

Huckel m.o. coefficients: Use in HW problems #1,#2

From, **Quantum Chemistry**, by J. P. Lowe, Academic Press, San Diego pp.503-504.

Two Centers

Ethylene (alternant) C_2H_2



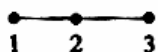
$$\text{all } q = 1.0, p_{12} = 1.0,$$

$$E_{\pi} = 2\alpha + 2\beta$$

n	x	c_1	c_2
2	-1.000	0.7071	0.7071

Three Centers

Allyl radical (alternant) C_3H_5



$$\text{all } q = 1.0, p_{12} = 0.707,$$

$$E_{\pi} = 3\alpha + 2.8284\beta$$

n	x	c_1	c_2	c_3
2	-1.4142	0.5000	0.7071	0.5000
1	0.0000	0.7071	0.0000	-0.7071

Cyclopropenyl radical (nonalternant) C_3H_3



$$\text{all } q = 1.0, p_{12} = 0.5,$$

$$E_{\pi} = 3\alpha + 3.0000\beta$$

n	x	c_1	c_2	c_3
2	-2.0000	0.5774	0.5774	0.5774
$\frac{1}{2}$	1.0000	-0.8165	0.4082	0.4082
$\frac{1}{2}$	1.0000	0.0000	0.7071	-0.7071

Four Centers

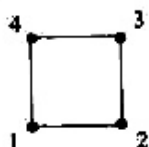
Butadiene (alternant) C_4H_6



$$\text{all } q = 1.0, p_{12} = 0.8944, p_{23} = 0.4472, \\ E_\pi = 4\alpha + 4.4721\beta$$

n	x	c_1	c_2	c_3	c_4
2	-1.6180	0.3718	0.6015	0.6015	0.3718
2	-0.6180	0.6015	0.3718	-0.3718	-0.6015

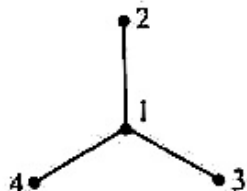
Cyclobutadiene (alternant) C_4H_4



$$\text{all } q = 1.0, p_{12} = 0.5, E_\pi = 4\alpha + 4.000\beta$$

n	x	c_1	c_2	c_3	c_4
2	-2.0000	0.5000	0.5000	0.5000	0.5000
2	0.0000	0.5000	0.5000	-0.5000	-0.5000

2-Allylmethyl (alternant) C_4H_6

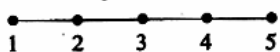


$$\text{all } q = 1.0, p_{12} = 0.5774, E_\pi = 4\alpha + 3.4641\beta,$$

n	x	c_1	c_2	c_3	c_4
2	-1.7320	0.7071	0.4082	0.4082	0.4082
1	0.0	0.0000	0.7071	-0.7071	0.0000
1	0.0	0.0000	0.4082	0.4082	-0.8165

Five Centers

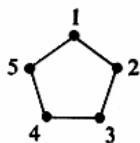
Pentadienyl radical (alternant) C_5H_7



$$\text{all } q = 1.0, p_{12} = 0.7887, p_{23} = 0.5774, \\ E_n = 5\alpha + 5.4641\beta$$

n	x	c_1	c_2	c_3	c_4	c_5
2	-1.7320	0.2887	0.5000	0.5774	0.5000	0.2887
2	-1.0000	0.5000	0.5000	0.0000	-0.5000	-0.5000
1	0.0000	0.5774	0.0000	-0.5774	0.0000	0.5774

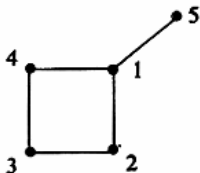
Cyclopentadienyl radical (nonalternant) C_5H_5



$$\text{all } q = 1.0, p_{12} = 0.5854, E_n = 5\alpha + 5.8541\beta$$

n	x	c_1	c_2	c_3	c_4	c_5
2	-2.0000	0.4472	0.4472	0.4472	0.4472	0.4472
$\frac{3}{2}$	-0.6180	0.6325	0.1954	-0.5117	-0.5117	0.1954
$\frac{3}{2}$	-0.6180	0.0000	-0.6015	-0.3718	0.3718	0.6015
0	1.6180	0.6325	-0.5117	0.1954	0.1954	-0.5117
0	1.6180	0.0000	0.3718	-0.6015	0.6015	-0.3718

Cyclobutadienylmethyl radical (alternant) C_5H_5



$$\text{all } q = 1.0, p_{12} = 0.3574, p_{23} = 0.6101, \\ p_{15} = 0.8628, E_n = 5\alpha + 5.5959\beta$$

n	x	c_1	c_2	c_3	c_4	c_5
2	-2.1358	0.5573	0.4647	0.4351	0.4647	0.2610
2	-0.6622	-0.4351	0.1845	0.5573	0.1845	-0.6572
1	0.0000	0.0000	-0.7071	0.0000	0.7071	0.0000