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A Spreadsheet To Facilitate Group Theory Calculations and Display of Character Tables

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Supporting Information

ABSTRACT: A Microsoft Excel workbook is described that can be used to perform group theory calculations using character tables for 50 chemically significant point groups. The workbook will reduce arbitrary representations, calculate direct products, and identify erroneous representations. In addition, the character tables can be projected for use in the classroom or copied to a word-processor for publication.

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

KEYWORDS: *Upper-Division Undergraduate, Inorganic Chemistry, Computer-Based Learning, Group Theory/Symmetry, MO Theory, Spectroscopy*

The use of symmetry and group theory to solve problems in chemical structure and spectroscopy is an important topic in inorganic and physical chemistry.[1] Character tables encapsulate the mathematical representation of molecular symmetry and are used for a variety of calculations that are tedious, but necessary, in order to arrive at a deeper understanding of molecular bonding and behavior. Once students have mastered the calculations, it is desirable to give them a method of performing the calculations quickly so that they can focus on chemical interpretation of the results. In addition, while teaching group theory, it is often necessary to project character tables in a lecture hall.[2] Finally, it is occasionally necessary to reproduce character tables in printed documents, such as exams.

O'Brien and Schmidt published an MS-DOS program that will perform group theory calculations in some of the important point groups.[3] Condren suggested using a spreadsheet to decompose reducible representations and a method for performing the calculations.[4] More recently, Vitz published a spreadsheet containing templates to perform group theory calculations in several point groups.[5] The resources produced by O'Brien and Schmidt and by Vitz both provide chemical interpretation (e.g., matching orbitals by symmetry and predicting vibrational modes) in addition to performing calculations. However, O'Brien and Schmidt's program cannot be expanded to include point groups that were not originally included, and Vitz's spreadsheet requires that the templates be copied and modified by hand to solve problems other than those included as examples.

I have chosen to take a different approach in teaching the use of character tables in my courses. I have produced a spreadsheet containing character tables for all 50 of the chemically significant point groups as listed by Cotton[6] and by Wörner and Merkt.[7] The spreadsheet will decompose arbitrary representations to irreducible representations and calculate direct products of representations. Therefore, it takes care of the tedious calculations, but leaves all chemical interpretation to the user. Using the methods suggested by Carter, the spreadsheet performs calculations on tables containing imaginary characters,[8] and in the infinite-order linear groups.[9] In addition, the errors in commonly available character tables pointed out by Shirts[10] have been corrected. Using the spreadsheet during lecture, character tables can be projected and, if desired, used to perform calculations on-the-fly. The character tables have been carefully formatted so that they can be printed directly or copied into other software for more formal presentation.

In addition to using the spreadsheet during my lecture classes, I allow students to use it for their homework. Once they have completed an assignment proving that they can perform group theory calculations by hand, I distribute copies of the spreadsheet for their use on future assignments. This allows them to focus on the structural and spectroscopic insights gained from the analysis rather than on the calculations. One difficulty students often encounter is determining whether they cannot successfully reduce a representation because they are making a mistake in the calculations or because they are starting with an incorrect representation. This spreadsheet will highlight the representation if it is not a correct linear combination in the current point group. This allows the students to focus their error-checking efforts on determining the correct representation if necessary.

■ ASSOCIATED CONTENT

Supporting Information

The Microsoft Excel workbook containing instructions and a worksheet for each point group is available. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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