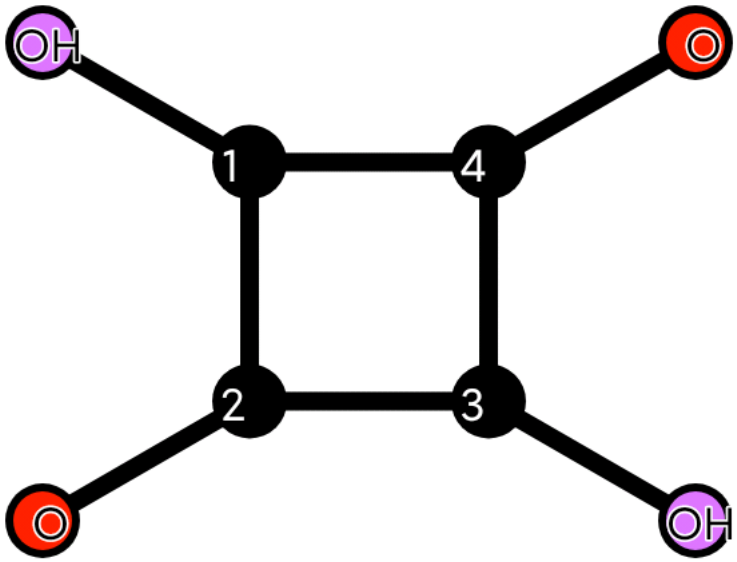
Print calculated values

Report generated by:root, 18.02.2020 - 15:28:29

The following determinant is calculated:

-x	1.0	0.0	1.0	0.0	0.0	0.0	0.9
1.0	-x	1.0	0.0	0.0	1.93	0.0	0.0
0.0	1.0	-x	1.0	0.0	0.0	0.9	0.0
1.0	0.0	1.0	-x	1.93	0.0	0.0	0.0
0.0	0.0	0.0	1.93	-x+1.18	0.0	0.0	0.0
0.0	1.93	0.0	0.0	0.0	-x+1.18	0.0	0.0
0.0	0.0	0.9	0.0	0.0	0.0	-x+2.0	0.0
0.9	0.0	0.0	0.0	0.0	0.0	0.0	-x+2.0

It is about this molecule:

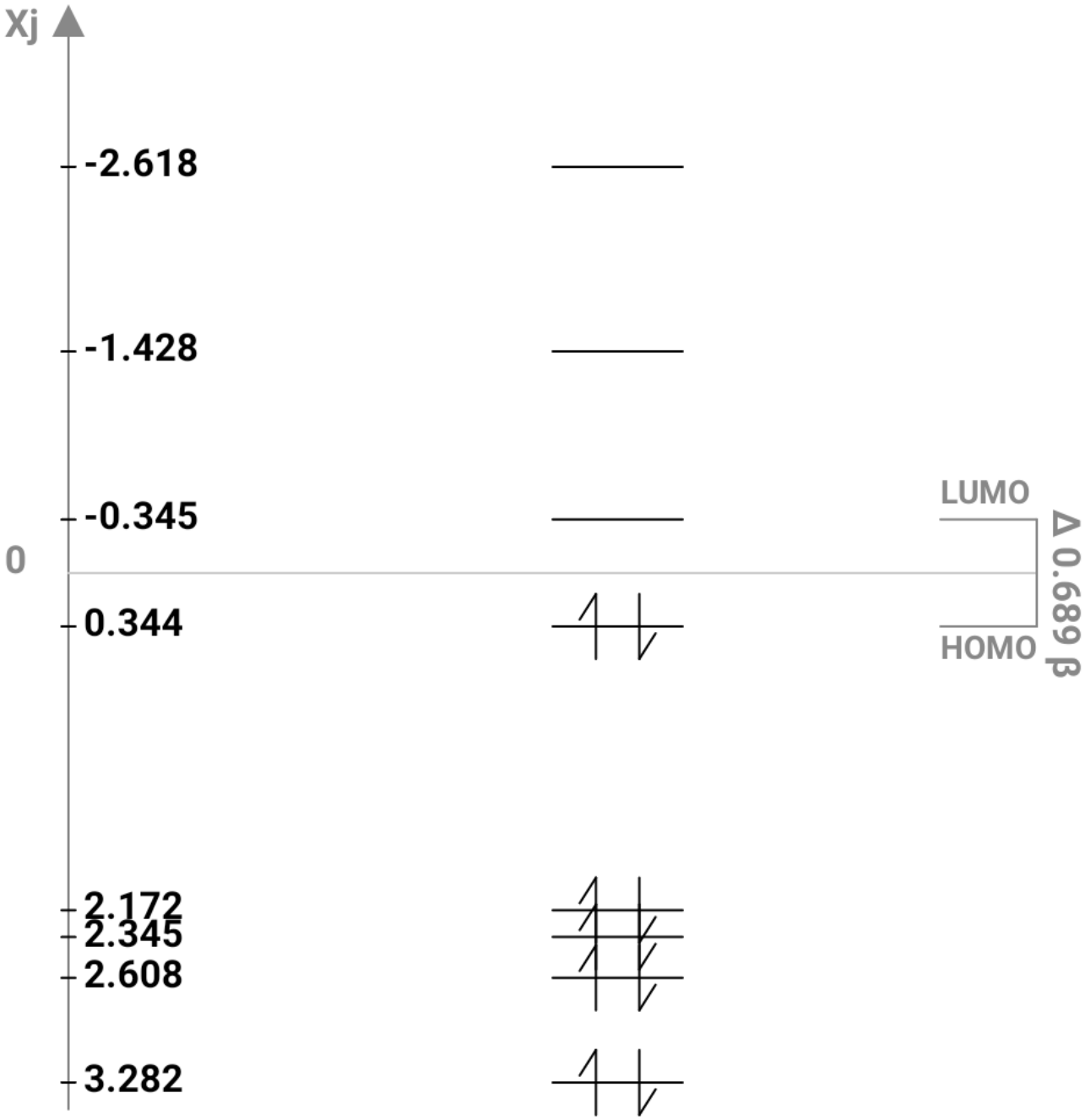


HMO-Energies

x1 = 3.282; x2 = 2.608; x3 = 2.345; x4 = 2.172; x5 = 0.344; x6 = -0.345; x7 = -1.428; x8 = -2.618;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 8α + 21.502β -

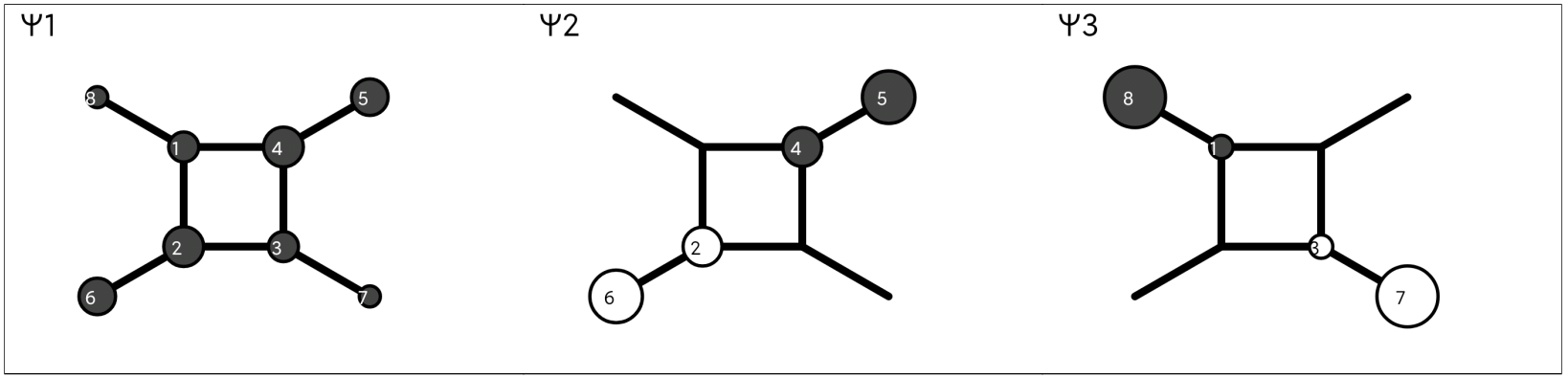
this corresponds to one πelectron: 2.15β

