

A Simple Nomenclature for Complex Organic Free Radicals

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The usual way of naming an organic free radical is to use the name the radical would have if it were a substituent in a compound. The terms "methyl, alkyl, hydroxyl, acetyl, and glycyI," *etc.* may then be used to refer to groups substituted for hydrogen in various compounds and as well to the corresponding free radicals if they exist. To qualify for a name then a free radical must be related to a group of such importance as a substituent in compounds that a "radical" name has already been coined for it. Even for such a simple radical as $\dot{\text{C}}\text{H}_2\text{COOH}$ this is not the case, and authors who have reported this species have apparently preferred to designate it by its formula rather than resort to such a label as methylene carboxylic acid. It seems most natural to regard it as being derived from acetic acid by removal of one of the

methyl hydrogens to leave a vacant bond. In fact, a search of the literature shows that all so far reported free radicals produced by irradiation of organic crystals could be converted into more or less familiar compounds by the insertion of a hydrogen atom into the dangling bond. These considerations lead us to propose the following rules for naming complex organic free radicals.

(1) Regard the unsatisfied valence as containing a hypothetical monovalent "substituent" called the kenon (Gk. *κενον*, empty) and the radical species as being therefore a keno derivative of a parent compound. Hence $\dot{\text{C}}\text{H}_2\text{COOH}$ is called kenoacetic acid by analogy with chloroacetic acid and $\text{HOOC}\dot{\text{C}}\text{H}_2\dot{\text{C}}\text{HCOOH}$ is called kenosuccinic acid by analogy with chlorosuccinic acid. Kenosuccinic acid can in fact be made by

radiation damage in crystals of aminosuccinic (aspartic) acid,¹⁾ replacing the amino group of the amino acid with a "hole" or kenon.

(2) Use the ordinary rules for specifying the position of the substituent kenon. Thus $\dot{\text{C}}\text{H}_2\text{-CH}_2\text{COOH}$ becomes β -kenopropionic acid as distinct from the α -keno compound, $\text{CH}_3\text{-}\dot{\text{C}}\text{HCOOH}$. Similarly $\text{HO}\langle\bigcirc\rangle\cdot$ becomes p -kenophenol; the compound $\text{CH}_3\dot{\text{C}}\text{HCO}(\text{CH}_2)_{10}\text{-CH}_3$ acquires the name 2-keno-3-tetradecanone while $\dot{\text{S}}\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$ is called β -keno-thio- α -aminopropionic acid.

(3) Radicals such as methyl, $\dot{\text{C}}\text{H}_3$ can be regarded either as kenomethane or methyl kenide. Since a free radical can be given a kenide name only if the corresponding bound radical has already been named, such a term is of little use unless one wishes to emphasise the free radical character by attaching the redundant term kenide.

1) T. S. Jaseja and R. S. Anderson, *J. Chem. Phys.*, **36**, 2727 (1962).

The use of some sort of "hole" or "vacancy" language such as this is so helpful in describing free radical phenomena in irradiated organic crystals, that even if only for this purpose it is necessary to coin a name for the hole. For example,²⁾ we can refer to "kenon diffusion" instead of "transfer and diffusion of the free radical state by hydrogen atom jumping" and the phrase "kenon trapping on impurities" sufficiently designates that process whereby the free radical state is localised on impurities which have a bond to hydrogen which is weaker than the bonds to hydrogen of the molecules of the host crystal. Principally, however, the proposed nomenclature has to its advantage that it names simply and unambiguously any free radical by using the resources of the existing nomenclature, regarding the radical as a "substituted" compound, and signifies its free radical character immediately by the presence of the tags "keno" or "kenide."

2) D. R. Cutten and L. G. Ericson, International Conference on Electron Diffraction and the Nature of Defects in Crystals, Melbourne II A-2, 1965.