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Transfer learning-driven artificial intelligence model for glass transition temperature estimation of molecular glass formers mixtures

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ABSTRACT

Predicting binary mixtures' glass transition temperature (T_g) is crucial in various fields, particularly for industrial materials affected by this property during production processes and in service-life. On the other hand, from the fundamental point of view, this predictive capability is relevant for understanding the chemical interactions between the two components and how this affects the T_g of the mixture. In this sense, some models provide different approaches for describing the T_g of the mixture. Among them, the Gordon-Taylor approach has been widely used since it only relies on the relationship between the T_g of the pure components, their weight fraction, and only one fitting parameter. Although simple, this approach still requires measurements of T_g of the pure components and at least some intermediated composition for the fitting procedure. In a previous work, our research has focused on neural networks methods for predicting T_g values directly from the chemical structure of monomers and molecules, but the scarcity of experimental data for binary mixtures limits the application of a similar approach. To address this problem, we propose to use in this work a transfer learning method that relays on the previous acquired knowledge of the chemical structure - T_g relationship, for the prediction of the T_g of the binary mixtures. Therefore, pure component characteristics are derived from chemical fingerprints originated in a pre-trained network, and enables a training process focused on their behavior within the mixtures. This approach successfully estimated K with very low deviations, even allowing for the exploration of the embedded chemical structure's relation to previously unknown mixtures.

1. Introduction

Predicting the glass transition temperature (T_g) of binary mixtures hold significant importance across various fields, especially to industrial materials for which production processes are heavily affected by this property. Knowledge of its behavior enables the optimization of processing conditions (such as temperature, mixing energy and heating–cooling rates) to achieve the desired results during manufacturing processes. In addition, it is crucial for their mechanical and chemical stability, and shelf-life in fields like pharmaceutical [1–5], food industries [6–14] (it significantly impacts texture and other organoleptic properties), and materials in general [15–20].

There are several models for describing the glass transition of binary mixtures, like Gordon Taylor (GT), Fox, Kwei or Couchman –Karasz [21–24]. Among these, the Gordon Taylor approach is widely used because it provides a useful approximation by just considering the relationship between the T_g of pure components, their weight fraction in the mixture and a single fitting parameter (K). This approach offers a simplified and quick method for describing the T_g of mixtures without the need for many experimental measurements. In addition, it can be applied to a wide range of mixtures, including molecules and polymers, and can be easily extended to pseudobinary systems [25–27]. The physical meaning of the GT fitting parameter can be approximated from thermodynamic considerations, and for weakly interacting systems it can be related to the change in heat capacity (ΔC_P) of the pure components, their molecular weight and the Flory-Huggings interaction parameter, $\chi_{1,2}$ (defined for the pair of components in the blend labeled as 1 and 2).

In our previous research, we have developed several neural network approaches to estimate the glass transition temperature of polymers and molecular glass-formers [28,29]. Besides using different architectures for the task, all these approaches involved mapping the chemical structure of either monomers or molecules to the corresponding T_g values [29–36]. Basically, during training, each neural network learned the various features within the encoded chemical structure [30,37] and therefore their correlation with the experimentally observed T_g. However, the scarceness of experimental data on the glass transition temperatures of mixtures as a function of their composition makes difficult

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the development of such an approach for this specific scenario. The main limitation that arises from this data scarcity is related to the mapping of the aforementioned chemical structure-glass transition temperature relationship, since training a network with only a few examples gives very inaccurate results. To overcome this challenge, we propose employing transfer learning techniques to use the previously acquired knowledge of the chemical structure-T_g relationship from our earlier networks, and to apply it to the prediction of glass transition temperatures of binary mixtures. In this new approach, the characteristics of each pure component are derived from their respective chemical fingerprints (as obtained from pre-trained models). Consequently, all training efforts are only concentrated on elucidating the chemical interactions between the two components in the mixture, a task for which the available amount of experimental data is enough. In this way, we have estimated K for several mixtures with very low deviations, thus opening the door for relating the embedded chemical structure to industrially relevant mixtures whose behavior was not experimentally reported.

