Standardisation of gas chromatographic analyses of essential oils

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5. **Summary**

The subject of standardisation is introduced as the selective restriction of the possible types of a product and the mutual interchangeability of the effect of the items produced. Its application to the chemical industry resulted first of all in standardisation of the methods for measuring product characteristics. For essential oils for the assessment of the composition, which ultimately determines the product characteristics, the method of choice is analysis by gaschromatography. Standardisation of this method of analysis is the subject of this study.

The gaschromatographic analysis results either in a fingerprint, used for assessing identity and purity of an oil, or in the determination of the proportion of a specified component. The content of the concept "fingerprint" is discussed. In fingerprints peak identity is not important, it is the pattern that counts. Representation of that pattern in standardised form is recommended.

Reviewing the advantages and disadvantages of the different systems to describe positions in a chromatogram one may conclude that the retention index, although being a relative system, is the best suited.

Important in gaschromatography are the concepts of resolution and polarity. Expressions for the resolving power are reviewed and for standardisation purposes the German definition is preferred for its simplicity.

With regard to the concept of polarity it is stated that the sequence of elution and the separation is a result of the interaction between the compound and the whole of the column between injection point and detector entrance and not solely of the stationary phase. After having pointed out the disadvantages of the Rohrschneider polarity system the concept of the alkane index of the column is developed on base of the Pierotti equation for the activity coefficient. For standardisation purposes the alkane index is rejected because of the difficulty of its assessment and its restriction to isothermal operation.

As a practical approach the observation was used that on a non-polar column compounds elute in sequence of boiling point and not in sequence of molecular mass. By relating a compound by its boiling point to a hypothetical normal alkane with the same boiling point, it is related also to the molecular mass of that alkane. The polarity factor of a compound is now defined as the quotient of the molecular mass of that hypothetical normal alkane and that of the compound.

Similarly, by way of the retention index, the polarity factor due to the interaction of the compound with the column is defined as the quotient of the molecular mass of the hypothetical alkane with the same retention index as the compound and of the molecular mass of that compound.

For a certain column the interaction polarity factors may be calculated from the compound polarity factors using a quadratic equation. The polarity factor of a column is now defined as being equal to the interaction polarity factor in the event of the compound polarity factor being one.

The coefficients of the quadratic function are calculated from the retention indices of the components of a test mixture, consisting of limonene,

acetophenone, linalol, naphthalene, linalyl acetate and cinnamic alcohol. The resolution of the column may be found from a specified pair of compounds of this test mixture. Linalyl acetate is used to check possible decomposition properties of the column.

This system of the polarity factors is explored and its use discussed. Finally the standardisation of the whole procedure is laid down in a draft standard, together with a draft for determining a specified component.

Applications of gaschromatographic analysis are given in the form of fingerprints for several oils and also discussed are the results obtained on a number of essential oil samples.

A table of retention indices of some constituents of essential oils concludes the study.