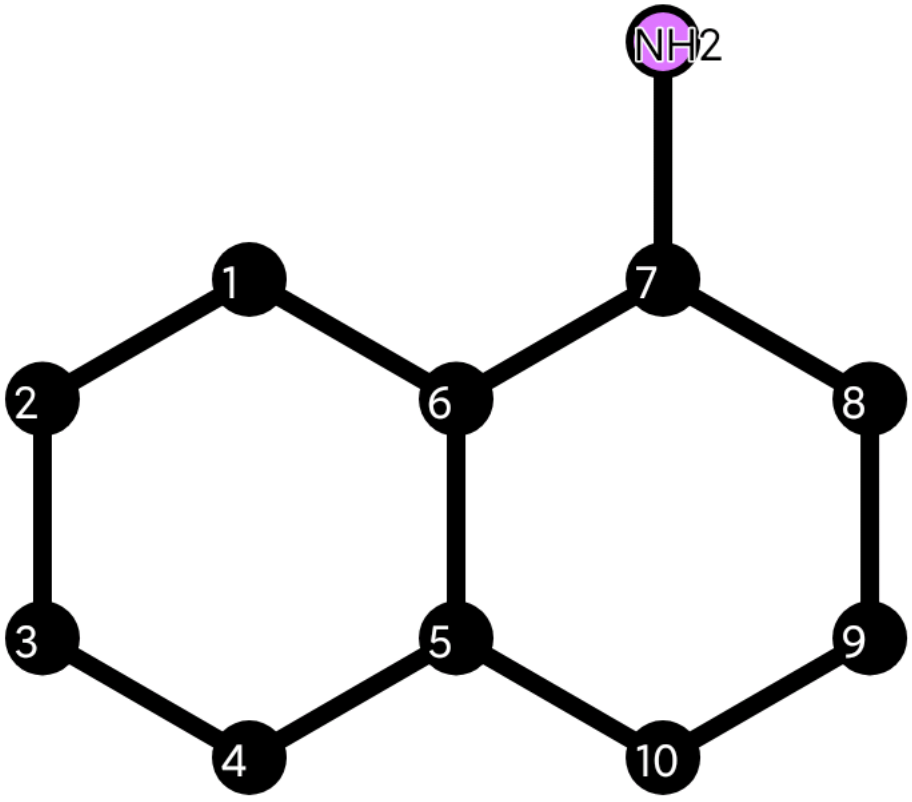
Print calculated values

Report generated by:root, 18.02.2020 - 12:04:51

The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	1.0	0.0
1.0	0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0	1.3
0.0	0.0	0.0	0.0	0.0	0.0	1.0	-x	1.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	-x	1.0	0.0
0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	-x	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	-x+1.47

It is about this molecule:

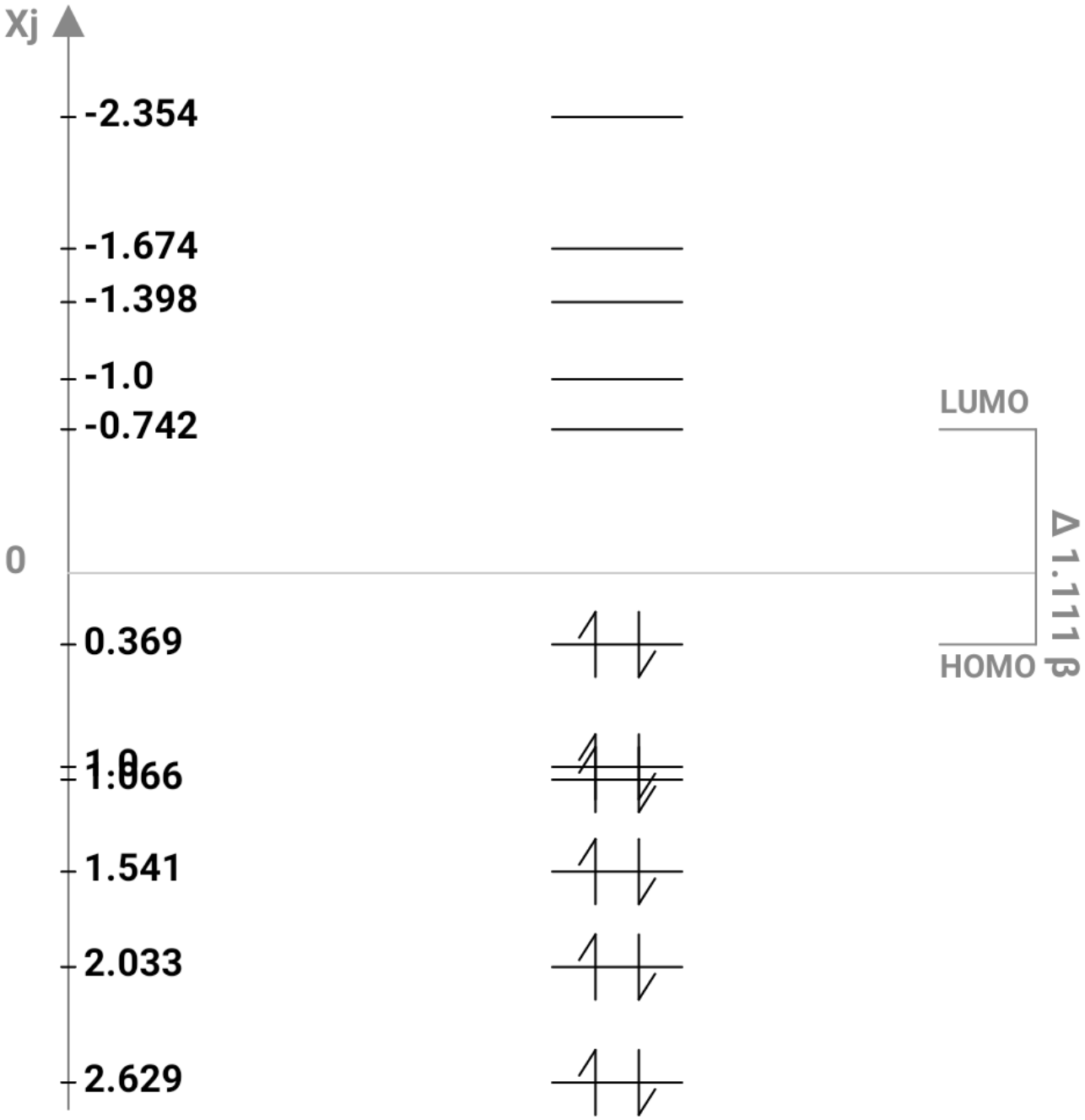


HMO-Energies

x1 = 2.629; x2 = 2.033; x3 = 1.541; x4 = 1.066; x5 = 1.0; x6 = 0.369; x7 = -0.742; x8 = -1.0;
x9 = -1.398; x10 = -1.674; x11 = -2.354;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 17.276β -

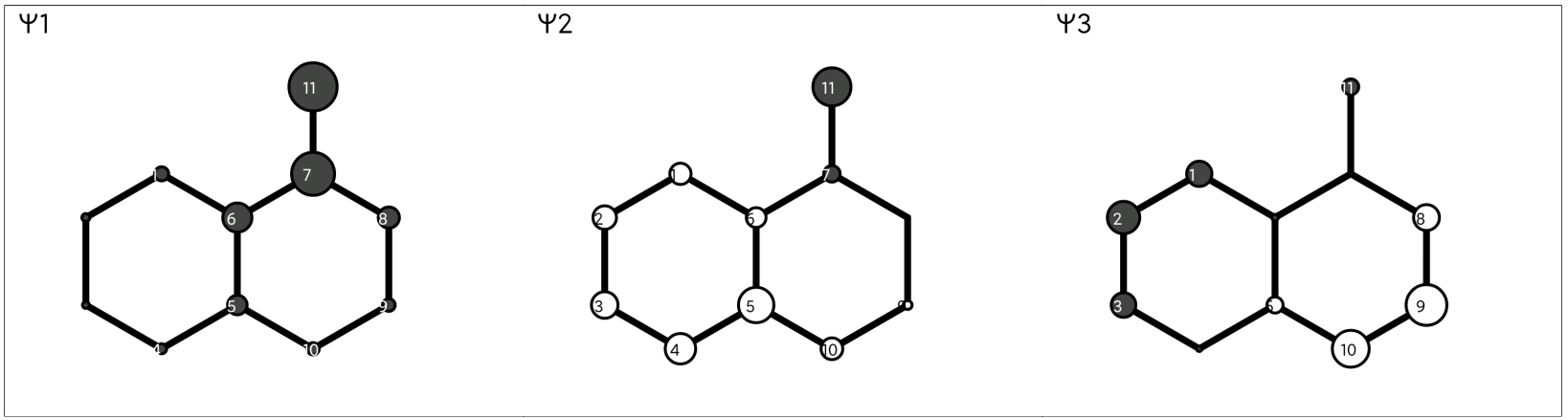
this corresponds to one πelectron: 1.44β