2. Theoretical background

2.1. Glass transition in miscible binary mixtures

As for pure materials, miscible binary mixtures exhibit a single glass transition temperature, which in turn depends on their composition [25]. In some cases, the T_g of the mixture may show a linear relationship with composition and the T_g values of the pure components (this behavior is commonly observed for ideal polymer blends). However, for more complex systems, the T_g of the mixture may deviate from linearity due to interactions between the components (these interactions can lead to changes in molecular mobility and therefore affect the observed T_g). Therefore, the presence of strong specific interactions such as hydrogen bonding can significantly affect the T_g behavior in the mixtures [27].

2.2. Gordon Taylor approach

The Gordon Taylor approach is a widely used method for estimating the glass transition temperature of blends and mixtures [21–23,25]. The key concept behind the Gordon Taylor approach is that the T_g can be estimated based on a relationship between the T_g of the pure components ($T_{g,1}$, $T_{g,2}$) and their weight fractions (w_1, w_2) in the mixture, and a fitting parameter known as K.

$$T_g^{mixture} = \frac{T_{g,1}w_1 + T_{g,2}w_2K}{w_1 + w_2K} \tag{1}$$

Among other ways, the Gordon Taylor expression can be obtained from the enthalpy balance in the vicinity of the glass transition of the mixture. As a result, an expression relating thermodynamic parameters of the single components (through specific heats) and intermolecular interactions (through Flory Huggings interaction parameter) can be obtained. From this general expression, GT equation is obtained and the fitting parameter can be thus related to physically meaningful quantities [38].

$$K \approx k + A/(T_{g,2} - T_{g,1}) \tag{2.1}$$

$$A = \frac{-\chi R(T_{g,2} - T_{g,1})}{\Delta C_{p,1}^{mass} M_1} \tag{2.2}$$

$$k = \Delta C_{p,2}^{mass} / \Delta C_{p,1}^{mass} \tag{2.3}$$

where $\Delta C_{p,1}^{mass}$,M_1 and χ stand for: heat capacity diference between glass and liquid state, molecular weight of component 1, and Flory Huggings interaction parameter, respectively. As a result, and by using this model as an indicator of the complexity level, it is possible to infer that the training process should deal with a highly multidimensional system (with only the chemical structure of the materials as input data). In this model aproximation, we can already identify several thermodynamic quantities involved: $T_{g,1}$, $T_{g,2}$, $\Delta C_{p,1}^{mass}$,M_1 and χ. This imposes a huge strain on the data pipeline, since a lot of examples would be required for this learning task.

2.3. Chemical embedding

We have previously developed neural networks applied to predicting glass transition temperature of molecular glass formers. We have shown that their embedding process can encode the relevant chemical features of the glass transition in a vector of m dimensions (that can be thought as coordinates in an m dimensional space). Therefore, we propose a transfer learning process that uses the knowledge in these vectors or chemical fingerprints in the new problem at hand. As a result, the new network has only to learn the interactions in the mixtures rather than all the features of each component plus mixtures from scratch. We have also previously shown that these embeddings carry information on the chemical structure-glass transition temperature relationship (both through molecular weight and interactions), but it is worth noticing that in the here proposed approach we are implicitly assuming that some info about the ΔC_P has also to be present. Finally, the way the components interact, as represented in K through the interaction parameter, has to be learned from the blend examples in the current training process.

