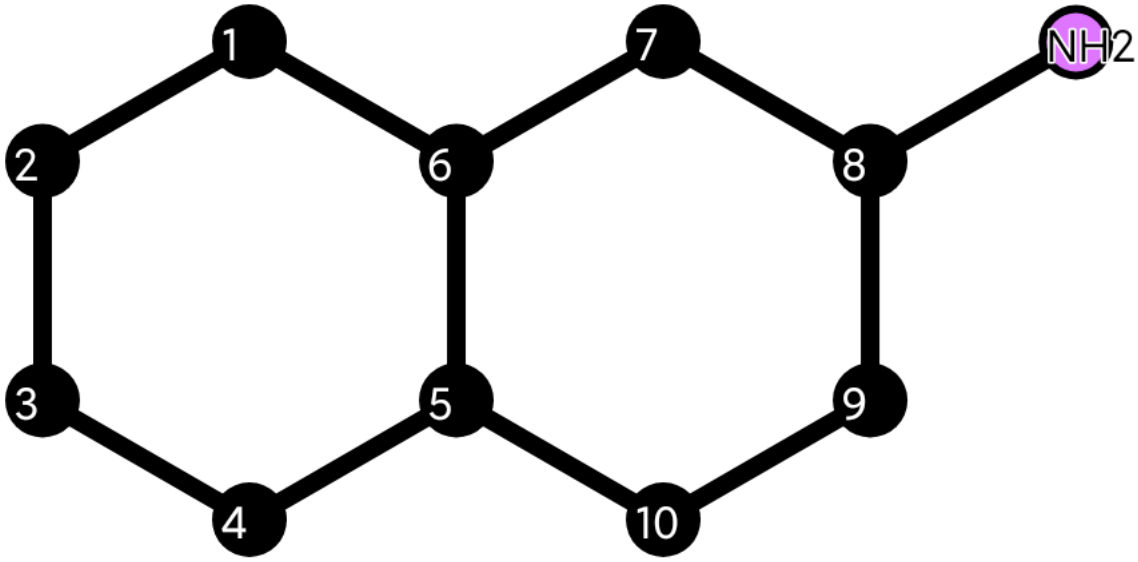
Print calculated values

Report generated by:root, 18.02.2020 - 12:03:43

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

It is about this molecule:

