

Teaching undergraduates about structure using database examples

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Throughout undergraduate curriculum in North America, the requirement for understanding structure is explicit. For example, in first year general chemistry, Valence Shell Electron Pair Repulsion (VSEPR) theory is used to predict the geometric shape of a molecule based on its electron repulsion forces. The shape of the molecule is determined by minimizing (bonding and non-bonding) electron group repulsions surrounding the central atom(s). [1] Methodology to achieve understanding of concepts related to structure, however, is ordinarily not explicit, and in the case of VSEPR, student learning activities have traditionally involved modeling molecular shapes using manufactured kits, or with materials that are readily available (for example, Styrofoam balls, or marshmallows and toothpicks.) [2] These activities are based on ideal geometry assumptions, and lead to the question, for molecules with a combination of bonding and non-bonding electron groups, how much is "less than" ideal angles? Similarly, in senior chemistry courses, students face structural questions related to resonance, coordination number, the explanation of spectroscopic features, and magnetic properties. The use of active learning engagement through structural database explorations can be employed to address questions at both first-year, and senior levels. Practical approaches to these questions will be explored, with an emphasis on using information available from the Cambridge Structural Database. [3]

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2. Gillespie, R. J. (1992) *Chem. Rev.* 59.

3. Groom, C. R. et al. (2016) *Acta Cryst.* B72, 171.

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