3. Methods

3.1. Dataset

We collected glass transition temperature vs concentration experimental data for 40 binary mixtures, a total of around 400 temperature-composition points. The experimental data was then fit with Gordon-Taylor approach in order to obtain K for each mixture. It is worth noticing that approximately 30 % of the dataset is composed of mixtures in which one of the two components is water. In these cases, we need to make some assumptions due to the intense debate existing in the literature about the value of the water's glass transition temperature. Some authors hold that the T_g is around 136 K [39–42], while others consider it is higher [43–45]. Although the debate is still open, in this work we use the value of 136 K because most of the mixtures show a consistent picture when extrapolating to this value for pure water (see also SI 1). The rest of the dataset is mainly composed by alcohol and pharmaceutical drugs mixtures, and, when not explicitly stated, T_g of pure components was either obtained from literature or extrapolated from the graph (see SI 1 and SI 2).

3.2. Neural network

In previous works we developed a recurrent neural network (RNN) able to predict the glass transition temperature of molecular glass formers. The dataset from which the RNN was trained is composed of around 500 molecules, including alcohols, pharmaceutical drugs, additives, sugars and carbohydrates [37]. The architecture was designed to deal with sequential inputs and we employed a bidirectional long short-term memory layer, which reads each sequence both from the beginning to the end and viceversa. The molecular structure of the compounds was expressed by the Simplified Molecular-Input Line-Entry System (SMILES) as an alpha-numerical string of characters, which was then converted in a numerical format [46,47]. The network was able to predict T_g with a mean absolute percentage error (MAPE) of 8.1 %. In this study, we use such network to obtain vectorial representations of the molecules in an m-dimensional space, where «m» is the number of neurons of the last layer. As a result, we obtain an embedding array of 16 neurons for each component, which contains the encoding for the relationship between T_g and molecular structure [30,37]. We then used these arrays as an input for a fully connected architecture and the fitted *K* as the output (see Fig. 1). In this way, we can take advantage of the structure-T_g information and focus the training in the mixing effects on the T_g. Therefore, the aim of the fully connected network is to find the correlation between the molecular structure expressed in the T_g-oriented space and the *K* of the mixtures. This network is composed by two fully connected hidden layers (50–50) with leaky ReLU activations. A more detailed description of the network and the hyperparameters optimization can be found in section SI 3.

4. Results and discussion

We employed the model described in previous section for predicting *K* for different binary mixtures, by using only a fingerprint of the chemical structure as input. Even with the very limited amount of available training data there is good correlation between the predicted *K* and the value of the experimental *K* (see Fig. 2). We obtained MAPE values of 7, 15 and 18 % respectively for the training, test and validation sets (a detailed list of RMSE values for all mixtures in the dataset is presented in the SI).

A more intuitive comparison can be observed from Fig. 3, where we show the results of the mixture behaviour derived from predicted *K*(red line) with respect to the experimental T_g-composition data (empty circles) for binary mixtures in the test set. In addition, we show the GT fitting of experimental data (blue line), which in turn shows the experimental *K*.

The predicted (red) GT lines present low deviations with respect to the experimental (blue) lines, therefore suggesting that the training procedure has been able to generalize the mixture behaviour. This is especially valid for some mixtures (like propanol- pentanol and ibuprofen-naproxen in Fig. 3), where experimental and predicted glass transition temperatures are really close to each other. In these cases, we assume that the embedded chemical structure of the input is accurately describing the characteristics of each component, and that the fully connected network is then able to generalize the interactions between these components.

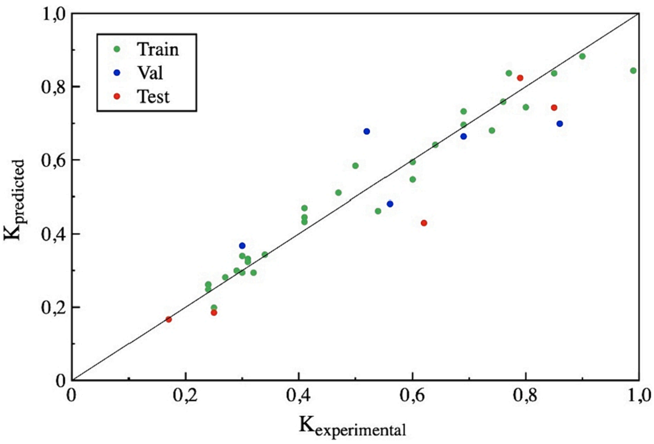

Fig. 2. Predicted vs experimental K. The black line represents the bisector (K predicted = K experimental), showing the good accordance between the experimental and the predicted K. We obtained a mean absolute percentage error (MAPE) values of 7, 15 and 18 % respectively for the training, test and validation sets.