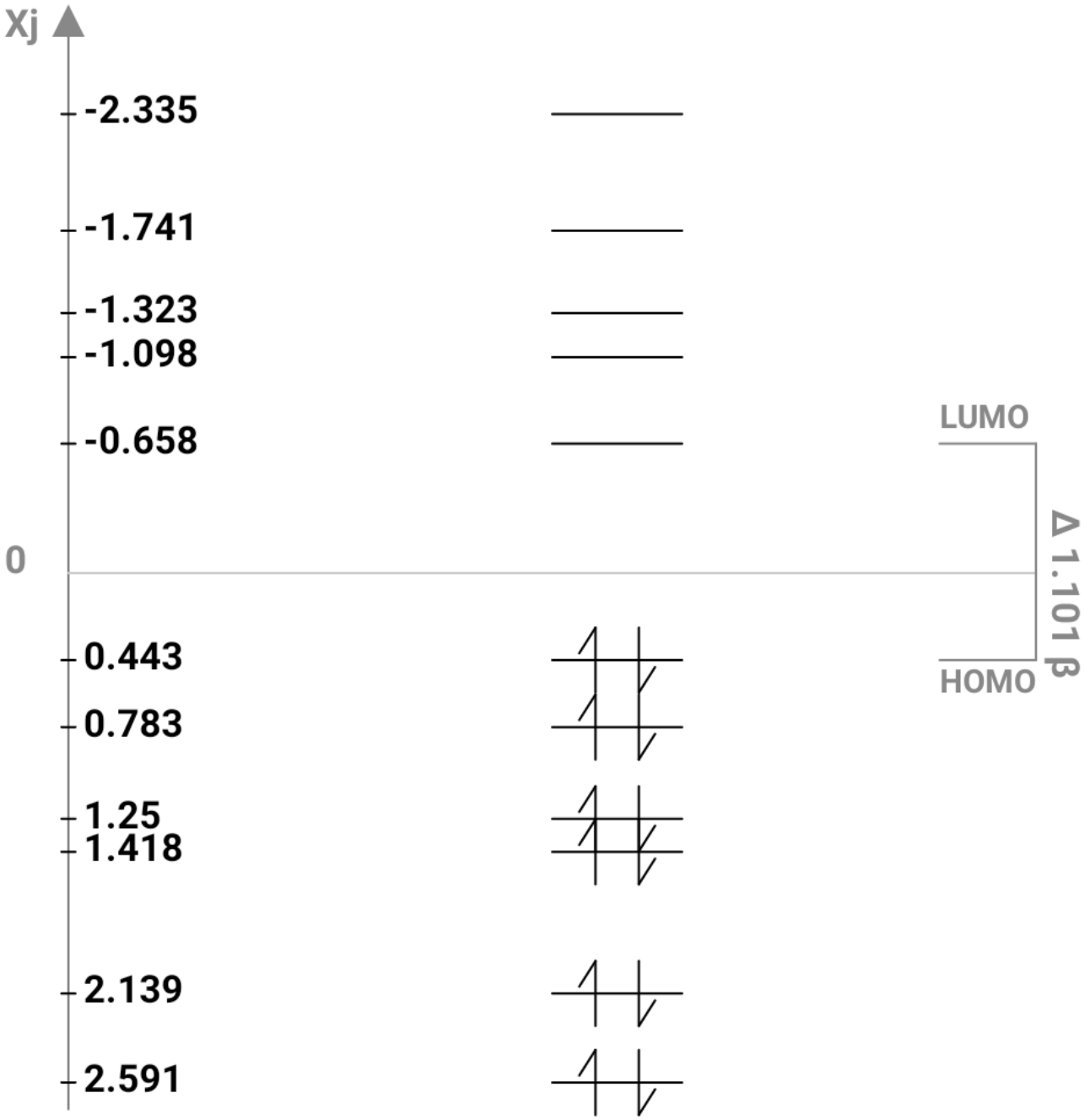


HMO-Energies

x1 = 2.591; x2 = 2.139; x3 = 1.418; x4 = 1.25; x5 = 0.783; x6 = 0.443; x7 = -0.658; x8 = -1.098; x9 = -1.323; x10 = -1.741; x11 = -2.335;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 11α + 17.248β -

