

- [54] **METHOD AND APPARATUS FOR DETERMINING THE CHEMICAL STRUCTURE OF AN UNKNOWN SUBSTANCE**
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- [58] **Field of Search** 364/496, 497, 498, 499, 364/413; 356/303, 319, 326; 436/43, 173; 324/307, 312

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[57] **ABSTRACT**

A method and apparatus for determining the chemical structure of an unknown substance wherein spectral data of the unknown substance is detected, a point-assessment is calculated which expresses the degree of possibility of partial structures being contained in the unknown substance based on the spectral data and prememorized chemical shift values corresponding to the partial structures of known substances, it is judged whether the point-assessment is a predetermined threshold value or more and the partial structures with a large possibility of being contained in the unknown substance based on the output of the judgement results are found and displayed. The partial structures thus found are used to determine a molecular structure of the unknown substance.

24 Claims, 7 Drawing Figures