In this sense, our method relies on two training processes in series, and we can thus identify three main error sources. On the one hand, the first training process relies on a larger dataset for learning and encoding the chemical structure-glass transition relationship of molecular glass formers, on the other hand, the second one uses these encoded arrays for predicting mixture behaviour. As a result, it is reasonable to think that observed deviations can be originated from a poor chemical description of the components (i.e. from the model in the first step) or a poor description of the interactions in the mixture (from the model in the second step). We have throroughly characterized the performance of the first model with respect to the chemical structure of the inputs, and it was found that low deviations were obtained the closer the compound to a chemical confidence area (see Fig. 4). In particular, within this area we found no bias due to molecular weight or intermolecular forces. The observation of the embeddings with dimensionality reduction techniques shown that there are 3 main regions: 1) which mainly consist of low-molecular-weight, flexible linear carbonated chains and weak

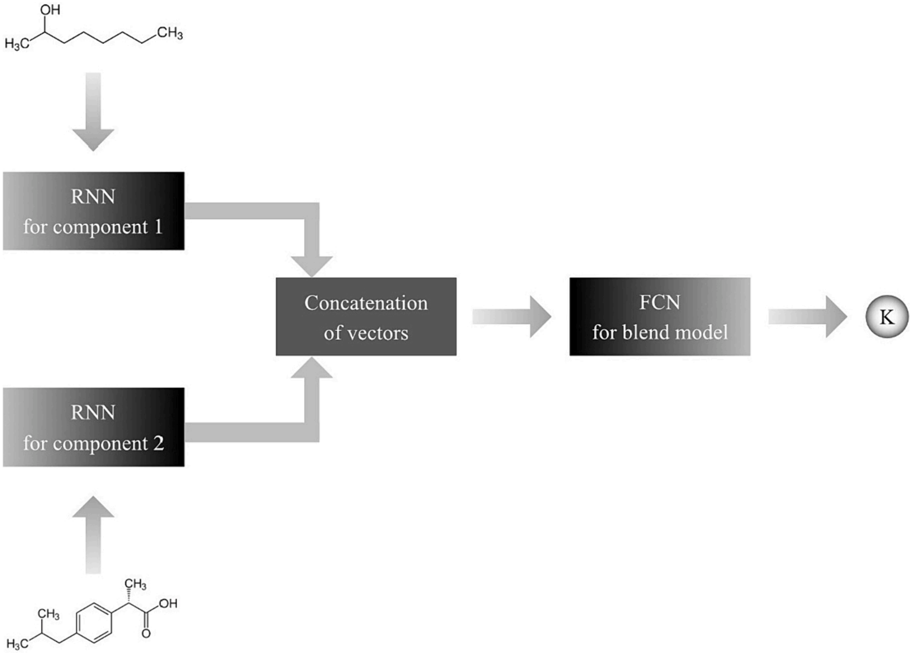

Figure 1. Scheme of the process. First, we feed the RNN with a representation of the molecular structure of each component, then we obtain the vector of the last layer of the RNN and feed them to the trainable mixture model which predicts the K.

