Print calculated values

Report generated by:root, 20.01.2020 - 12:25:56

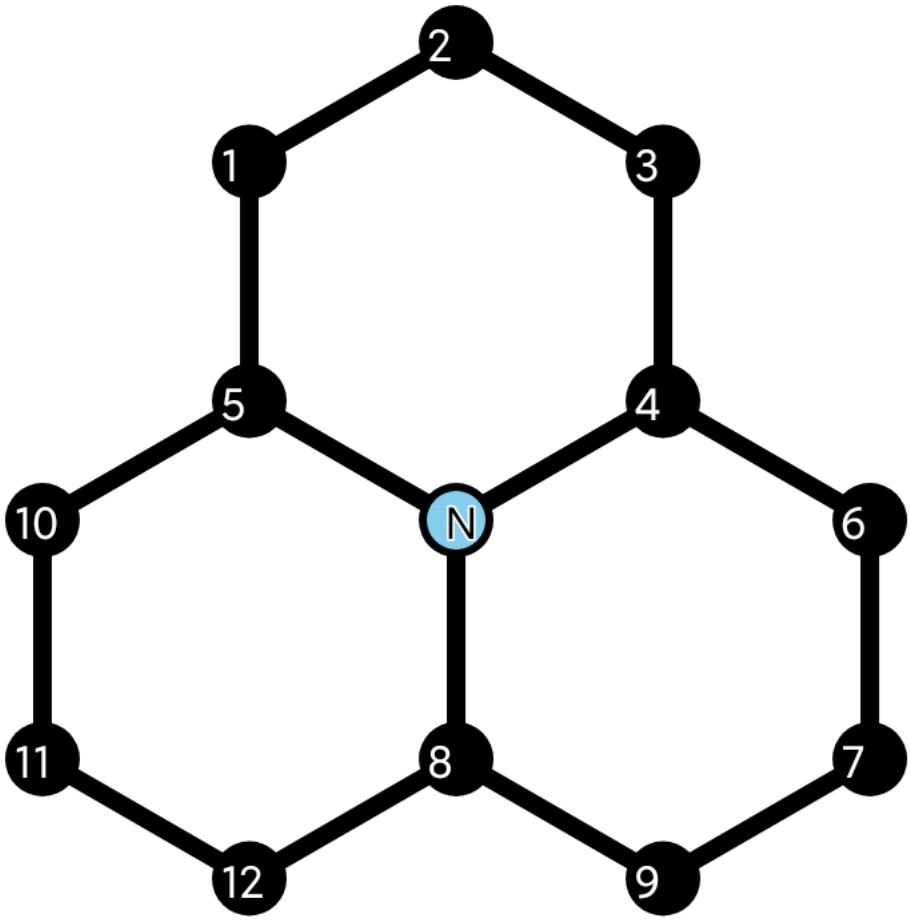
The following determinant is calculated:

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

It is about this molecule:

HMO-Energies

x1 = 3.377; x2 = 1.732; x3 = 1.732; x4 = 1.423; x5 = 1.0; x6 = 1.0; x7 = 0.0; x8 = -0.851;
x9 = -1.0; x10 = -1.0; x11 = -1.732; x12 = -1.732; x13 = -2.479;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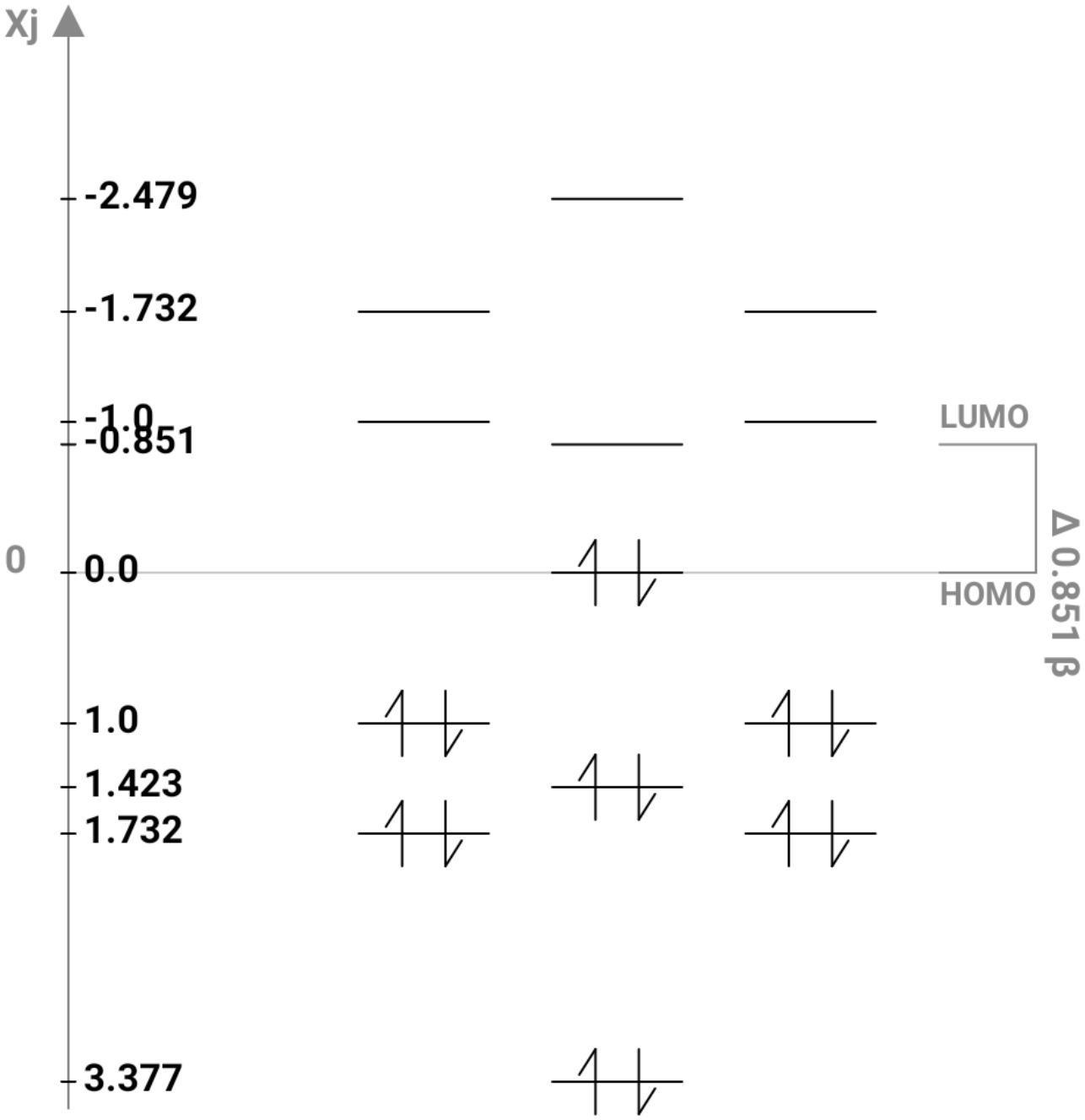
1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 13α + 20.528β -

