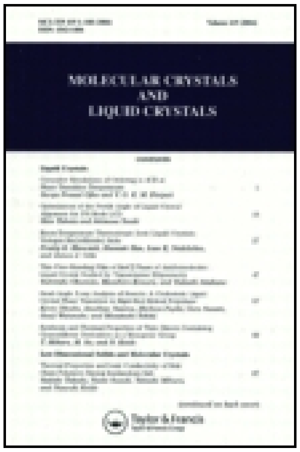

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Analysis of Infrared Spectra of Liquid Crystal Mixtures by Neural Networks Methods

Khin M. Yin [a] & Takashi Kayano [b]

[a] School of Technology, Kent State University, Kent, Ohio, USA

[b] Department of Information Science, Shimane University, Matsue, Japan

Version of record first published: 04 Oct 2006

To cite this article: Khin M. Yin & Takashi Kayano (1997): Analysis of Infrared Spectra of Liquid Crystal Mixtures by Neural Networks Methods, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 304:1, 435-439

To link to this article: http://dx.doi.org/10.1080/10587259708046993

Mol. Cryst. Liq. Cryst., 1997, Vol. 304, pp. 435–439
Reprints available directly from the publisher
Photocopying permitted by license only

ANALYSIS OF INFRARED SPECTRA OF LIQUID CRYSTAL MIXTURES BY NEURAL NETWORKS METHODS

KHIN M. YIN
School of Technology, Kent State University, Kent, Ohio, USA

TAKASHI KAYANO
Department of Information Science, Shimane University, Matsue, Japan

Abstract We have used neural network approach to the classification of infrared spectra of binary mixtures of 4-n-nonyl-4'-cyanobiphenyl (9CB) and 4-n-pentylphenyl-trans-4'-pentylcyclohexane-1-carboxylate (5H5). We built the neural networks, using nonlinear back propagation algorithm (BPN). The input neurons represent selected spectral intensities in the range of 1000-40000 wave numbers/cm. The output neurons represent the concentrations of the mixtures, the phases (isotropic, nematic and smectic) at the experimental temperatures. In the classifier mode, the network correctly classifies the smectic liquid crystal phases.[1] The training of the neural networks was carried out fairly well. The predictions of compositions of the mixtures agree qualitatively.

INTRODUCTION

Artificial neural networks are implementations of computational algorithms that create dynamic data structures that animate some simple functions of human brains. Neural networks are capable of learning patterns and making predictions. They are useful in classifying sets of patterns that may have similarities and dissimilarities. In molecular spectroscopy, such as in the infrared molecular spectroscopy, a spectrum indicates structural motions of the constituent molecules. Since these molecular motions take place in some thermodynamic environment, the phase properties of these substances are related to the molecular properties. Using neural networks, we may be able to extract properties of liquid crystals from experimental data that the experiments do not provide directly.

In the case of liquid crystal mixtures, infrared spectra obtained at different temperatures and compositions show differences in spectral densities and the relative positions of the lines. Phase diagrams and spectra of the liquid crystal mixtures, 9CB and 5H5, are reported[2]. In Figure 1, we show a spectrum adapted from the paper.

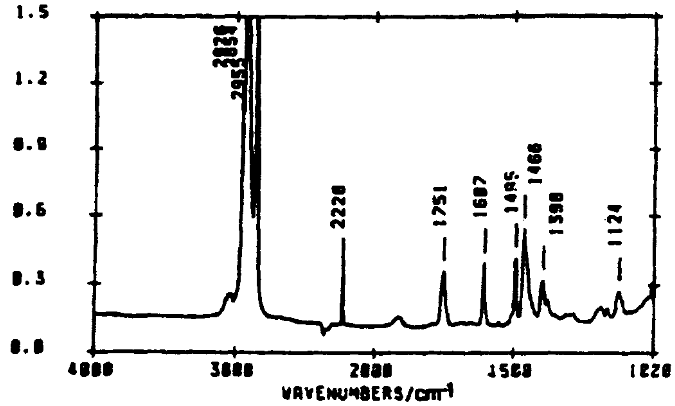

FIGURE 1. Infrared Spectrum of the mixture, 90%(weight) of 9CB and 10%(weight) of 5H5 at 27°C

It shows the spectrum for the mixture 90% of 9CB and 10% of 5H5 (by weight) at 27°C (smectic-A). A spectrum (not shown here) of the same mixture at 60°C (nematic) is quite different.

