

Why chemists care about graph theory

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Graph theory has had close links with chemistry for at least a century and a half, from the early preoccupation with structural enumeration, through quantum mechanical models of electronic structure, to systematic nomenclature, study of the links between structure and properties of molecules, and the advent of ‘combinatorial chemistry’. This talk starts with a personal perspective on what makes chemistry an ideal field for the application of graph theory, and goes on to describe some ideas in the burgeoning field of *molecular conduction*, which give yet another reason for chemists to ‘care about graph theory’.

The talk includes work done in collaboration with Martha Borg, Rasthy De Los Reyes, Wendy Myrvold, Barry Pickup, Tomaz Pisanski, Irene Sciriha, and Tsanka Todorova.