C9930, 6. přednáška, 7. 4. 2021

3. EHT: dokončení

Literatura: John P. Löwe, Quantum Chemistry

Kapitola 10

3. Rozšířená Hückelova metoda

3.1 Souřadnice jader (Lowe 10-1.A)

3.2 Báze pro MO-LCAO (Lowe 10-1.B)

3.3 Matice překryvu (Lowe 10-1.C)

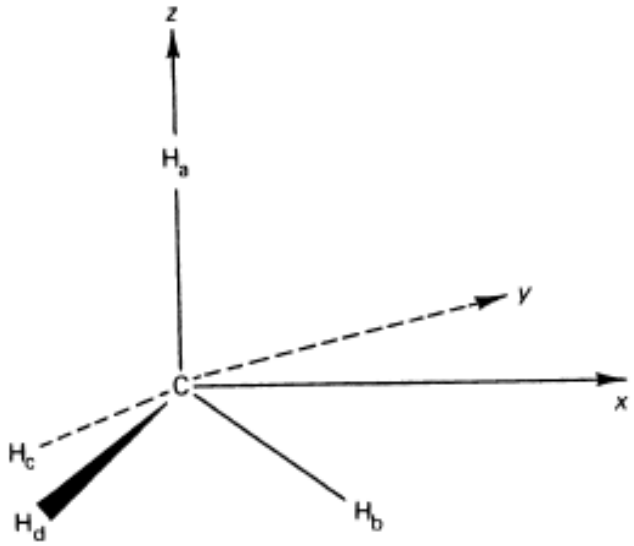


Figure 10-1 ▶ Orientation of methane in a Cartesian axis system.

TABLE 10-2 ▶ Basis AOs for Methane

AO no.	Atom	Type	n^a
1	C	2s	2
2	C	$2p_z$	2
3	C	$2p_x$	2
4	C	$2p_y$	2
5	H_a	1s	1
6	H_b	1s	1
7	H_c	1s	1
8	H_d	1s	1

TABLE 10-3 ▶ Overlap Matrix for STOs of Table 10-2

	1	2	3	4	5	6	7	8
1	1.0000	0.0	0.0	0.0	0.5133	0.5133	0.5133	0.5133
2	0.0	1.0000	0.0	0.0	0.4855	−0.1618	−0.1618	−0.1618
3	0.0	0.0	1.0000	0.0	0.0	0.4577	−0.2289	−0.2289
4	0.0	0.0	0.0	1.0000	0.0	0.0	0.3964	−0.3964
5	0.5133	0.4855	0.0	0.0	1.0000	0.1805	0.1805	0.1805
6	0.5133	−0.1618	0.4577	0.0	0.1805	1.0000	0.1805	0.1805
7	0.5133	−0.1618	−0.2289	0.3964	0.1805	0.1805	1.0000	0.1805
8	0.5133	−0.1618	−0.2289	−0.3964	0.1805	0.1805	0.1805	1.000

3.2 Báze pro MO-LCAO (Lowe 10-1.B)

3.3 Matice překryvu (Lowe 10-1.C)

3.4 Matice Hamiltoniánu (Lowe 10-1.D)

TABLE 10-4 ► The Extended Hückel Hamiltonian Matrix for CH_4[a]

	1	2	3	4	5	6	7	8
1	−0.7144	0.0	0.0	0.0	−0.5454	−0.5454	−0.5454	−0.5454
2	0.0	−0.3921	0.0	0.0	−0.3790	0.1263	0.1263	0.1263
3	0.0	0.0	−0.3921	0.0	0.0	−0.3573	0.1787	0.1787
4	0.0	0.0	0.0	−0.3921	0.0	0.0	−0.3094	0.3094
5	−0.5454	−0.3790	0.0	0.0	−0.5000	−0.1579	−0.1579	−0.1579
6	−0.5454	0.1263	−0.3573	0.0	−0.1579	−0.5000	−0.1579	−0.1579
7	−0.5454	0.1263	0.1787	−0.3094	−0.1579	−0.1579	−0.5000	−0.1579
8	−0.5454	0.1263	0.1787	0.3094	−0.1579	−0.1579	−0.1579	−0.5000

[a] All energies in a.u.