2. Hueckel-coefficient

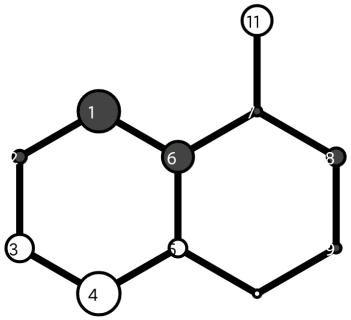
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 2.629	x2= 2.033	x3= 1.541	x4= 1.066	x5= 1.0	x6= 0.369	x7= -0.742	x8= -1.0	x9= -1.398	x10= -1.674	x11= -2.354
1	-0.174	0.262	-0.312	-0.489	0.0	-0.237	0.49	0.0	0.364	0.232	-0.286
2	-0.098	0.29	-0.4	-0.155	-0.408	-0.264	-0.24	0.408	-0.237	-0.403	0.208
3	-0.085	0.327	-0.304	0.324	-0.408	0.139	-0.312	-0.408	-0.032	0.443	-0.203
4	-0.124	0.376	-0.069	0.501	0.0	0.315	0.471	0.0	0.282	-0.338	0.27
5	-0.242	0.437	0.198	0.209	0.408	-0.023	-0.038	0.408	-0.362	0.124	-0.432
6	-0.36	0.244	-0.081	-0.366	0.408	0.177	-0.124	-0.408	-0.271	0.015	0.466
7	-0.53	-0.204	-0.011	-0.11	0.0	0.325	-0.361	0.0	0.377	-0.38	-0.379
8	-0.261	-0.047	0.319	-0.211	-0.408	0.441	0.116	0.408	-0.034	0.417	0.258
9	-0.157	0.109	0.502	-0.115	-0.408	-0.162	0.275	-0.408	-0.33	-0.319	-0.229
10	-0.152	0.268	0.455	0.089	0.0	-0.501	-0.32	0.0	0.495	0.117	0.281
11	-0.594	-0.47	-0.196	0.354	0.0	-0.383	0.212	0.0	-0.171	0.157	0.129

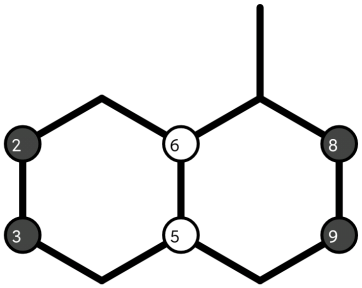
2.2. Molecule orbital presentation:



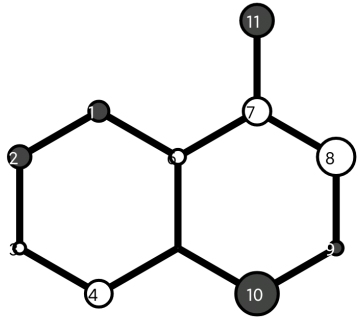
Ψ4



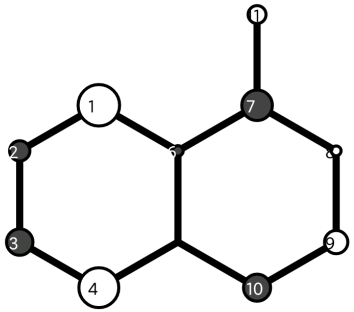
Ψ5



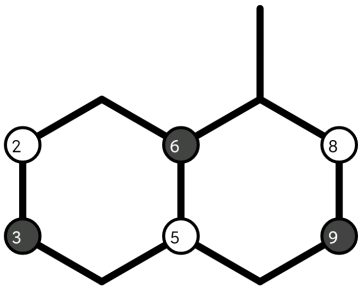
Ψ6



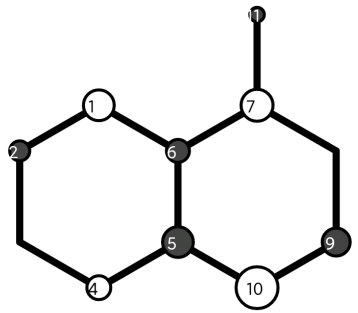
Ψ7



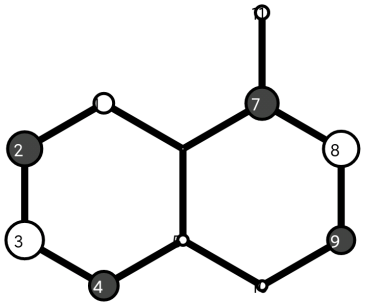
Ψ8



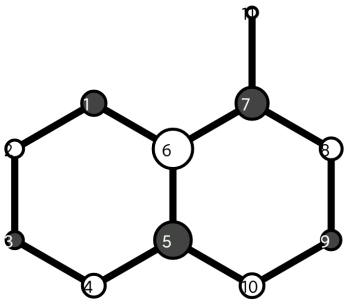
Ψ9



Ψ10



Ψ11

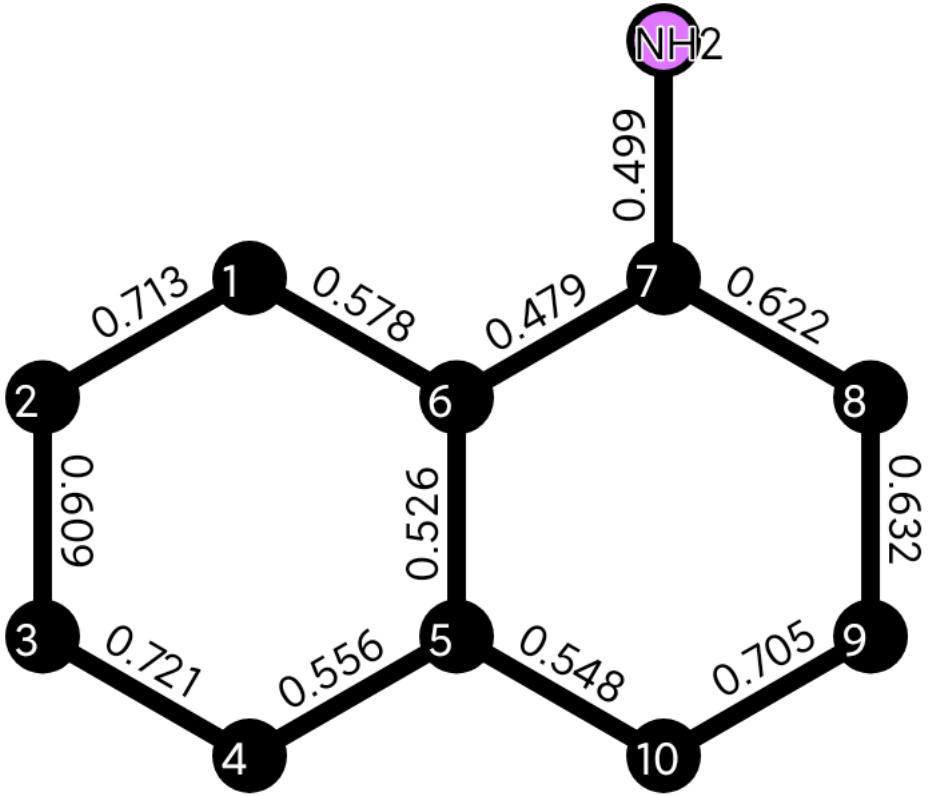


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.984										
2	0.713	1.029									
3	0.008	0.609	0.996								
4	-0.356	-0.025	0.721	1.023							
5	-0.004	-0.244	0.002	0.556	0.998						
6	0.578	-0.036	-0.252	0.028	0.526	1.055					
7	0.039	-0.143	-0.018	0.074	0.013	0.479	0.88				
8	-0.135	-0.065	0.139	0.053	-0.23	0.091	0.622	1.156			
9	-0.013	0.147	0.006	-0.165	-0.004	-0.222	0.031	0.632	0.99		
10	0.06	0.059	-0.157	-0.05	0.548	-0.076	-0.303	-0.134	0.705	1.121	
11	-0.083	0.094	0.035	-0.067	-0.036	-0.165	0.499	-0.258	-0.07	0.196	1.769

