

## The Valence Bond Matrix in Chemistry

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For a chemical graph, a new matrix called the valence bond matrix (VBM) is proposed. Diagonal terms are linked to bonds and off-diagonal terms to pairs of bonds connected to a common atom. The new matrix has been developed in two versions: including all bonds to hydrogen atoms or a single "bonds to hydrogen" column and line. All bonds are "oriented" having a "light" and a "heavy" end. The matrix is unsymmetrical, the upper triangle representing links to the "heavy" ends and the lower one links to "light" end. Neglecting differentiation between bond ends a symmetrical matrix can also be built. Rules are built for cyclic systems when "oriented" bonds are used. Starting from the VBM some local bond invariants (LOBs) are computed and new topological indices derived. Good correlations are obtained for the boiling points of C<sub>3</sub>-C<sub>10</sub> alkanes versus these new topological indices.