ARTIFICIAL NEURAL NETWORK CLASSIFIER

For the classification of the infrared spectra, we constructed a neural pattern classifier, using the formalism of the Minimum Distance Classifier[3]. The graphical representation of the neural classifier is shown in Figure 2. The output neurons represent the labeled cluster numbers. The outputs are further fed into the classifier. When all the spectra are classified, the outputs of the classifier are members of clusters, each with its member spectrum. The first pattern introduced is a cluster automatically. The next pattern belongs to the first if it is within a certain distance from the first cluster. If it is the case, the cluster center is reevaluated. If it is outside of the cluster distance, it forms a new cluster. The following patterns may belong to the previously established clusters or form another cluster. By controlling the size of the cluster radius, the total number of clusters can be controlled. The clustering is based on Euclidean distance, d_j. The value of d_j from a new pattern to the jth cluster is given as $(d_j)^2 = E_n(b_{ij} - x_j)^2$ where b_{ij} are the coordinates of the cluster centroid. Here E_n represents a summation. When a new pattern is presented, it is assigned to that cluster for which d_j^2 is the smallest, if d_j is less than cluster radius. This process continued until all input patterns are used. The output results include the input patterns with input tag numbers as belonging to the clusters. A suitably scaled algorithm implements the classifier.

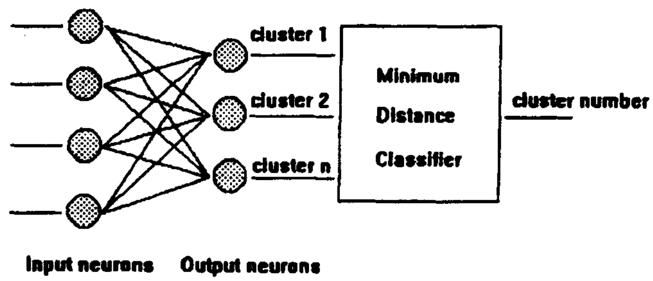

FIGURE 2. The graphical representation of the neural classifier

For this study, we selected 9 spectral patterns representing the isotropic, nematic and smectic phases. For each pattern, we used 100 spectral intensity values. The neural classifier places the 9 patterns into 3 clusters, 0,1,2. The results are shown in Table 1.

TABLE 1. Results of the classification by the Minimum Distance Classifier

Spectral Pattern	Cluster (Radius=3)	Liquid Crystal Phase
pattern-1	1	isotropic
pattern-2	0	isotropic
pattern-3	1	isotropic
pattern-4	0	isotropic
pattern-5	0	isotropic
pattern-6	1	nematic
pattern-7	2	smectic
pattern-8	2	smectic
pattern-9	2	smectic

Results in the table indicate that pattern-1 and pattern-3 do not agree with the other members of the pattern set. However, the classifier puts the patterns correctly for the smectic phase. The incomplete agreement may be due to some limitations in the preprocessing of the spectral data. We think that more data points and sets would make the difference in these neural experiments.