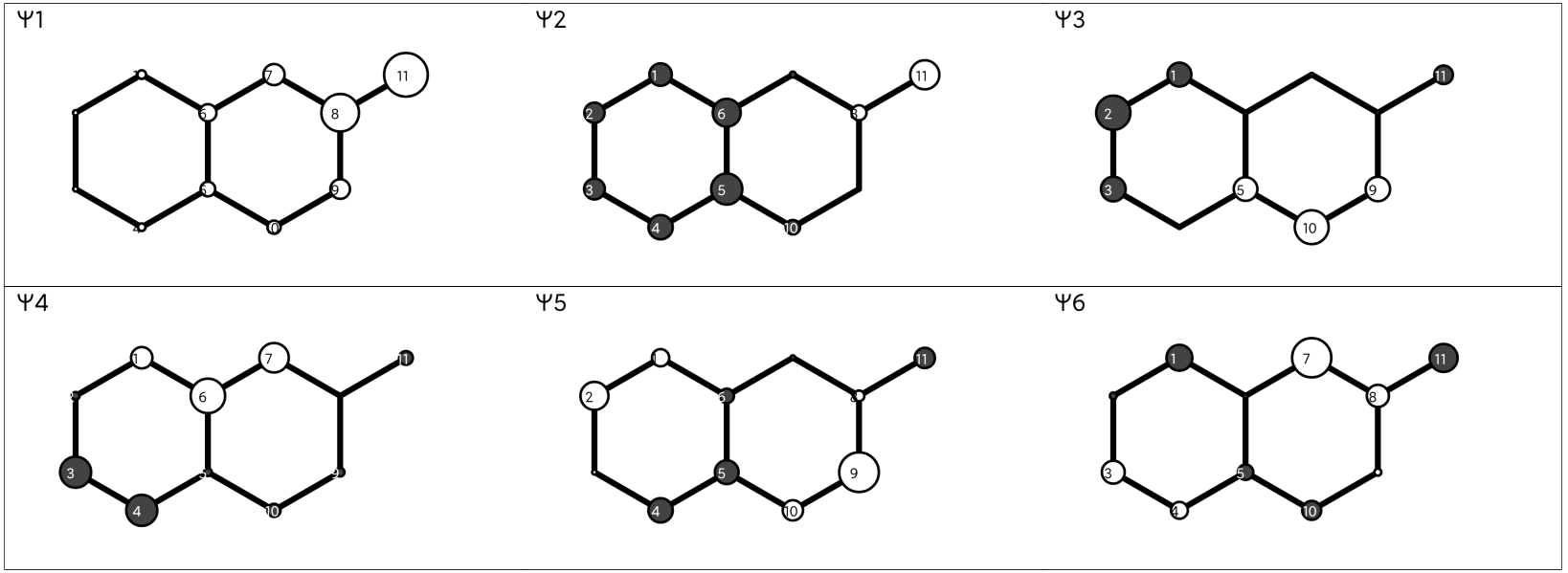
this corresponds to one πelectron: 1.437β

2. Hueckel-coefficient

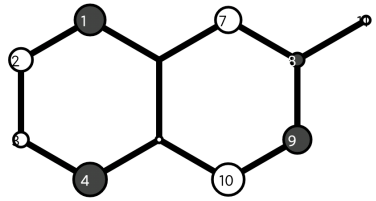
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11
	x1= 2.591	x2= 2.139	x3= 1.418	x4= 1.25	x5= 0.783	x6= 0.443	x7= -0.658	x8= -1.098	x9= -1.323	x10= -1.741	x11= -2.335
1	0.122	-0.318	-0.338	0.302	0.244	-0.366	-0.407	-0.08	0.41	0.256	-0.281
2	0.074	-0.286	-0.484	-0.11	0.396	-0.095	0.311	-0.386	-0.278	-0.366	0.209
3	0.07	-0.294	-0.349	-0.439	0.066	0.324	0.203	0.504	-0.043	0.381	-0.208
4	0.107	-0.343	-0.01	-0.439	-0.344	0.239	-0.444	-0.168	0.335	-0.297	0.276
5	0.207	-0.44	0.334	-0.11	-0.336	-0.218	0.09	-0.32	-0.4	0.136	-0.437
6	0.242	-0.394	0.005	0.487	-0.205	-0.067	-0.043	0.474	-0.265	-0.08	0.446
7	0.298	-0.085	0.011	0.416	-0.069	0.554	0.346	-0.12	0.34	-0.253	-0.323
8	0.531	0.212	0.01	0.033	0.152	0.312	-0.185	-0.342	-0.184	0.521	0.308
9	0.277	0.004	0.345	-0.122	0.56	0.099	-0.372	0.271	-0.208	-0.379	-0.26
10	0.187	-0.204	0.479	-0.185	0.287	-0.269	0.429	0.045	0.459	0.139	0.299
11	0.616	0.411	-0.263	-0.195	-0.287	-0.396	0.113	0.173	0.086	-0.211	-0.105

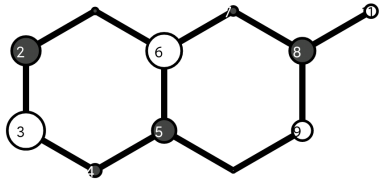
2.2. Molecule orbital presentation:



