contributing structure

The definition is based on the valence-bond formulation of the quantum mechanical idea of the wavefunction of a molecule as composed of a linear combination of wavefunctions, each representative of a formula containing bonds that are only single, double or triple with a particular pairing of electron spins. Each such formula represents a contributing structure, also called 'resonance structure' to the total wavefunction, and the degree to which each contributes is indicated by the square of its coefficient in the linear combination. The contributing structures, also called 'canonical forms', themselves thus have a purely formal significance: they are the components from which wavefunctions can be built. Structures may be covalent (or non-polar) or ionic (or polar). The representation is frequently kept qualitative so that we speak of important or major contributing structures and minor contributing structures. For example, two major non-equivalent contributing structures for the conjugate base of acetone are:

$$H_2C = \overset{O^-}{\underset{CH_3}{\diagup\diagdown}} \longleftrightarrow H_2C^- - \overset{O}{\underset{CH_3}{\diagup\diagdown}}$$
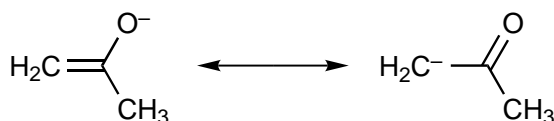
See also *delocalization, Kekulé structure, resonance.*
1994, *66,* 1100