3.2. Presentation of bond order:

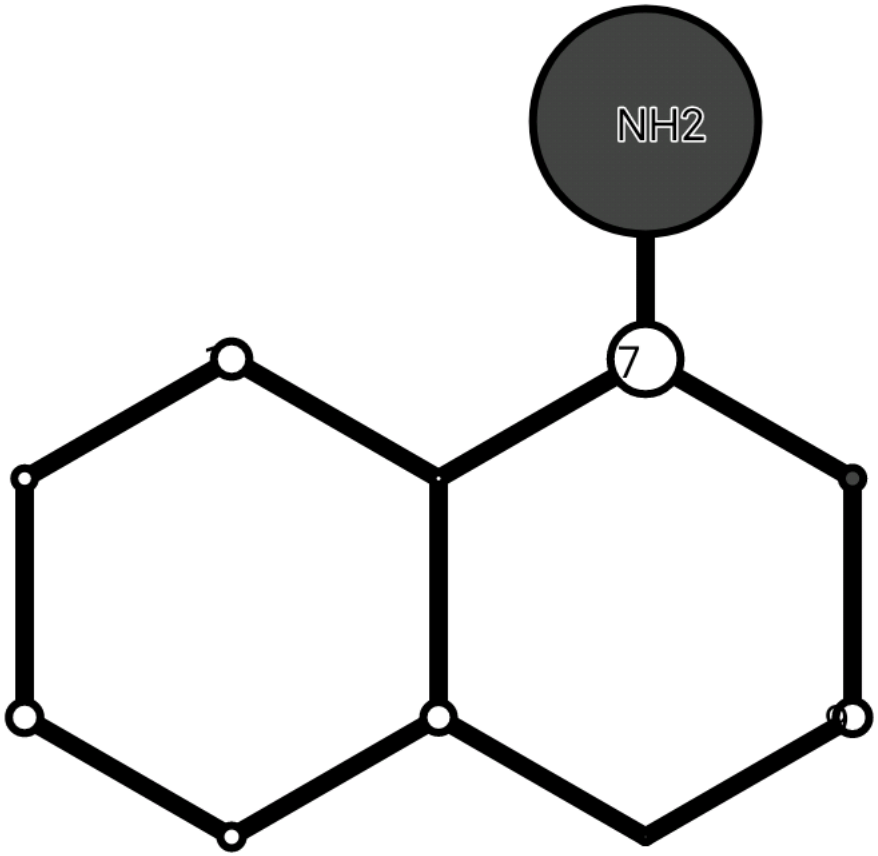

NH2
0.499
0.713
1
0.578
0.479
7
0.622
2
6
8
0.609
0.526
0.632
3
0.721
0.556
5
0.548
0.705
9
4
10

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.107										
2		0.062									
3			0.095								
4				0.068							
5					0.092						
6						0.036					
7							0.211				
8								-0.065			
9									0.101		
10										-0.03	
11											-0.678