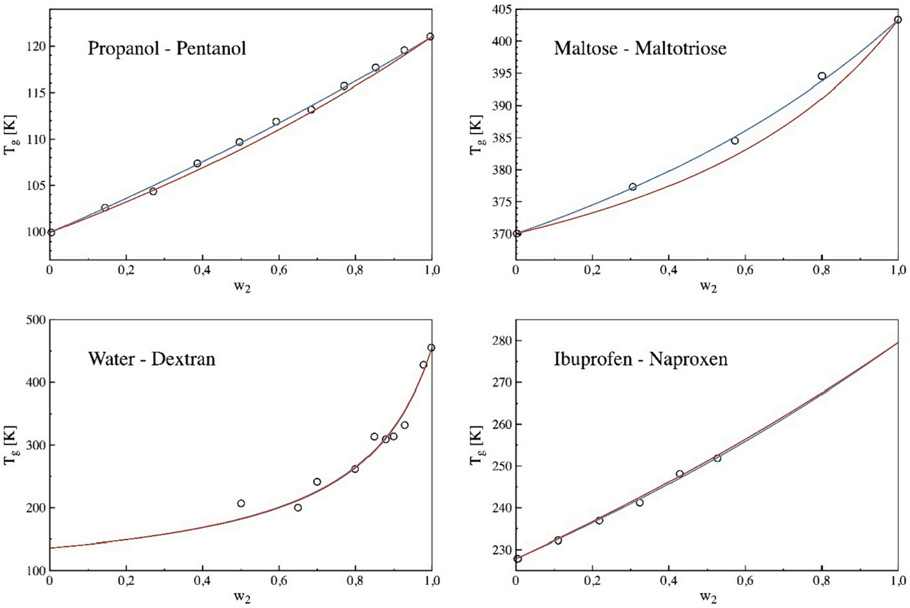

Fig. 3. Test set comparison between the GT fit (blue lines) and the GT model with the predicted K (red lines). Empty circles represent the experimental data.

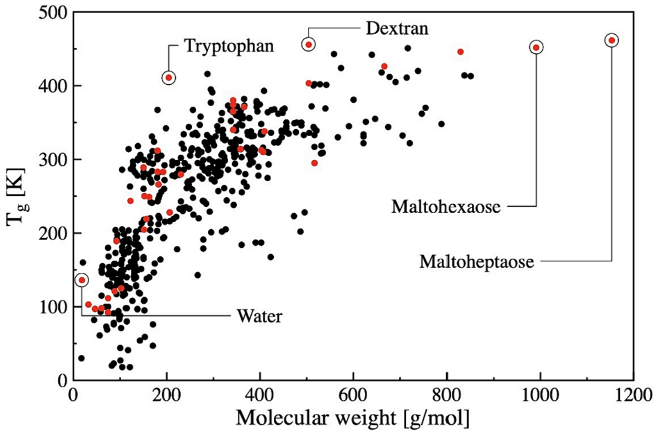

Fig. 4. Molecular weight dependence of the glass transition temperature for the training set molecules (black symbols). The pure components used in this work are shown in orange circles.

intermolecular forces; a middle section 2) with a tradeoff among intermolecular forces and the structural composition of the molecules as they progressively become more branched and incorporate bulkier molecular groups into their structure and; 3) composed of molecules with high-molecular weight, more rigid phenyl groups, and strong intermolecular forces. When pure components lie within this confidence area, the first error source can be assumed to be small in comparison with the rest of the process. Fig. 4 shows glass transition temperature as a function of molecular weight for the RNN's training set (which can be used as an approximation to the chemical space learned by the first model) and the molecular glass formers employed in this study. The latter are well within the confidence area, with the exception of water, dextran, maltohexaose and maltoheptaose, which slightly deviate from the other compounds behaviour (appear at higher temperatures due to comparatively strong hydrogen bonds).

The third source of deviations is related to the GT modelling of the experimental data. As shown in Fig. 3, some mixtures (like ibuprofen-naproxen) are not so well represented by the GT approach and therefore the "experimental" K is less accurate in these cases. In the case of water-dextran (or maltoheptaose-glucose) mixtures, we can assume that both the experimental error and a less accurate encoding (from their position quite on the outside of the chemical space) affect the final prediction (see Fig. 4).