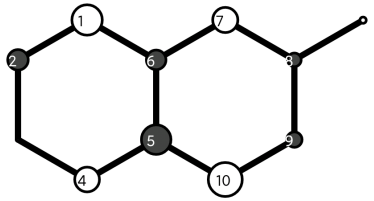
Ψ7



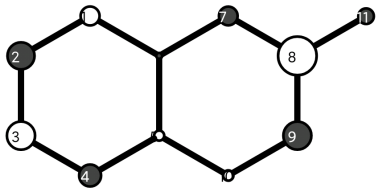
Ψ8



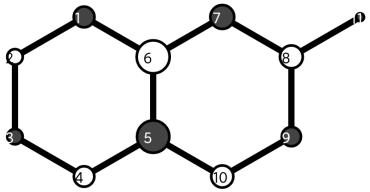
Ψ9



Ψ10



Ψ11

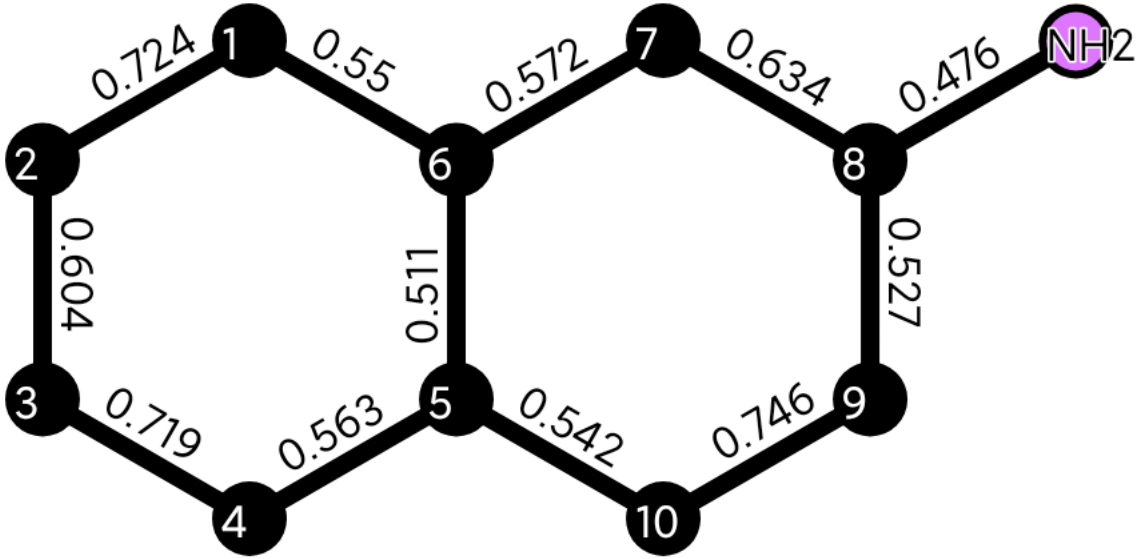


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	1.03										
2	0.724	1.0									
3	-0.03	0.604	1.03								
4	-0.357	0.0	0.719	0.996							
5	0.034	-0.241	-0.034	0.563	1.04						
6	0.55	0.0	-0.236	0.004	0.511	0.996					
7	-0.068	-0.169	0.068	0.068	-0.081	0.572	1.163				
8	-0.147	0.0	0.135	-0.016	-0.205	0.018	0.634	0.898			
9	-0.041	0.156	0.041	-0.182	-0.05	-0.227	0.103	0.527	1.069		
10	0.076	0.0	-0.161	0.007	0.542	-0.006	-0.335	0.029	0.746	0.989	
11	0.098	0.001	-0.096	0.034	0.124	-0.048	-0.27	0.476	-0.189	-0.069	1.789

