
Contents

1	Introduction	1
2	Linear Combination of Atomic Orbitals	5
2.1	H ₂ and He ₂ – The Simplest Examples	6
2.2	The Effect of Electronegativity	8
2.3	<i>p</i> -Orbitals and π -Overlap	11
2.4	Combining AOs to Build MOs	13
2.4.1.	Methylene, CH ₂	14
2.5	The AH ₂ Walsh Diagram	19
3	Larger Molecules	23
3.1	Ethylene	25
3.2	Cyclopropane	29
3.3	π -Systems	33
3.3.1	Linear Systems	34
3.3.2	Cyclic Systems	35
3.4	Hyperconjugation	37
3.4.1	The Ethyl Cation	37
3.4.2	The Cyclopropylcarbinyl Cation	40
3.4.3	Negative Hyperconjugation	41
3.4.4	The Anomeric Effect	43
4	Reactions	45
4.1	Lewis Acid/Lewis Base Interactions	45
4.1.1	S _N 2 Reactions	46
4.2	Selectivity; Frontier MO Theory	48
4.2.1	Nucleophilic Oxirane Ring-Opening	48
4.3	The Woodward-Hoffmann Rules	49

4.3.1	Electrocyclic Reactions	51
4.3.2	Cycloadditions	58
4.3.3	Sigmatropic Rearrangements	63
5	Elementary Symmetry	67
5.1	Symmetry Elements	67
5.1.1	The Identity	67
5.1.2	Proper Rotation Axes, C_n	68
5.1.3	Mirror Planes, σ	70
5.1.4	Improper Rotation Axes, S_n	73
5.1.5	Inversion Centres, i	73
5.2	Point Groups	74
5.3	Irreducible Representations and Character Tables	75
5.4	Degenerate Orbitals	78
6	Glossary	81
7	List of Molecules	87
8	General Information – Installation – Use	95

<http://www.springer.com/978-3-540-63726-4>

The Chemist's Electronic Book of Orbitals

Clark, T.; Koch, R.

1999, VIII, 96 p. 132 illus. With online files/update.,

Softcover

ISBN: 978-3-540-63726-4