2. Hueckel-coefficient

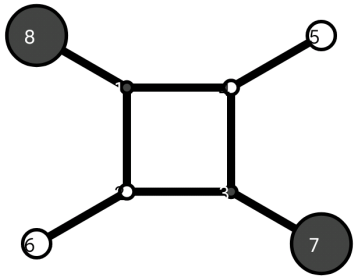
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8
	x1= 3.282	x2= 2.608	x3= 2.345	x4= 2.172	x5= 0.344	x6= -0.345	x7= -1.428	x8= -2.618
1	-0.325	0.0	-0.253	-0.118	0.457	-0.66	0.0	0.414
2	-0.431	0.421	0.0	0.149	0.19	0.0	-0.568	-0.506
3	-0.325	0.0	0.253	-0.118	0.457	0.66	0.0	0.414
4	-0.431	-0.421	0.0	0.149	0.19	0.0	0.568	-0.506
5	-0.396	-0.568	0.0	0.29	-0.44	0.0	-0.421	0.257
6	-0.396	0.568	0.0	0.29	-0.44	0.0	0.421	0.257
7	-0.228	0.0	0.66	-0.616	-0.248	-0.253	0.0	-0.081
8	-0.228	0.0	-0.66	-0.616	-0.248	0.253	0.0	-0.081

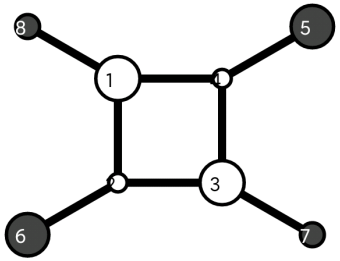
2.2. Molecule orbital presentation:



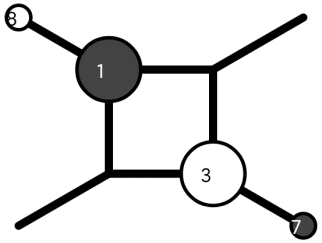
Ψ4



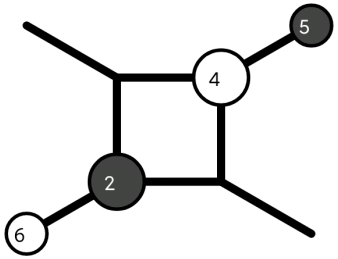
Ψ5



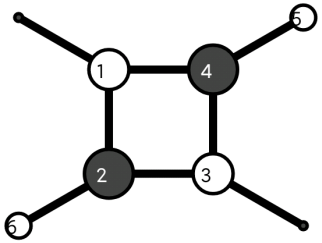
Ψ6



Ψ7



Ψ8

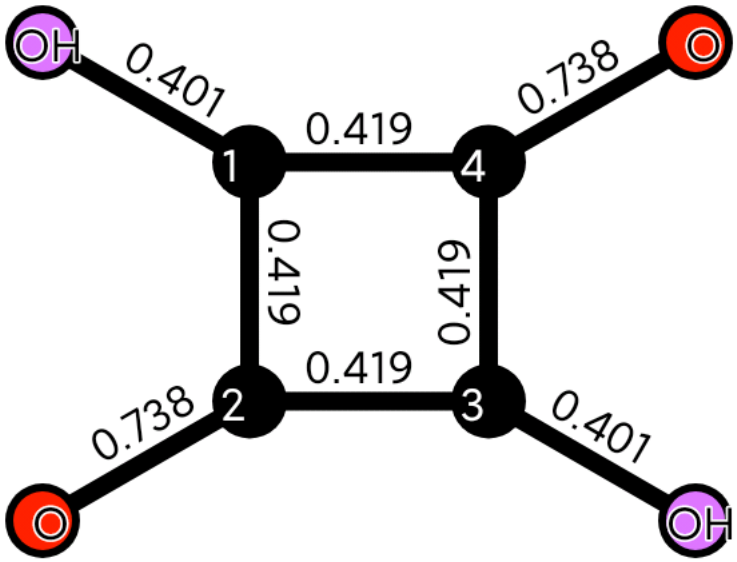


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.785							
2	0.419	0.842						
3	0.529	0.419	0.785					
4	0.419	0.134	0.419	0.842				
5	-0.213	-0.218	-0.213	0.738	1.514			
6	-0.213	0.738	-0.213	-0.218	0.222	1.514		
7	-0.268	-0.082	0.401	-0.082	0.041	0.041	1.859	
8	0.401	-0.082	-0.268	-0.082	0.041	0.041	0.115	1.859