3.2. Presentation of bond order:

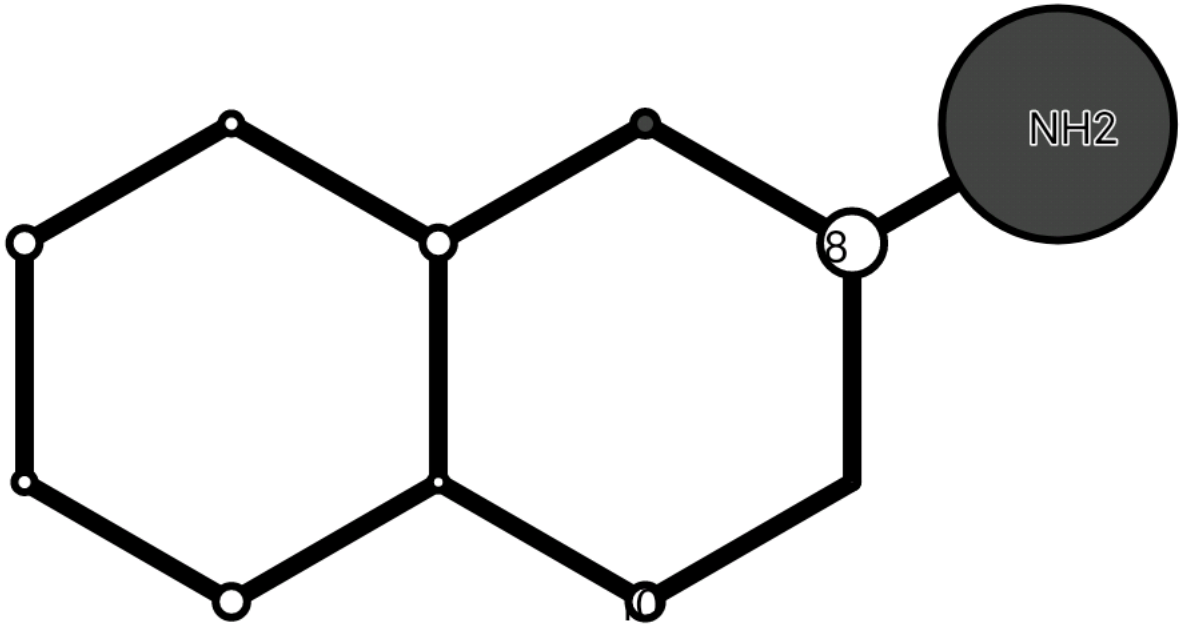

0.724
1
0.55
0.572
7
0.634
0.476
NH2
2
6
8
0.604
0.511
0.527
3
0.719
0.563
5
0.542
0.746
9
4
10

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.061										
2		0.091									
3			0.061								
4				0.095							
5					0.05						
6						0.095					
7							-0.072				
8								0.193			
9									0.022		
10										0.101	
11											-0.698