4.2. Presentation of molecule:

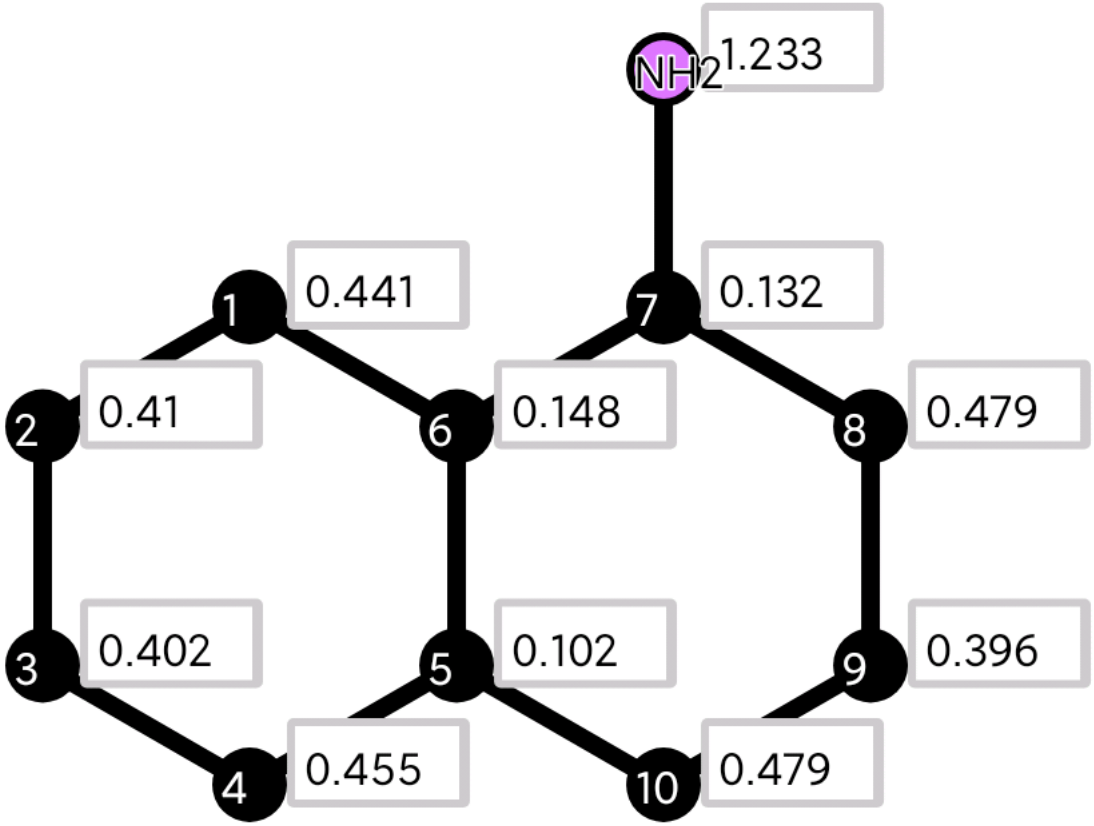

NH2
7

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.441	0.41	0.402	0.455	0.102	0.148	0.132	0.479	0.396	0.479	1.233

