

Curran, H. J., Pitz, W. J., and Westbrook, C. K., 2002
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All C_n species may be identified using the labeling scheme below.

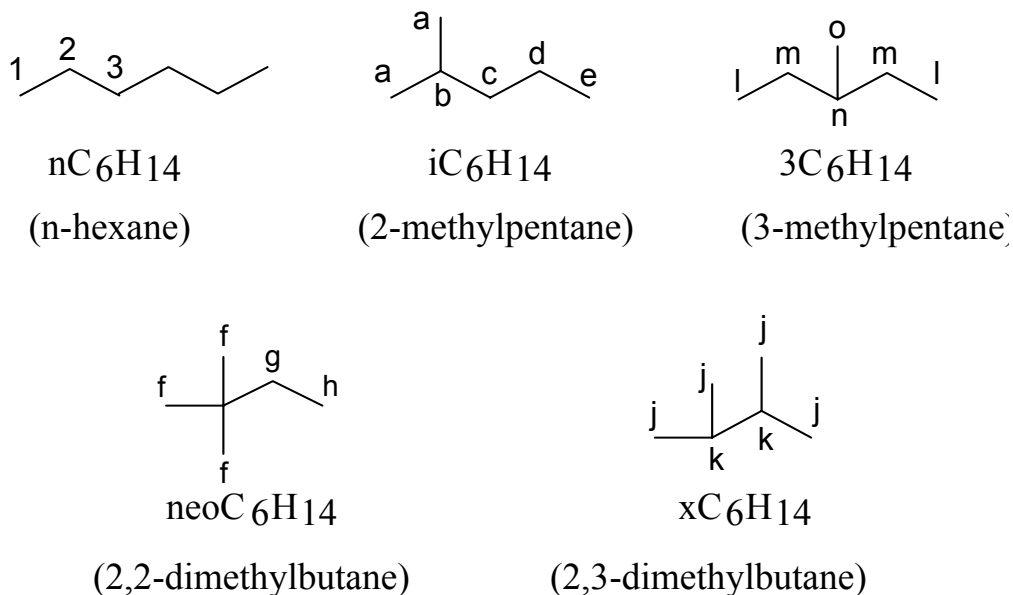


Figure 1: Labeling scheme for hexane isomers

For any alkyl-hydroperoxide species ($aC_nH_{(2n+1)}OOH$), a denotes the site of the hydroperoxyl group. Thus, for example, $1C_6H_{13}O_2H$ is 1-hexylperoxide and $1C_6H_{13}O_2$ is 1-hexyl-peroxyl radical. In addition, for $aC_nH_{2n}OOH-b$, a denotes the site of the hydroperoxyl group and b the radical site. Moreover, in $aC_nH_{(2n-1)}OOH-b$, a denotes the site of the double bond and b the site of the peroxy group. Finally, for xC_nketab , x denotes the particular isomer, a the site of the CO double bond and b the site of the peroxide group. For example, in $neoC_6ketg$ the CO double bond is at site g and the peroxide group is positioned at site f.

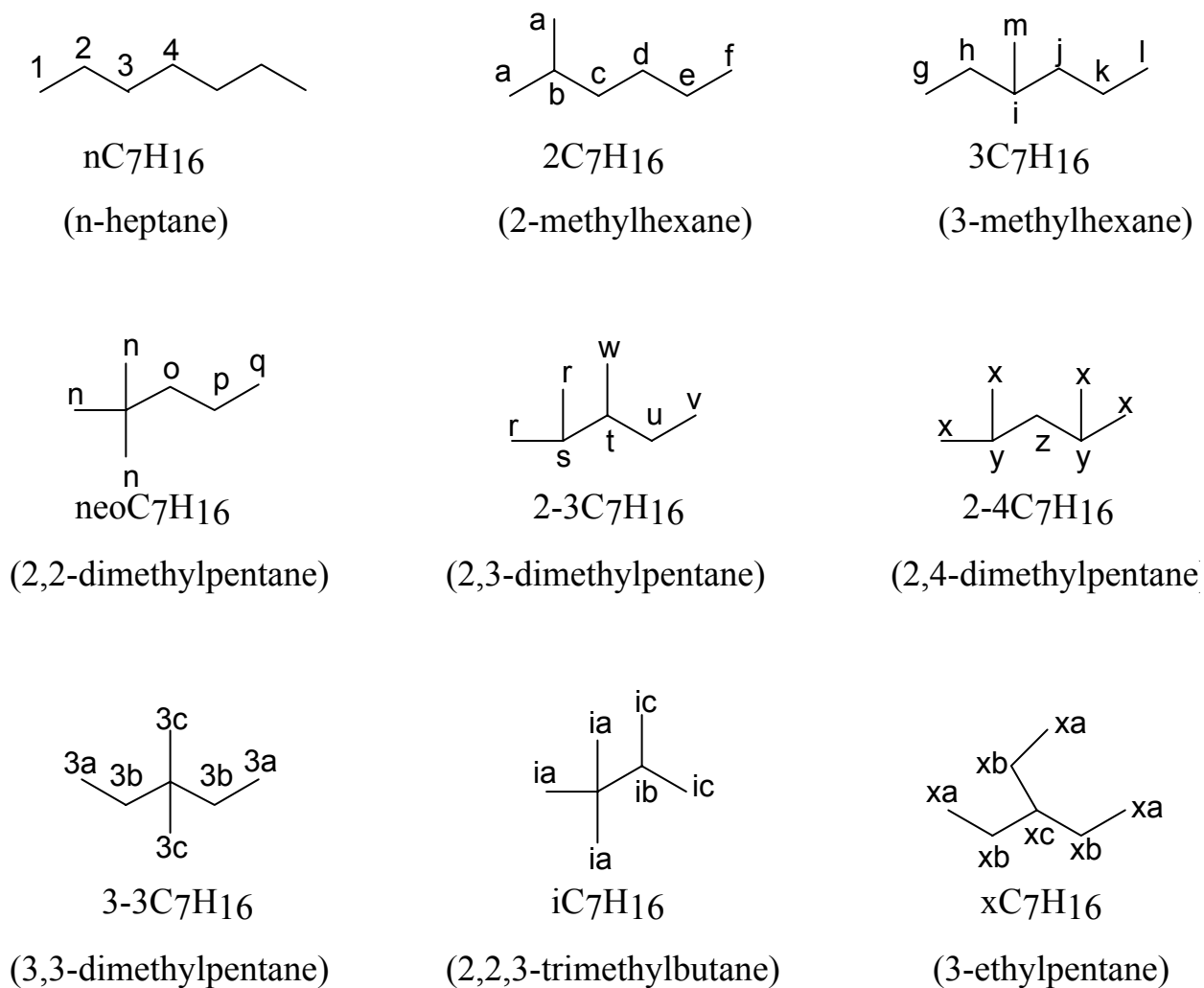


Figure 2: Labelling scheme for heptane isomers