4.2. Presentation of molecule:

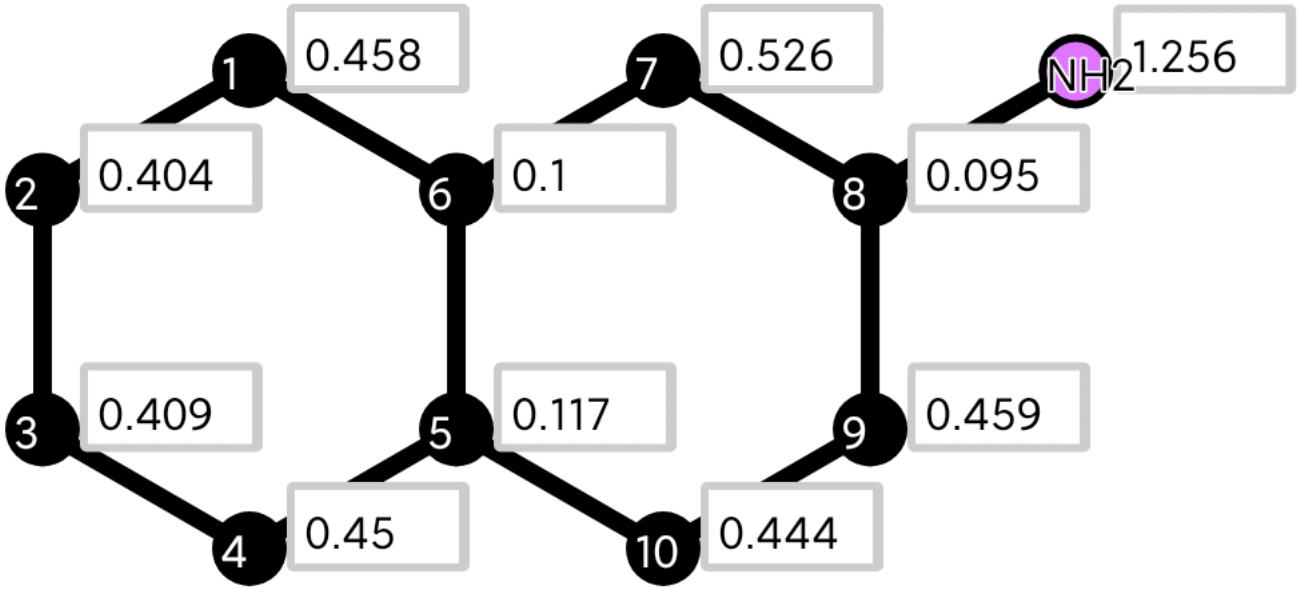

NH2
8
10

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11
0.458	0.404	0.409	0.45	0.117	0.1	0.526	0.095	0.459	0.444	1.256