5.2. Presentation of molecule:

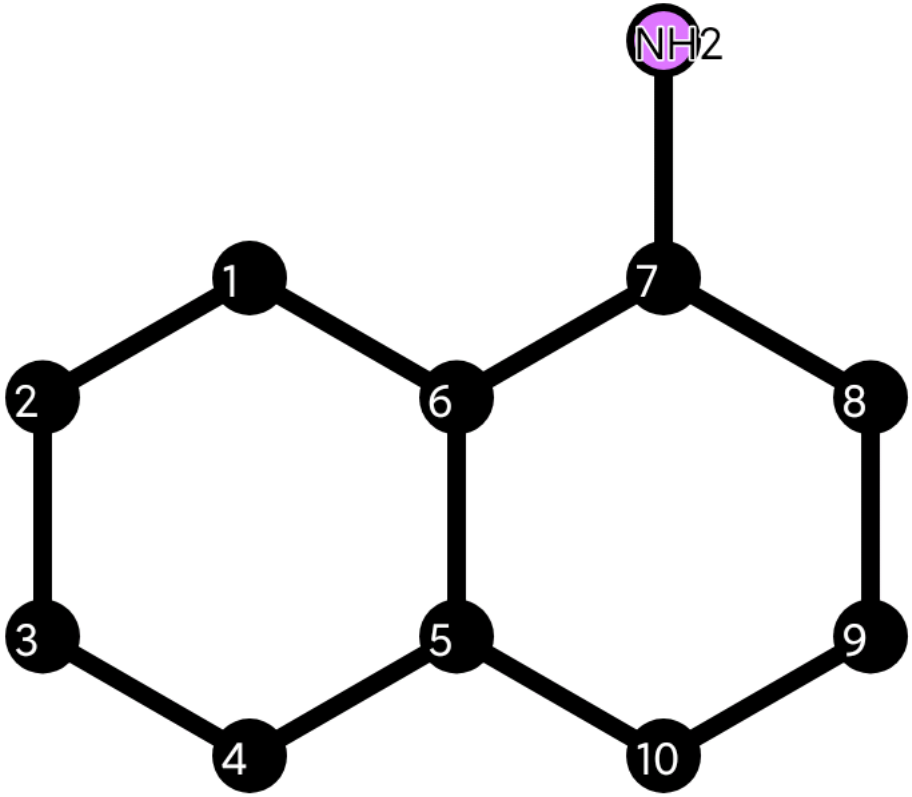

NH2
1.233
1
0.441
7
0.132
2
0.41
6
0.148
8
0.479
3
0.402
5
0.102
9
0.396
4
0.455
10
0.479

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.431										
2	-0.202	0.409									
3	0.016	-0.113	0.403								
4	-0.133	0.018	-0.209	0.445							
5	0.004	-0.05	0.007	-0.09	0.329						
6	-0.1	0.008	-0.053	0.001	-0.08	0.348					
7	0.015	-0.023	0.004	-0.018	0.002	-0.057	0.326				
8	-0.02	-0.008	-0.026	0.002	-0.045	-0.011	-0.143	0.426			
9	0.004	-0.029	0.0	-0.03	0.008	-0.041	0.01	-0.125	0.398		
10	-0.016	0.003	-0.027	0.025	-0.085	-0.002	-0.099	0.0	-0.195	0.447	
11	0.002	-0.012	0.001	-0.011	0.0	-0.012	-0.015	-0.05	0.001	-0.05	0.149

6.2. Presentation of molecule:

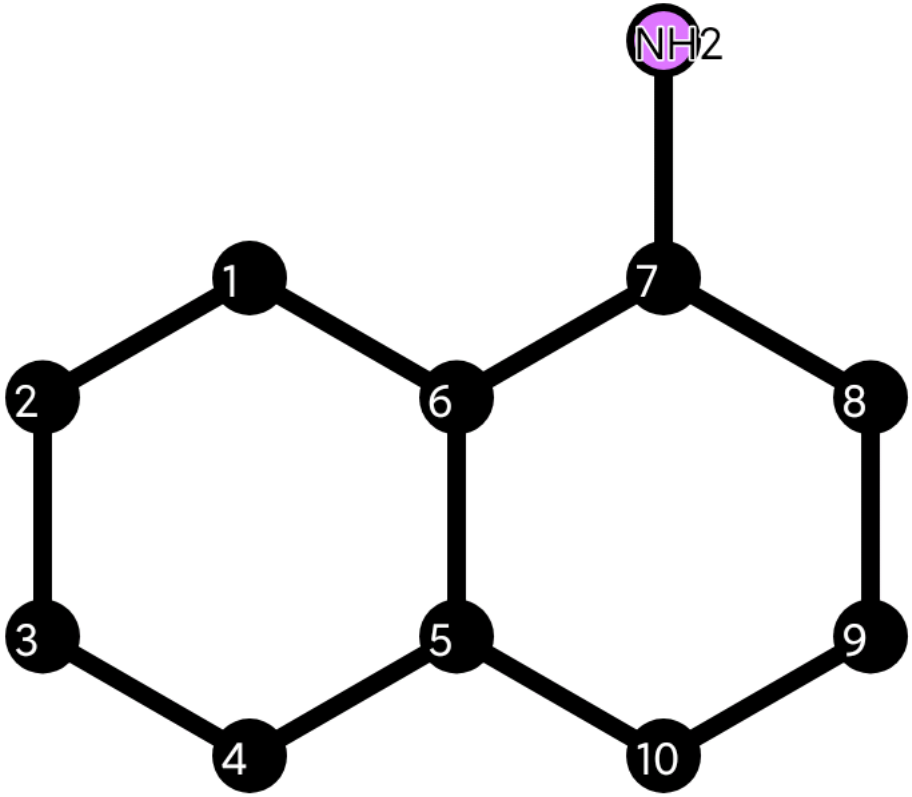

NH2
1
2
3
4
5
6
7
8
9
10

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	0.012	-0.012	-0.002	-0.013	-0.001	0.014	0.009	-0.012	0.003	-0.008	0.009
1 6	-0.005	0.018	0.0	0.016	0.001	-0.024	-0.015	0.017	-0.004	0.011	-0.016
2 3	-0.006	-0.012	-0.001	0.014	0.0	-0.012	-0.005	0.015	-0.001	0.013	-0.005
3 4	0.004	0.01	0.003	-0.012	0.0	0.009	0.003	-0.012	0.001	-0.01	0.003
4 5	-0.001	-0.008	-0.001	-0.008	0.0	-0.009	-0.001	0.015	0.0	0.014	-0.001
5 6	0.002	-0.011	0.0	-0.009	-0.002	-0.017	-0.005	0.023	0.001	0.022	-0.005
5 10	-0.001	0.018	0.001	0.017	0.002	0.023	0.005	-0.036	-0.001	-0.034	0.005
6 7	-0.007	-0.005	-0.003	-0.007	-0.002	0.006	0.04	-0.042	0.007	-0.027	0.041
7 8	0.01	-0.013	0.004	-0.01	0.002	-0.024	0.058	-0.033	-0.006	-0.048	0.061
7 11	-0.007	0.017	-0.002	0.015	-0.001	0.029	-0.056	0.088	-0.004	0.072	-0.151
8 9	-0.005	0.016	-0.001	0.014	0.0	0.022	-0.019	-0.068	-0.006	0.067	-0.02
9 10	0.004	-0.014	0.001	-0.012	0.0	-0.018	0.014	0.055	0.011	-0.057	0.015