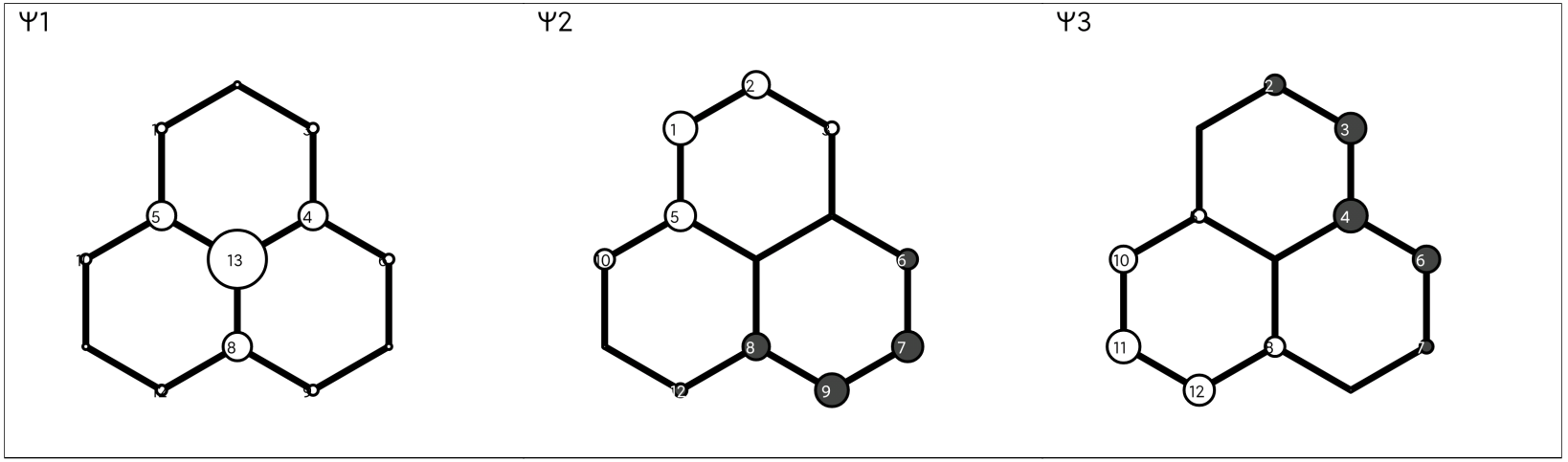
this corresponds to one πelectron: 1.466β

2. Hueckel-coefficient

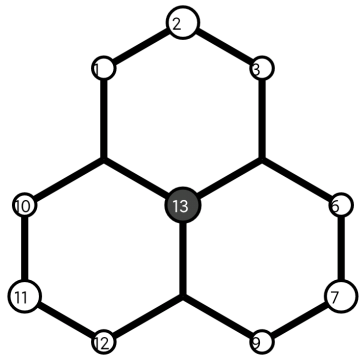
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12	Psi 13
	x1= 3.377	x2= 1.732	x3= 1.732	x4= 1.423	x5= 1.0	x6= 1.0	x7= 0.0	x8= -0.851	x9= -1.0	x10= -1.0	x11= -1.732	x12= -1.732	x13= -2.479
1	0.126	0.406	-0.047	0.265	0.31	0.265	-0.408	-0.167	-0.127	0.388	-0.289	0.289	-0.229
2	0.075	0.328	-0.244	0.372	0.385	-0.136	0.0	0.394	0.4	-0.084	0.106	-0.394	0.185
3	0.126	0.162	-0.375	0.265	0.075	-0.401	0.408	-0.167	-0.273	-0.304	0.106	0.394	-0.229
4	0.352	-0.047	-0.406	0.005	-0.31	-0.265	0.0	-0.251	-0.127	0.388	-0.289	-0.289	0.383
5	0.352	0.375	0.162	0.005	-0.075	0.401	0.0	-0.251	-0.273	-0.304	0.394	-0.106	0.383
6	0.126	-0.244	-0.328	0.265	-0.385	0.136	-0.408	-0.167	0.4	-0.084	0.394	0.106	-0.229
7	0.075	-0.375	-0.162	0.372	-0.075	0.401	0.0	0.394	-0.273	-0.304	-0.394	0.106	0.185
8	0.352	-0.328	0.244	0.005	0.385	-0.136	0.0	-0.251	0.4	-0.084	-0.106	0.394	0.383
9	0.126	-0.406	0.047	0.265	0.31	0.265	0.408	-0.167	-0.127	0.388	0.289	-0.289	-0.229
10	0.126	0.244	0.328	0.265	-0.385	0.136	0.408	-0.167	0.4	-0.084	-0.394	-0.106	-0.229
11	0.075	0.047	0.406	0.372	-0.31	-0.265	0.0	0.394	-0.127	0.388	0.289	0.289	0.185
12	0.126	-0.162	0.375	0.265	0.075	-0.401	-0.408	-0.167	-0.273	-0.304	-0.106	-0.394	-0.229
13	0.719	0.0	0.0	-0.403	0.0	0.0	0.0	0.422	0.0	0.0	0.0	0.0	-0.378

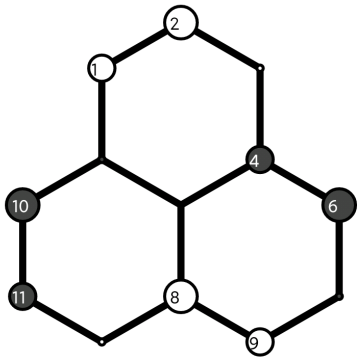
2.2. Molecule orbital presentation:



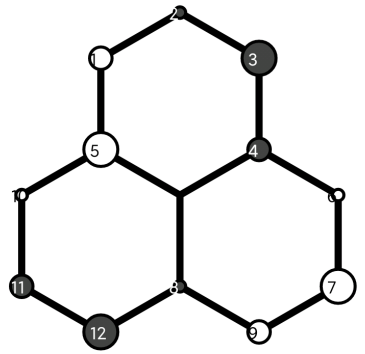
Ψ4



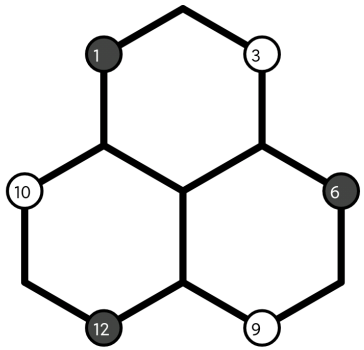
Ψ5



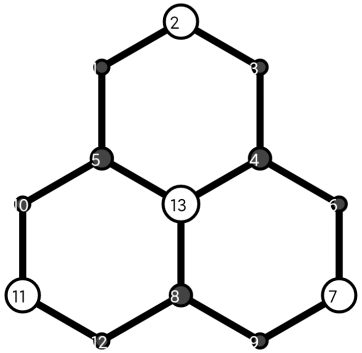
Ψ6



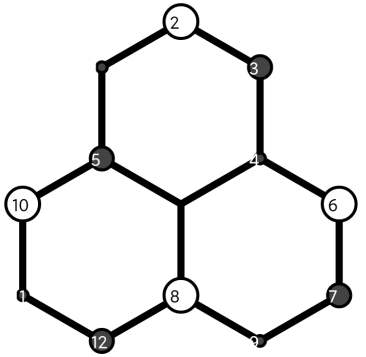
Ψ7



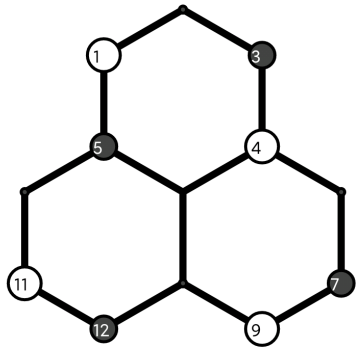
Ψ8



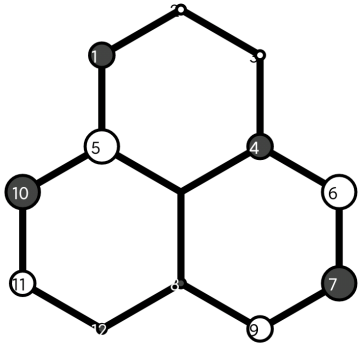
Ψ9



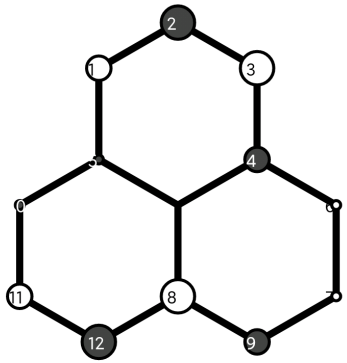
Ψ10



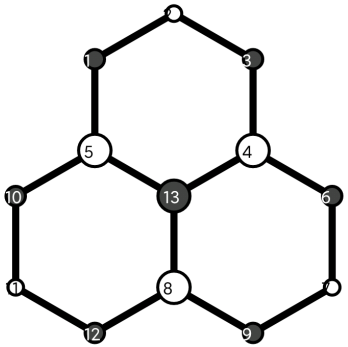
Ψ11



Ψ12



Ψ13

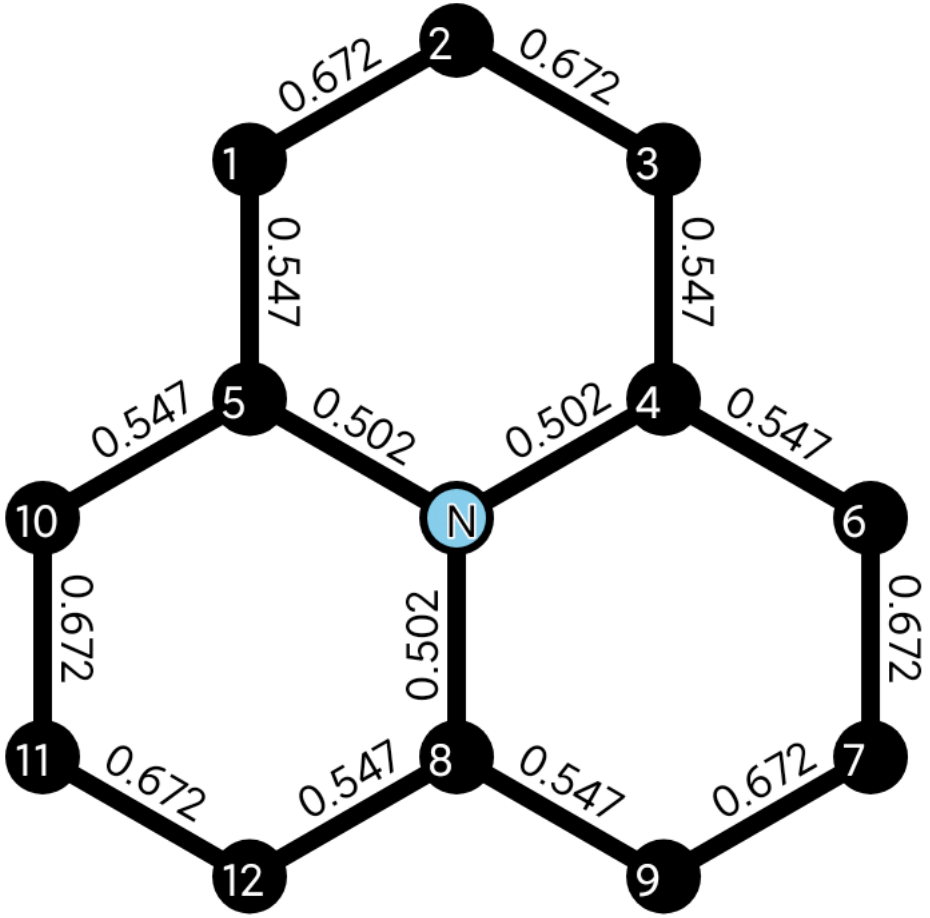


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	1.172												
2	0.672	0.955											
3	-0.161	0.672	1.172										
4	-0.242	0.056	0.547	0.914									
5	0.547	0.056	-0.242	-0.086	0.914								
6	0.172	-0.117	-0.161	0.547	-0.031	1.172							
7	0.094	-0.045	-0.117	0.056	0.056	0.672	0.955						
8	-0.031	0.056	-0.031	-0.086	-0.086	-0.242	0.056	0.914					
9	-0.161	0.094	0.172	-0.242	-0.031	-0.161	0.672	0.547	1.172				
10	-0.161	-0.117	0.172	-0.031	0.547	-0.161	0.094	-0.242	0.172	1.172			
11	-0.117	-0.045	0.094	0.056	0.056	0.094	-0.045	0.056	-0.117	0.672	0.955		
12	0.172	0.094	-0.161	-0.031	-0.242	0.172	-0.117	0.547	-0.161	-0.161	0.672	1.172	
13	-0.032	-0.192	-0.032	0.502	0.502	-0.032	-0.192	0.502	-0.032	-0.032	-0.192	-0.032	1.358

3.2. Presentation of bond order:

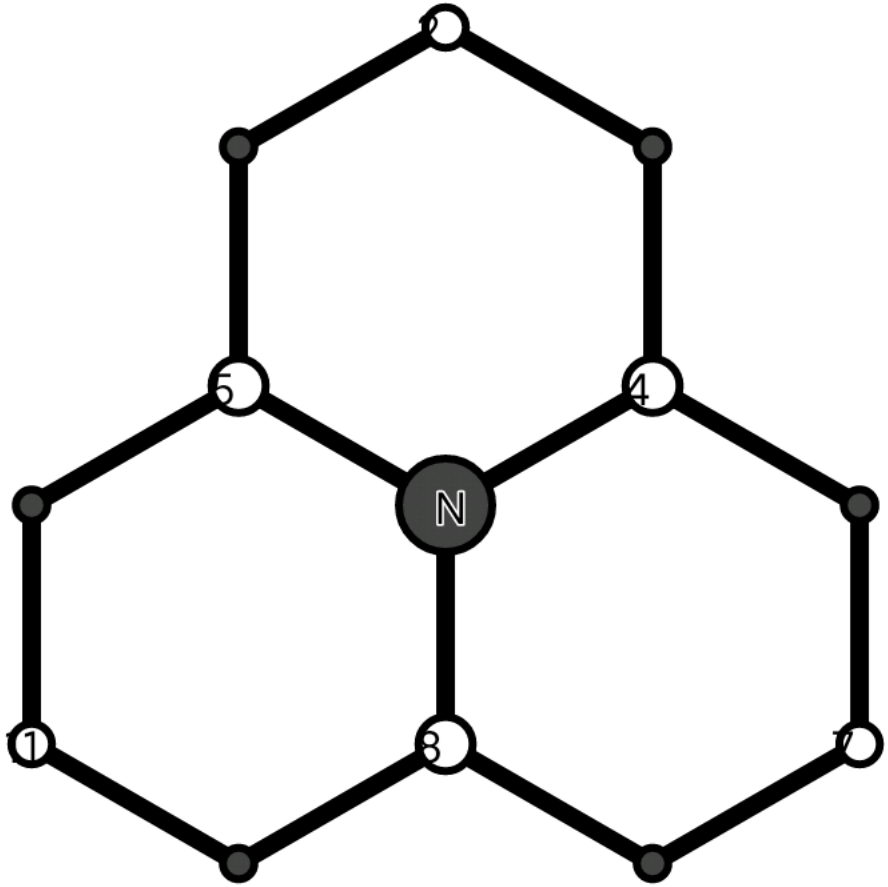

2
0.672
0.672
1
3
0.547
0.547
0.547
5
0.502
0.502
4
0.547
10
N
6
0.672
0.502
0.672
11
0.672
0.547
8
0.547
0.672
7
12
9

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	-0.095												
2		0.122											
3			-0.095										
4				0.163									
5					0.163								
6						-0.095							
7							0.122						
8								0.163					
9									-0.095				
10										-0.095			
11											0.122		
12												-0.095	
13													-0.281

4.2. Presentation of molecule:

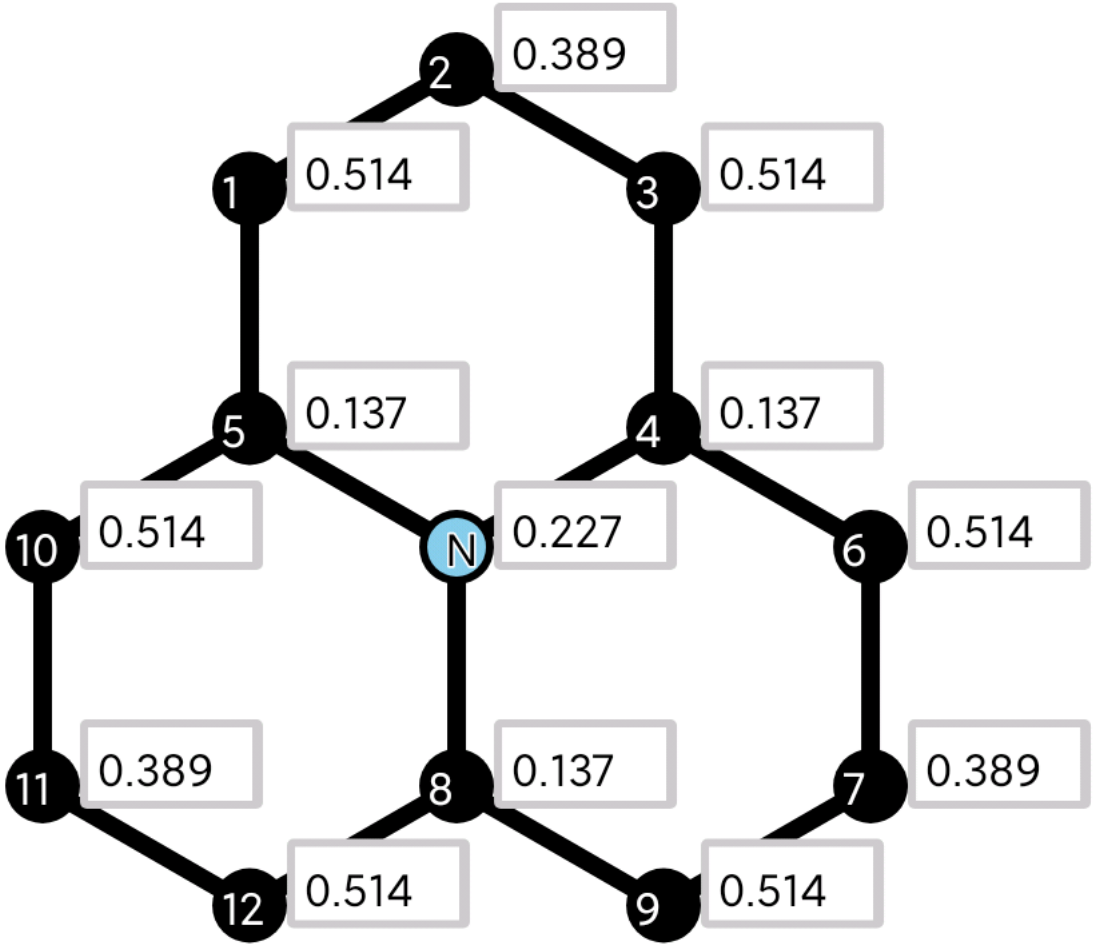

5
4
N
1
3

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12	13
0.514	0.389	0.514	0.137	0.137	0.514	0.389	0.137	0.514	0.514	0.389	0.514	0.227

5.2. Presentation of molecule:

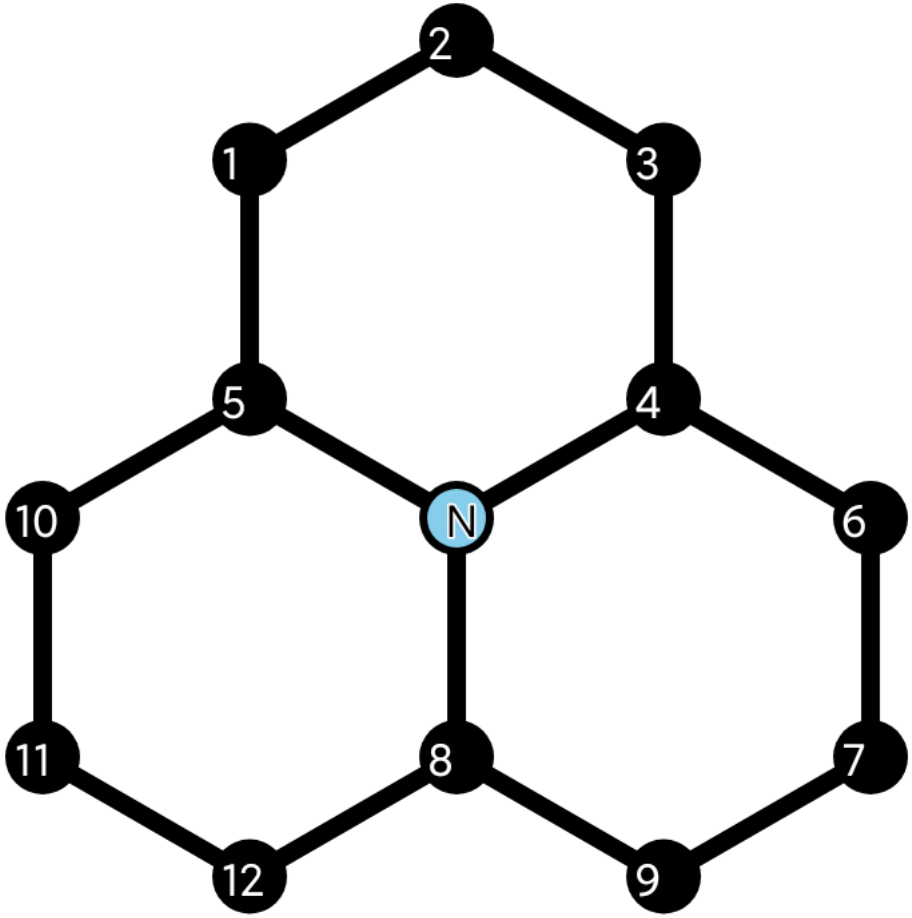

2
0.389
1
0.514
3
0.514
5
0.137
4
0.137
10
0.514
N
0.227
6
0.514
11
0.389
8
0.137
7
0.389
12
0.514
9
0.514

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0.463												
2	-0.16	0.389											
3	-0.007	-0.16	0.463										
4	-0.048	0.004	-0.086	0.314									
5	-0.086	0.004	-0.048	-0.001	0.314								
6	-0.038	-0.012	-0.007	-0.086	0.0	0.463							
7	-0.01	-0.003	-0.012	0.004	-0.002	-0.16	0.389						
8	0.0	-0.002	0.0	-0.001	-0.001	-0.048	0.004	0.314					
9	-0.059	-0.01	-0.038	-0.048	0.0	-0.007	-0.16	-0.086	0.463				
10	-0.007	-0.012	-0.038	0.0	-0.086	-0.059	-0.01	-0.048	-0.038	0.463			
11	-0.012	-0.003	-0.01	-0.002	0.004	-0.01	-0.003	0.004	-0.012	-0.16	0.389		
12	-0.038	-0.01	-0.059	0.0	-0.048	-0.038	-0.012	-0.086	-0.007	-0.007	-0.16	0.463	
13	0.003	-0.027	0.003	-0.05	-0.05	0.003	-0.027	-0.05	0.003	0.003	-0.027	0.003	0.212

6.2. Presentation of molecule:


2
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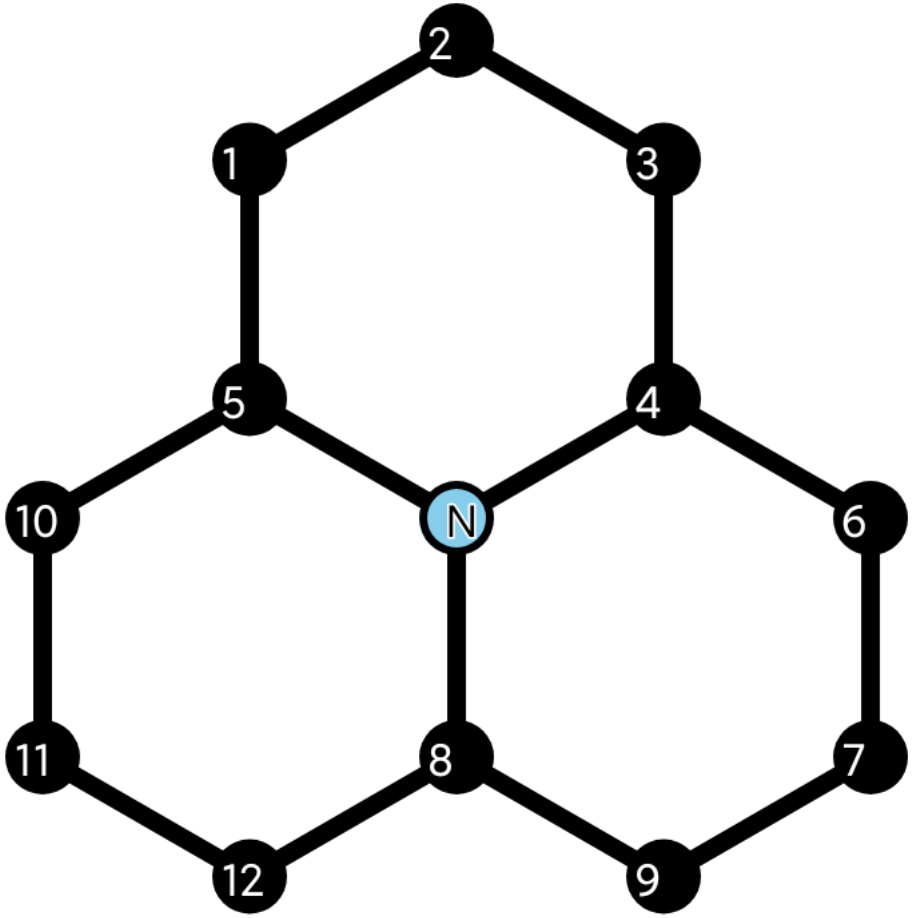
7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12	13
1 2	-0.091	0.015	0.086	0.011	-0.016	0.025	0.005	0.001	0.03	-0.024	-0.006	-0.031	-0.004
1 5	-0.047	-0.021	-0.059	-0.016	0.025	0.003	-0.006	-0.002	-0.003	0.05	0.007	0.06	0.008
2 3	0.086	0.015	-0.091	-0.016	0.011	-0.024	-0.006	0.001	-0.031	0.025	0.005	0.03	-0.004
3 4	-0.059	-0.021	-0.047	0.025	-0.016	0.05	0.007	-0.002	0.06	0.003	-0.006	-0.003	0.008
4 6	0.06	0.007	0.05	0.025	-0.002	-0.047	-0.021	-0.016	-0.059	-0.003	-0.006	0.003	0.008
4 13	-0.004	0.006	0.004	-0.015	0.019	0.004	0.006	0.019	-0.004	-0.001	0.011	-0.001	-0.045
5 10	0.05	0.007	0.06	-0.002	0.025	-0.003	-0.006	-0.016	0.003	-0.047	-0.021	-0.059	0.008
5 13	0.004	0.006	-0.004	0.019	-0.015	-0.001	0.011	0.019	-0.001	0.004	0.006	-0.004	-0.045
6 7	-0.031	-0.006	-0.024	-0.016	0.001	-0.091	0.015	0.011	0.086	0.03	0.005	0.025	-0.004
7 9	0.03	0.005	0.025	0.011	0.001	0.086	0.015	-0.016	-0.091	-0.031	-0.006	-0.024	-0.004
8 9	-0.003	-0.006	0.003	-0.016	-0.002	-0.059	-0.021	0.025	-0.047	0.06	0.007	0.05	0.008
8 12	0.003	-0.006	-0.003	-0.002	-0.016	0.06	0.007	0.025	0.05	-0.059	-0.021	-0.047	0.008
8 13	-0.001	0.011	-0.001	0.019	0.019	-0.004	0.006	-0.015	0.004	-0.004	0.006	0.004	-0.045
10 11	-0.024	-0.006	-0.031	0.001	-0.016	0.03	0.005	0.011	0.025	-0.091	0.015	0.086	-0.004
11 12	0.025	0.005	0.03	0.001	0.011	-0.031	-0.006	-0.016	-0.024	0.086	0.015	-0.091	-0.004

7.2. Presentation of molecule: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N
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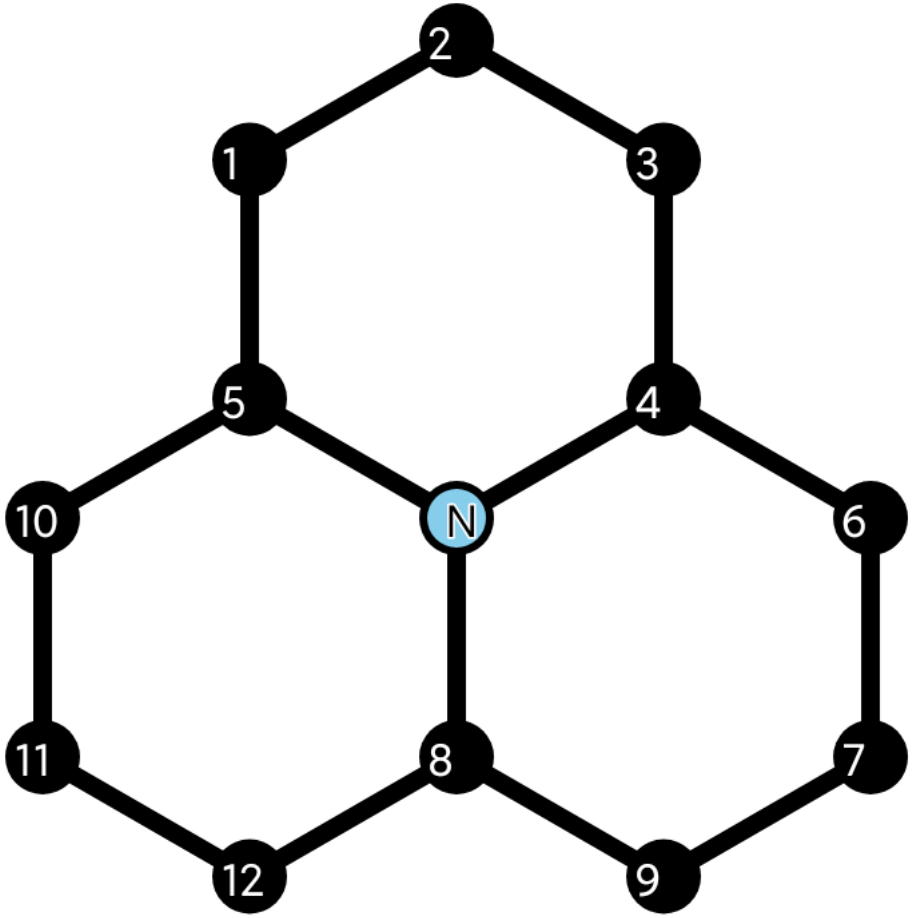
12
9

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 5	2 3	3 4	4 6	4 13	5 10	5 13	6 7	7 9	8 9	8 12	8 13	10 11	11 12
1 2	0.307														
1 5	-0.189	0.329													
2 3	-0.274	0.123	0.307												
3 4	0.123	-0.05	-0.189	0.329											
4 6	-0.057	0.005	0.068	-0.182	0.329										
4 13	-0.031	0.048	0.053	-0.096	-0.096	0.222									
5 10	0.068	-0.182	-0.057	0.005	-0.01	0.005	0.329								
5 13	0.053	-0.096	-0.031	0.048	0.005	-0.067	-0.096	0.222							
6 7	0.031	-0.008	-0.033	0.068	-0.189	0.053	0.011	-0.003	0.307						
7 9	-0.029	0.011	0.031	-0.057	0.123	-0.031	-0.008	-0.003	-0.274	0.307					
8 9	0.011	-0.01	-0.008	0.005	-0.05	0.048	0.005	0.005	0.123	-0.189	0.329				
8 12	-0.008	0.005	0.011	-0.01	0.005	0.005	-0.05	0.048	-0.057	0.068	-0.182	0.329			
8 13	-0.003	0.005	-0.003	0.005	0.048	-0.067	0.048	-0.067	-0.031	0.053	-0.096	-0.096	0.222		
10 11	-0.033	0.068	0.031	-0.008	0.011	-0.003	-0.189	0.053	-0.029	0.031	-0.057	0.123	-0.031	0.307	
11 12	0.031	-0.057	-0.029	0.011	-0.008	-0.003	0.123	-0.031	0.031	-0.033	0.068	-0.189	0.053	-0.274	0.307

8.2. Presentation of molecule:


2
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9