A New Visual Basic 6.0 Software Built-up For Solving-out Reduction Formula in Chemical Applications of Group Theory

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Abstract:

A need for computer software to solve-out the "Reduction Formula" for different Point Groups is beyond doubt. That would save time and effort to many chemists who are involved in different aspects of chemical applications of group theory. This presentation presents a computer software that has been constructed using Visual Basic 6.0 programming language. The input and output data are performed through software forms under Windows Vista environment. The software is able to perform the following functions:

1. Reducing Reducible Representations for most known Point Groups.

2. Finding Reducible Representations " Γ_{red} and Γ_{vib} " for Infinite Point Groups " $C_{\infty v}$ and $D_{\infty h}$ " and reducing them by S-L Method.

3. Finding Reducible Representation Γ_{3N} and reducing it for six chosen Point Groups "C_{2v} , C_{3v} , C_{4v} , D_{2h} , D_{4h} and T_d".

Solutions derived from the constructed software were tested by comparison with manual standard methods, and showed complete consistency.

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