5.2. Presentation of molecule:

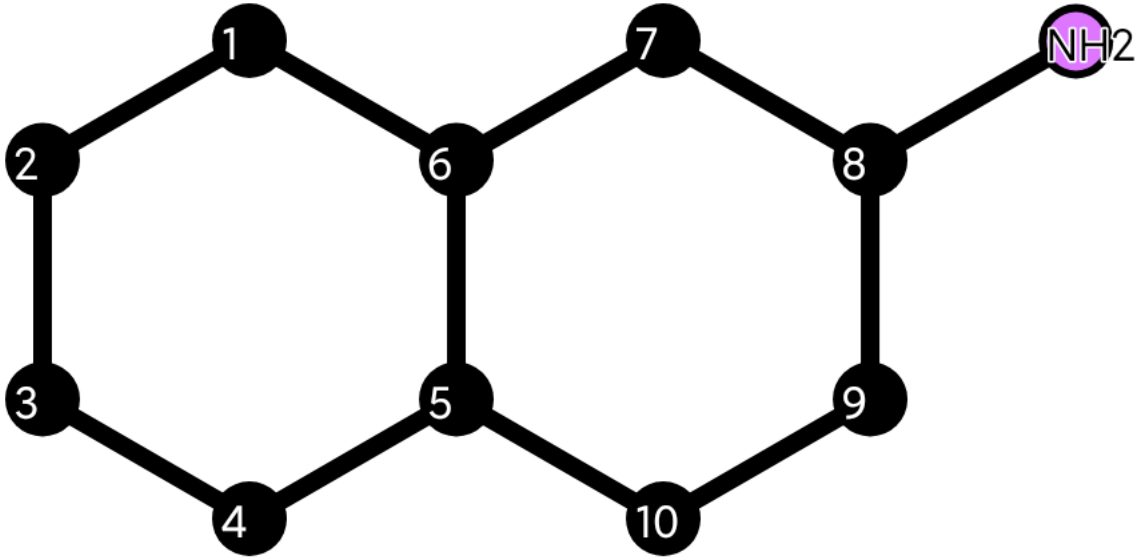


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1	0.448										
2	-0.213	0.405									
3	0.018	-0.11	0.409								
4	-0.135	0.018	-0.208	0.44							
5	0.0	-0.049	0.007	-0.093	0.336						
6	-0.086	0.007	-0.047	0.003	-0.073	0.327					
7	0.027	-0.032	0.002	-0.019	-0.003	-0.097	0.467				
8	-0.025	0.0	-0.026	0.004	-0.036	0.005	-0.155	0.311			
9	0.0	-0.033	-0.003	-0.036	0.009	-0.044	-0.01	-0.074	0.436		
10	-0.021	0.006	-0.029	0.025	-0.082	0.004	-0.122	0.011	-0.229	0.435	
11	-0.014	0.0	-0.014	0.001	-0.016	0.0	-0.059	-0.014	-0.016	0.001	0.13

6.2. Presentation of molecule:

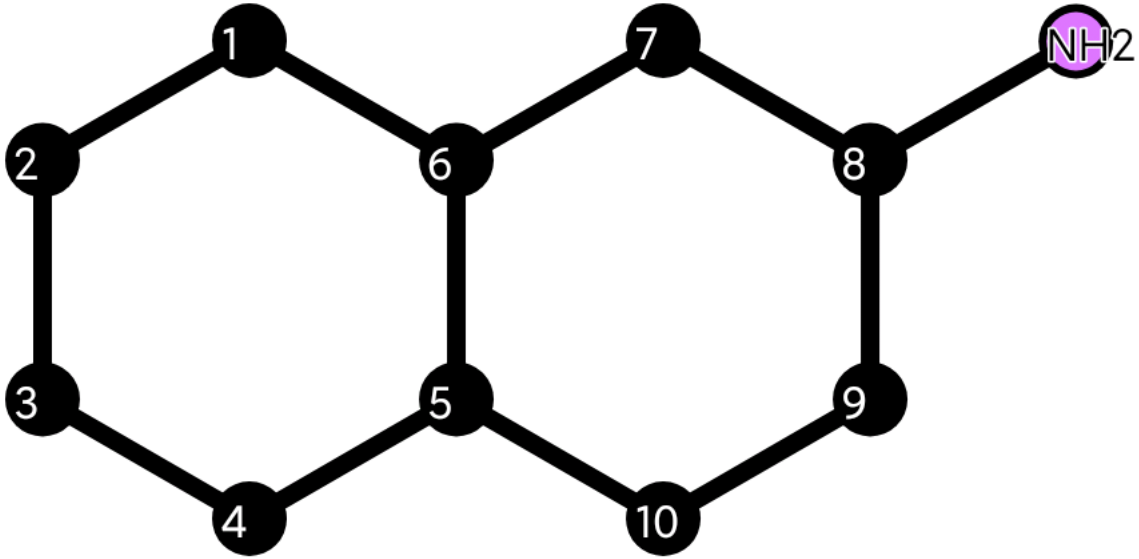

1
2
3
4
5
6
7
8
9
10
NH2

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11
1 2	-0.017	0.0	0.01	0.001	0.01	0.0	-0.017	0.0	0.01	0.001	0.001
1 6	-0.007	0.0	-0.008	0.002	-0.01	0.002	0.026	0.003	-0.012	0.0	0.004
2 3	0.018	0.0	-0.011	-0.001	-0.01	0.0	0.017	0.0	-0.01	-0.001	-0.001
3 4	-0.015	0.0	-0.015	0.005	0.012	0.001	-0.012	0.004	0.011	0.003	0.005
4 5	0.018	0.0	0.019	-0.003	-0.016	-0.001	0.013	-0.006	-0.014	-0.005	-0.007
5 6	-0.011	0.0	-0.009	-0.001	-0.009	0.003	0.027	0.005	-0.011	0.001	0.006
5 10	-0.008	0.0	-0.007	0.0	-0.008	0.001	-0.035	0.009	0.03	0.009	0.01
6 7	0.019	0.0	0.019	-0.001	0.022	-0.004	-0.06	-0.01	0.026	0.0	-0.012
7 8	-0.01	0.0	-0.013	0.003	-0.017	-0.003	-0.039	0.047	-0.033	0.011	0.053
8 9	-0.011	0.0	-0.009	-0.002	-0.008	0.004	-0.052	0.037	0.008	-0.009	0.041
8 11	0.019	0.0	0.02	-0.002	0.025	-0.002	0.099	-0.051	0.038	-0.005	-0.14
9 10	0.009	0.0	0.009	-0.001	0.012	0.0	0.046	-0.013	-0.043	-0.004	-0.015