These tendencies are also reflected in the Validation set, where predicted results describe quite closely the experimental data. As shown in Fig. 5, all pure components are apparently well described by the first model encoding, and some minor uncertainties related to the GT fitting are observed in the case of diethyl ether mixtures-pentanol. In overall, the proposed approach provides an excellent description of the experimental results, therefore encouraging us to explore relevant but unknown mixtures.

4.1. *Virtual laboratory: predicting the glass transition of unknown mixtures*

As stated before, the glass transition temperature plays a crucial role in shaping the behavior of the mixtures' properties, that in turn affect various industrial processes. This becomes evident when considering parameters that present a large change in the vicinity of T_g such as viscosity, modulus, and diffusion coefficient, among others. For example, the diffusion coefficient is of paramount importance in industries like food and pharmaceuticals, where precise knowledge of substances diffusion is crucial for product quality and performance. On the other hand, viscosity is also heavily changed near the T_g and plays a pivotal role in determining transport properties in industrial processes across various sectors, since it affects the uniformity of mixing and blending processes, as well as energy expenditure (high-viscosity materials require more energy to mix effectively and may lead to incomplete dispersion or uneven distribution of ingredients). Finally, the glass transition temperature in binary mixtures can also affect several other key properties like drug release rates through the drug release kinetics.

For the above stated reasons, we believe that a fully predictive model holds value at the moment of performing exploratory analysis, saving time and effort by giving clues on the potential behaviour of materials. Therefore, we applied our trained model to the prediction of the glass transition temperature as a function of composition for several mixtures with, to the best of our knowledge, no reported experimental values. In order to study the effect of the chemical structure of the system's components on the results, we have analysed mixtures by keeping one component constant while changing the other. Fig. 6 shows the mixture T_g as a function of concentration for Water – 1,2,6-Hexanetriol,