3.2. Presentation of bond order:

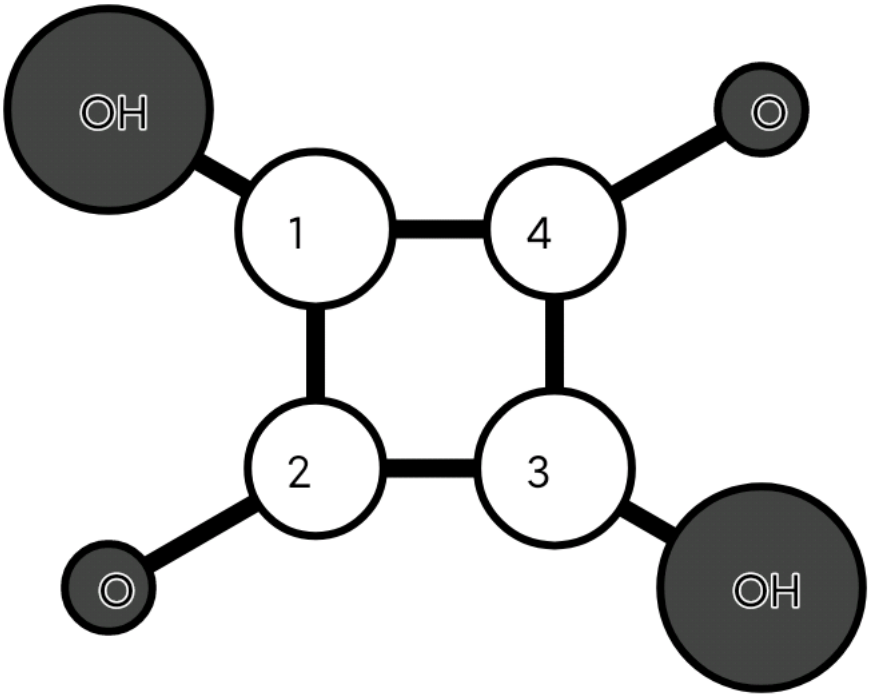


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.465							
2		0.408						
3			0.465					
4				0.408				
5					-0.264			
6						-0.264		
7							-0.609	
8								-0.609

4.2. Presentation of molecule:

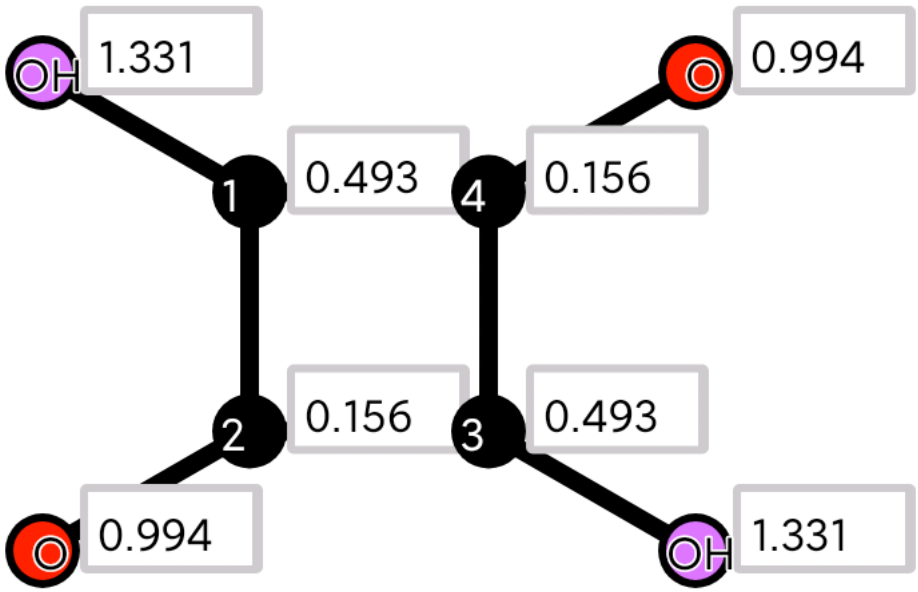


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8
0.493	0.156	0.493	0.156	0.994	0.994	1.331	1.331