THE NEURAL NETWORKS FOR LEARNING AND CONSULTING

For the learning networks, we chose the network architecture consisting of 100 input neurons, one hidden layer with 50 neurons and an output layer with 5 neurons. Figure 3 shows the network architecture. The input neurons represent the spectral patterns prepared from the infrared spectra. Each input pattern is a representation of the relative intensities of each spectrum. The neurons are connected in feed forward manner. The output neurons represent the phase properties of the liquid crystal mixtures: %-weight of 9CB, %-weight of 5H5, presence or absence of isotropic phase, presence or absence of nematic phase, and presence or absence of smectic phase. The values range from 0 to 1, 0 meaning absence and 1 meaning presence. We used a modified form of a back-propagation algorithm[4] which we briefly described.

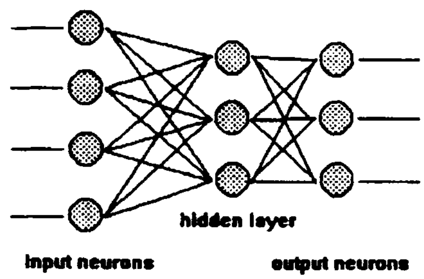

FIGURE 3. The Learning Neural Network

The general idea of back propagation is to establish the data stored in the neurons of the hidden layers so that the input pattern relates to the output pattern within desired accuracy. This is done by propagating incremental values (errors) repeatedly. This process is often called learning by the neural network. For one specific input/output pair, the error at any output is $e_k= t_k-o_k$, where t is the desired target output and o is the actual output. The total error for the input pattern is $e_k=(1/2)E_k(t_k-o_k)^2$. Here E_k represents summation over the index k. This error is reduced repeatedly by correcting the weights and possibly threshold values. At any iteration, the correction to the weight is $dw_{ki}=ld_ko_j$, where l is learning rate parameter. The error signal d_k at an output unit k is given by $d_k=(t_k-o_k)f(net_k)= (t_k-o_k)o_k(1-o_k)$.

For internal neurons, the values of the d_k at the nodes in the hidden layer j can be inferred from d values at an upper layer, and the estimated value is a linear combination of the higher layer d. The error propagated backward is $d_j=o_j(1-o_j)E_kd_kw_{kj}$ and $dw_{ji}=ld_jo_j$ .To increase the learning rate, we may use a momentum parameter, so that the correction at the (n+1)th step is dependent on the nth step:

$$dw_{ki}(n+1) = ld_ko_j + md_wk_j(n) \qquad \text{[Generalized Delta Rule]}$$

where m is selectable momentum parameter. This iterative procedure to reduce the error is carried out until the system error is acceptably small. In our case, the l and m values are selectable by the human trainer.

SUMMARY OF RESULTS

Isotropic phase: Using the cluster 0 patterns, a back propagation neural network was constructed and trained using the GDR. The network learned well, that is, the system errors are less than the experimental errors. The number of iterations is less than 1000 in most cases. This trained neural network was used to consult, i.e., to generate output neural values from an input pattern that belonged to the set. The trained neural network correctly predict the phase: isotopic phase.

Smectic phase: Using the cluster 2 patterns, a back propagation neural network similar to the one in isotropic phase was constructed and trained using the GDR. Again the system errors were reduced to below the experimental values, within 1000 iterations. We used two input patterns from the set that represent smectic phase. The predicted values of the %-weights of 9CB and 5H5 are in fair agreement.

In short, the neural network classifiers work well. The back propagation neural networks for learning and consulting concentration predict fairly well. Currently we are making refinements for better results.

The authors are grateful to Dr. Mary Neubert of the Liquid Crystal Institute, Kent State University, for information on liquid crystals and helpful discussion.

REFERENCES

1. K. M. Yin and T. Kayano, EXPERSYS-94 Expert Systems Applications and Artificial Intelligence, 1, 673 (1994).
2. C. David and D. Baeyens-Volant, Liquid Crystals, 6, 2, 247-261(1989).
3. Y. Pao, Adaptive Pattern Recognition and Neural Networks (Addison Wesley Pub. Co.) Second Edition, 1991.
4. D. Rumelhart and J. McClelland, Parallel Distributed Processing 1 and 2. Sixth Printing (MIT Press, 1987).