## reactivity index

Any numerical index derived from quantum mechanical model calculations that permits the prediction of relative reactivities of different molecular sites. Many indices are in use, based on a variety of theories and relating to various types of reaction. The more successful applications have been to the substitution reactions of conjugated systems where relative reactivities are determined largely by changes of  $\pi$ -electron energy.

## Source:

PAC, 1994, 66, 1077 (Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)) on page 1159