3.3 Matice překryvu (Lowe 10-1.C)

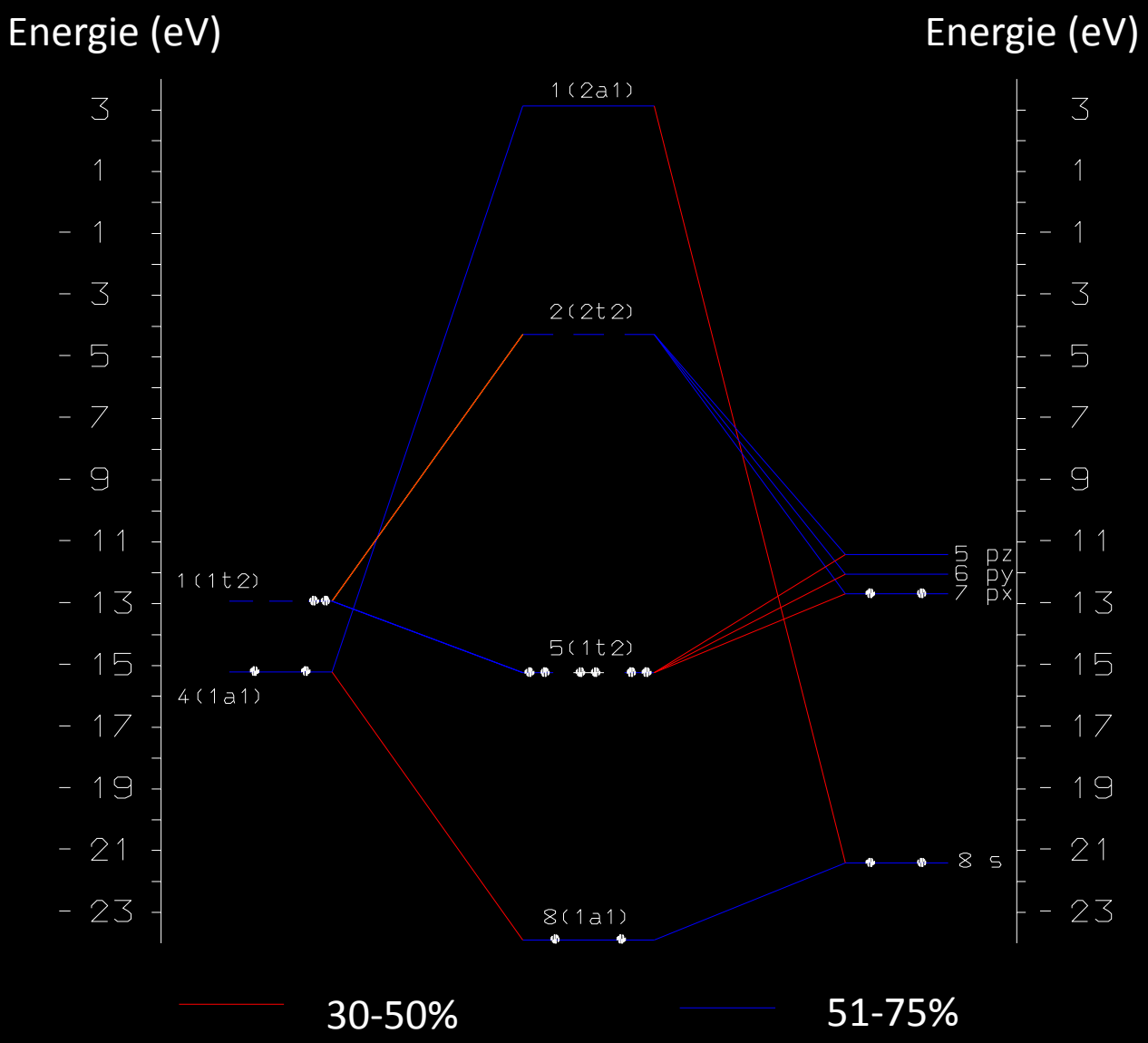
3.4 Matice Hamiltoniánu (Lowe 10-1.D)

3.5 Vlastní funcke a vektory (Lowe 10-1.E)

TABLE 10-5 ▶ Energies for Methane by the Extended Hückel Method

MO no.	Energy (a.u.)	Occ. no.
8	1.1904	0
7	0.2068	0
6	0.2068	0
5	0.2068	0
4	−0.5487	2
3	−0.5487	2
2	−0.5487	2
1	−0.8519	2

Interakční diagram molekuly CH_4 vypočtený programem C.A.C.A.O.*



* (Computer Aided Composition of Atomic Orbitals) . The package consists of an EHC program (SIMCON), an orbital analysis program (MOAN) and a display program for atomic orbitals (CACAO). Davide M. Proserpio, Universita di Milano.