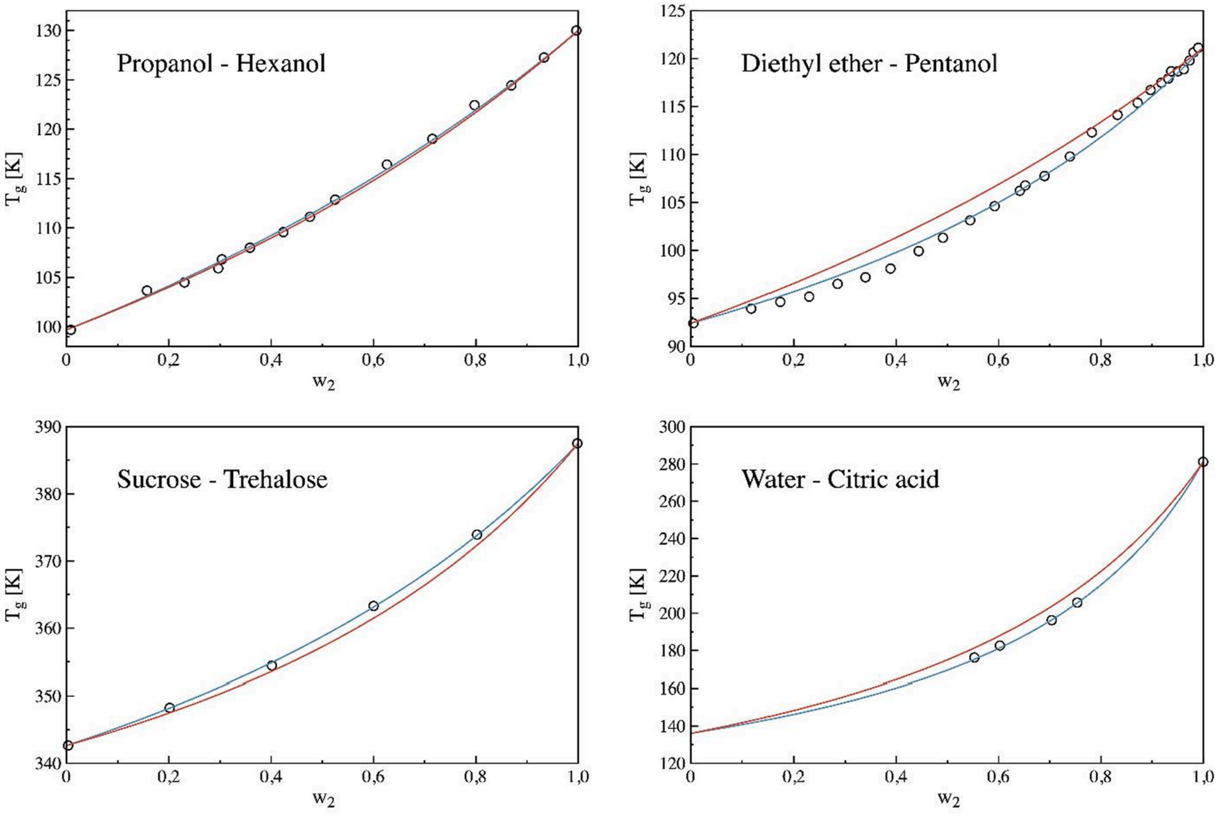

Fig. 5. Validation set comparison between the GT fit (blue lines) and the GT model with the predicted K_{GT} (red lines). Empty circles represent the experimental data.

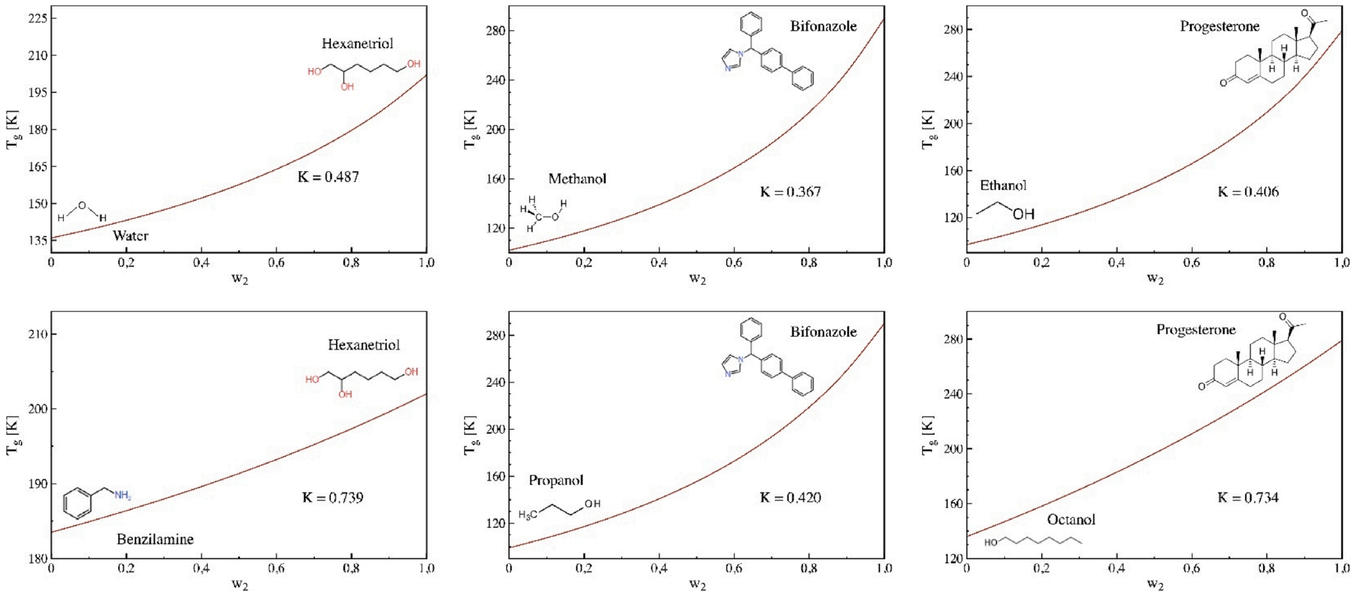

Fig. 6. T_g of various experimentally unknown mixtures of interest.