7.2. Presentation of molecule:


1
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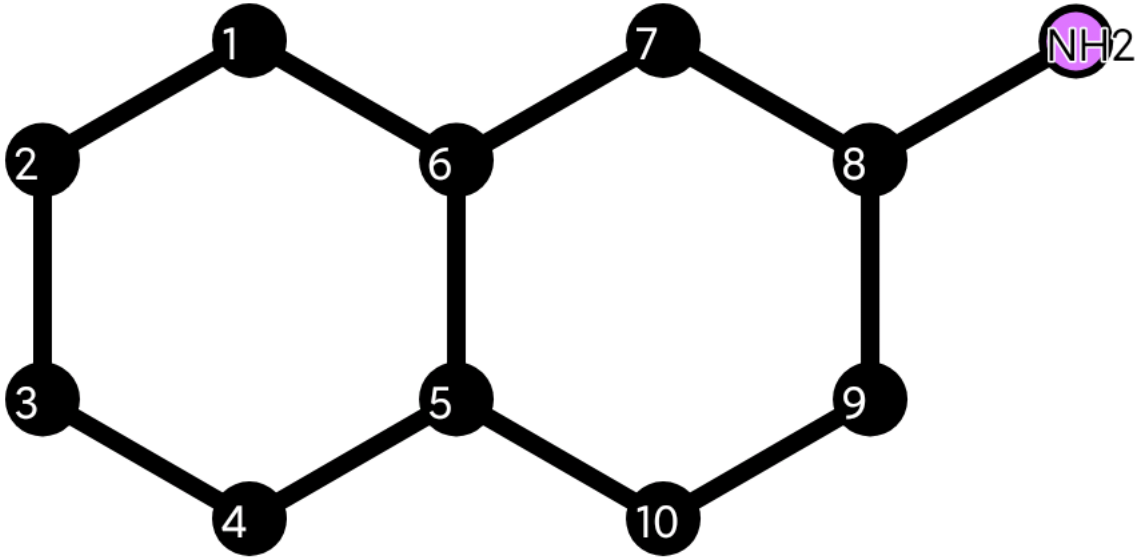
10
NH2

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	8 9	8 11	9 10
1 2	0.213											
1 6	-0.18	0.292										
2 3	-0.212	0.11	0.298									
3 4	0.124	-0.071	-0.209	0.217								
4 5	-0.075	0.091	0.112	-0.188	0.291							
5 6	0.064	-0.102	-0.039	0.067	-0.109	0.26						
5 10	0.025	-0.023	-0.045	0.061	-0.146	-0.106	0.3					
6 7	0.061	-0.154	-0.046	0.02	-0.019	-0.12	0.089	0.3				
7 8	-0.028	0.056	0.028	-0.012	0.015	0.063	-0.054	-0.168	0.246			
8 9	0.029	-0.036	-0.03	0.033	-0.045	-0.032	0.105	0.086	-0.131	0.3		
8 11	-0.001	-0.008	0.001	-0.01	0.014	-0.012	-0.022	0.027	-0.141	-0.116	0.338	
9 10	-0.02	0.023	0.033	-0.036	0.066	0.062	-0.192	-0.067	0.089	-0.189	0.035	0.21

8.2. Presentation of molecule:


1
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7
8
9
10
NH2