7.2. Presentation of molecule:

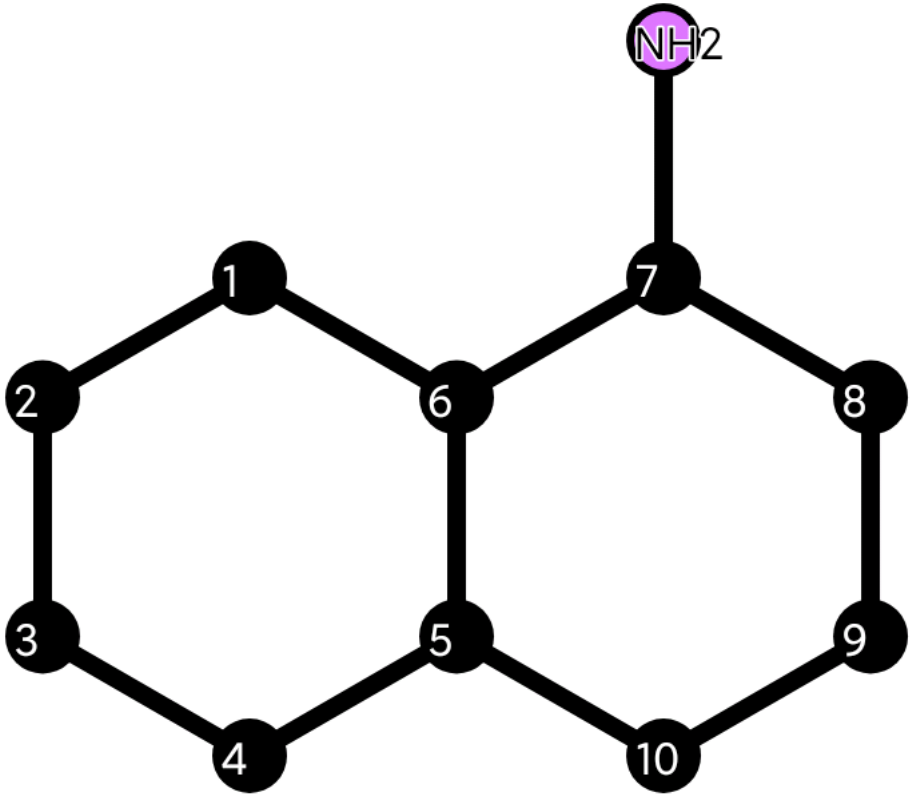

NH2
1
2
3
4
5
6
7
8
9
10

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	2 3	3 4	4 5	5 6	5 10	6 7	7 8	7 11	8 9	9 10
1 2	0.219											
1 6	-0.194	0.289										
2 3	-0.208	0.115	0.294									
3 4	0.125	-0.078	-0.212	0.213								
4 5	-0.072	0.096	0.112	-0.18	0.288							
5 6	0.072	-0.119	-0.043	0.068	-0.109	0.26						
5 10	0.018	-0.018	-0.044	0.057	-0.146	-0.118	0.302					
6 7	0.057	-0.131	-0.042	0.025	-0.024	-0.093	0.085	0.289				
7 8	-0.015	0.029	0.021	-0.014	0.021	0.049	-0.058	-0.102	0.26			
7 11	-0.02	0.038	0.011	-0.007	0.002	0.012	-0.011	-0.115	-0.16	0.353		
8 9	0.021	-0.029	-0.027	0.028	-0.044	-0.04	0.108	0.077	-0.197	0.047	0.306	
9 10	-0.012	0.014	0.028	-0.029	0.059	0.063	-0.178	-0.051	0.123	-0.034	-0.234	0.239

8.2. Presentation of molecule:


NH2
1
2
3
4
5
6
7
8
9
10