Benzylamide – 1,2,6-Hexanetriol, Methanol – Bifonazole, Propanol – Bifonazole, Ethanol – Progesterone and Octanol – Progesterone.

The first study case involves 1,2,6-Hexanetriol, which is known for its ability to adjust viscosity, enhance solubility, and improve stability of mixtures in a range of industries that include cosmetics, pharmaceuticals, agriculture, and coatings [48]. As shown in Fig. 6, 1,2,6-Hexanetriol mixtures with water and Benzylamide yield very different concentration dependence, reflected by a change of nearly 40 % on their predicted *K* values. On the one hand, the small water molecule largely interacts with the OH groups of the alcohol through hydrogen bonding, while the amide presents both a larger (non-interacting) mass due to its phenyl group and comparatively lower intermolecular forces that yield a *K* value closer to 1.

In our second study case, we study Bifonazole, which is a multifaceted compound with applications ranging from the treatment of fungal infections to its role as a solubility-enhancing agent for very poorly soluble drugs. To overcome the challenge of its relatively low aqueous solubility, researchers have explored methods like cosolvency to increase the solubility of bifonazole in water. For this purpose, recent studies have focused on mixtures of bifonazole with various alcohols [49]. As shown in Fig. 6, mixtures of Bifonazole with methanol and propanol yield similar K values, which are consistent with the previous observations where the most interacting component presents the smallest values.

Finally, we analysed Progesterone, which is a crucial drug with a wide range of applications in healthcare. It is commonly utilized for the treatment of various conditions, including menopause, hormone deficiency, fertility issues, contraceptive preparations, support during pregnancy, and the management of gynecological disorders. However, when administered orally, progesterone faces a significant challenge in terms of bioavailability. This is primarily due to its low solubility in aqueous environments and its relatively short half-life resulting from enzymatic degradation in the mouth and stomach. To address these challenges and optimize drug delivery, it is essential to study progesterone's solubility in different solvents (being octanol one of the most employed references) [50]. As shown in Fig. 6, ethanol and octanol yield very different K values, also consistent with the previously observed trend in which the more massive and non-interacting molecule yields K values closer to 1.

This approach successfully predicts K for binary mixtures, therefore demonstrating its ability to generalize mixture behaviour effectively. The combination of transfer learning and two-step training allowed us to address challenges related to data scarcity and accurately estimate T_g for various mixtures from the chemical structure of pure components alone.

5. Conclusions

We have successfully employed a two-step training for estimating the glass transition of various binary mixtures by using only the chemical structure of the pure components as input. Despite the limited amount of available training data, our model demonstrated excellent correlation between the predicted K and the experimental values. We have characterized our approach by identifying the main error sources, which are related to the first training process, the second training process or the experimental model. Some compounds, like water, dextran, maltohexaose, and maltoheptaose, slightly deviate due to comparatively strong hydrogen bonds. Our findings indicate that complex relationships between molecular weight, intermolecular forces, and structural composition learned by the first model contain relevant information and can be used as a fingerprint. To further show the potential applications of such models, we predicted the composition dependence of unmeasured mixtures of interest. The insights gained from this study provide valuable guidance for further improving the model's performance and expanding its application to more complex mixtures in various fields of material science.

CRediT authorship contribution statement

Claudia Borredon: Validation, Visualization, Software, Writing – review & editing. **Luis A. Miccio:** Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **Gustavo A. Schwartz:** Conceptualization, Analysis, Visualization, Investigation, Methodology, Supervision, Funding acquisition, Project administration, Resources, Validation, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.commatsci.2024.112931.

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