5.2. Presentation of molecule:

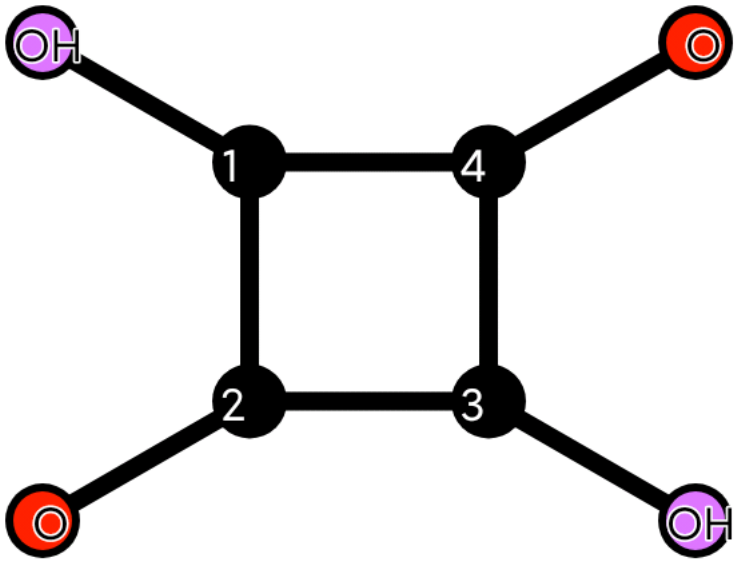


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8
1	0.702							
2	-0.041	0.226						
3	-0.493	-0.041	0.702					
4	-0.041	-0.014	-0.041	0.226				
5	-0.023	-0.037	-0.023	-0.086	0.219			
6	-0.023	-0.086	-0.023	-0.037	-0.048	0.219		
7	-0.113	-0.003	0.033	-0.003	-0.001	-0.001	0.112	
8	0.033	-0.003	-0.113	-0.003	-0.001	-0.001	-0.023	0.112

6.2. Presentation of molecule:

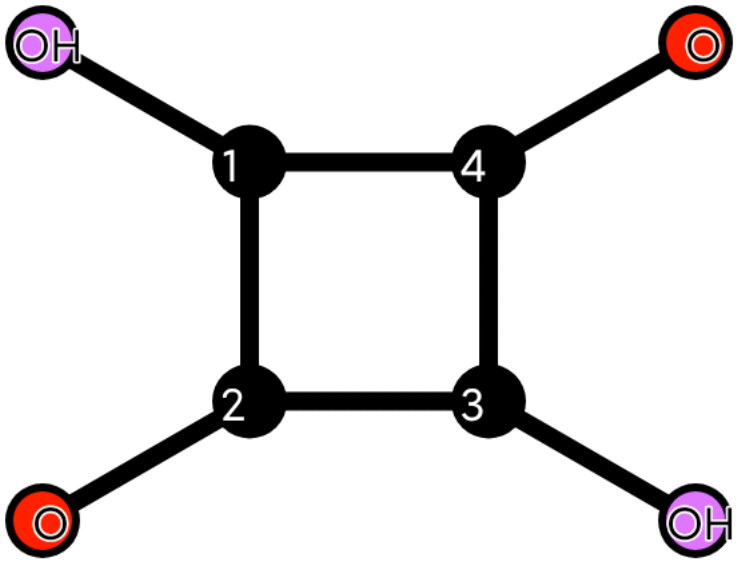


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8
1 2	0.111	0.039	-0.154	-0.029	-0.04	0.071	-0.028	0.029
1 4	0.111	-0.029	-0.154	0.039	0.071	-0.04	-0.028	0.029
1 8	-0.166	0.012	0.239	0.012	0.005	0.005	0.052	-0.159
2 3	-0.154	0.039	0.111	-0.029	-0.04	0.071	0.029	-0.028
2 6	0.033	-0.007	0.033	0.026	0.044	-0.133	0.002	0.002
3 4	-0.154	-0.029	0.111	0.039	0.071	-0.04	0.029	-0.028
3 7	0.239	0.012	-0.166	0.012	0.005	0.005	-0.159	0.052
4 5	0.033	0.026	0.033	-0.007	-0.133	0.044	0.002	0.002

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 4	1 8	2 3	2 6	3 4	3 7	4 5
1 2	0.295							
1 4	-0.041	0.295						
1 8	-0.132	-0.132	0.511					
2 3	-0.041	-0.124	0.136	0.295				
2 6	-0.143	0.075	-0.017	-0.143	0.21			
3 4	-0.124	-0.041	0.136	-0.041	0.075	0.295		
3 7	0.136	0.136	-0.226	-0.132	-0.017	-0.132	0.511	
4 5	0.075	-0.143	-0.017	0.075	-0.074	-0.143	-0.017	0.21

8.2. Presentation of molecule: