoms divided by the total surface area of the repeating unit. This descriptor quantifies the ability of a polymer to form hydrogen bonds, and is calculated by eq 4, where S_A is the exposed surface area of a hydrogen acceptor atom, N_A is the number of hydrogen acceptor atoms capable to form hydrogen bond, and S is the total surface area of the repeating unit fragment:

$$HASA2/TFSA = \frac{\sum_A^{N_A} \sqrt{S_A}}{S} \qquad (4)$$

The *fractional positive partial charged surface area* (FPSA-3) is defined as the ratio between the positively charged surface area and total surface area of the repeating unit[24] and describes electrostatic interactions between molecules. FPSA-3 is calculated by eq 5, where S_A is the surface area of a positively charged atom, q_A is the corresponding positive atomic charge, N_A is the number of the positively charged atoms in the repeating unit, and S is the total surface area of the repeating unit:

$$FPSA3 = \frac{\sum_A^{N_A} S_A q_A}{S} \qquad (5)$$

As already discussed, it is more appropriate to correlate T_g/M (where M is the molecular weight of the repeating unit) rather than T_g itself. Indeed, conversion of the predicted T_g/M values into T_g values and comparison with experimental T_g values reduces the correlation coefficient R^2 to 0.754 (Figure
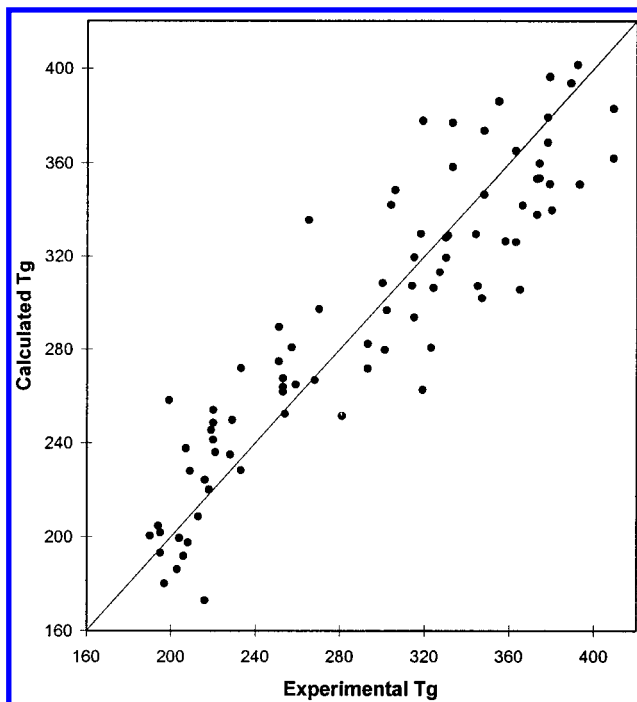
Figure 4. Plot of predicted T_g values (calculated from predicted T_g/M values) versus experimental values of T_g after removing outliers ($R^2 = 0.830$).

Table 3. Descriptors Involved in the Best Five Parameter QSPR Model Derived for T_g/M After Removing Outlyers ($R^2 = 0.964$, $R_{cv}^2 = 0.957$, $F = 412.66$, $s^2 = 0.08$)

descriptor	X	ΔX	t test	$R^{2\ a}$
intercept	3.31	0.16	20.96	
moment of inertia I_C	73.14	5.62	13.00	0.458
HASA-2/TFSA [semi-MO PC]	39.70	2.43	16.32	0.112
log (Kier shape index (2nd order) + 1)	−1.33	0.096	−13.87	0.693
most negative atomic charge	22.51	0.48	4.67	0.042
FPSA-3 fractional PPSA (PPSA-3/TFSA) [semi-MO PC]	14.30	1.76	8.11	0.035

^{a} Correlation coefficient of the descriptor with the molecular weight.

3); the standard error of predicted T_g values is 32.9°. According to calculated 95% confidence interval, four polymers are outliers: poly(1,1-dichloroethylene), poly[p-(n-butyl)styrene], poly(vinyl chloride), poly(methyl methacrylate). Removing these outliers improves R^2 between the experimental and predicted T_g values to 0.830 (Figure 4), and the standard error decreased to 27.5°. The regression of recalculated T_g/M values also improved the R^2 to 0.964, by omitting these four outliers, whereas the corresponding regression coefficients remain almost unchanged (Table 3 versus Table 2).

Additional cross-validation analysis was considered both to test our QSPR model for stability and the suitability of its application to unknown systems. We first divided our data, sorted by experimental T_gs into three subsets based on the data set in this order. Then, we combined two of the subsets, recalculated the QSPR model, predicted T_gs for the third subset, and calculated the correlation coefficient for this third data set. We applied similar procedures to calculate the correlation coefficients for the other two subsets. The average correlation coefficient for the three subsets was 0.935, which is comparable with the cross-validated cor-

relation coefficient[21] ($R_{cv}^2 = 0.938$) calculated by stepwise elimination of every single data point.

CONCLUSION

We have presented a successful five-parameter correlation for T_gs temperatures of a variety of high molecular weight polymers. The molecular descriptors involved in the correlation relate rationally to the physical phenomena, because T_g is believed to be determined both by shape/bulkiness of the repeating units (which are reflected in our equation by the moment of inertia and the Kier shape index) and by intermolecular electrostatic interactions (accounted by most negative atomic charge, HASA-2/TFSA and FPSA-3). The R^2 of the correlation for T_g/M values was 0.946 and the standard error was 0.33 K mol g^{-1}. The approach used here relies solely on descriptors calculated from the chemical structure of the molecule, so this approach is applicable in principle to regular linear polymers of any chemical structure. This result encourages the further application of QSPR methods to other classes of polymer, such as copolymers, cross-linked polymers, and biopolymers.

ACKNOWLEDGMENT

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