Print calculated values

Report generated by:root, 17.02.2020 - 11:17:59

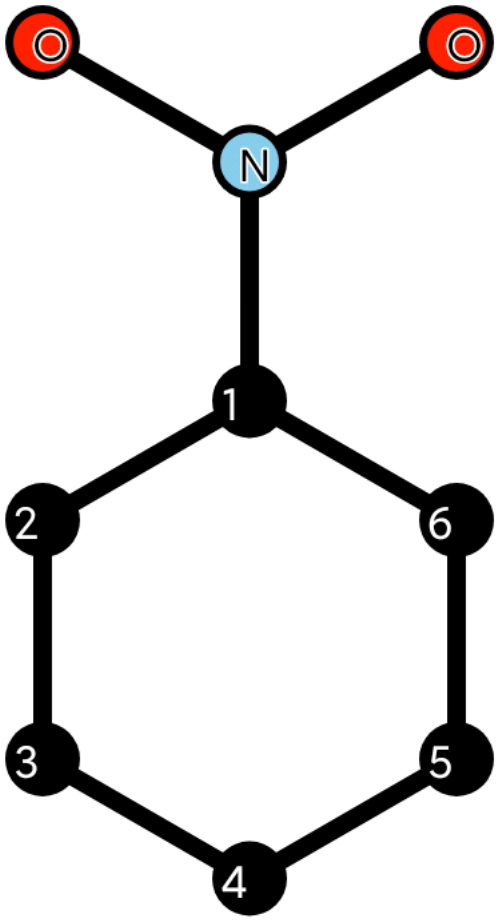
The following determinant is calculated:

-x	1.0	0.0	0.0	0.0	1.0	1.3	0.0	0.0
1.0	-x	1.0	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	1.0	-x	1.0	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	0.0	0.0	1.0	-x	0.0	0.0	0.0
1.3	0.0	0.0	0.0	0.0	0.0	-x+1.47	1.95	1.95
0.0	0.0	0.0	0.0	0.0	0.0	1.95	-x+1.18	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.95	0.0	-x+1.18

It is about this molecule:

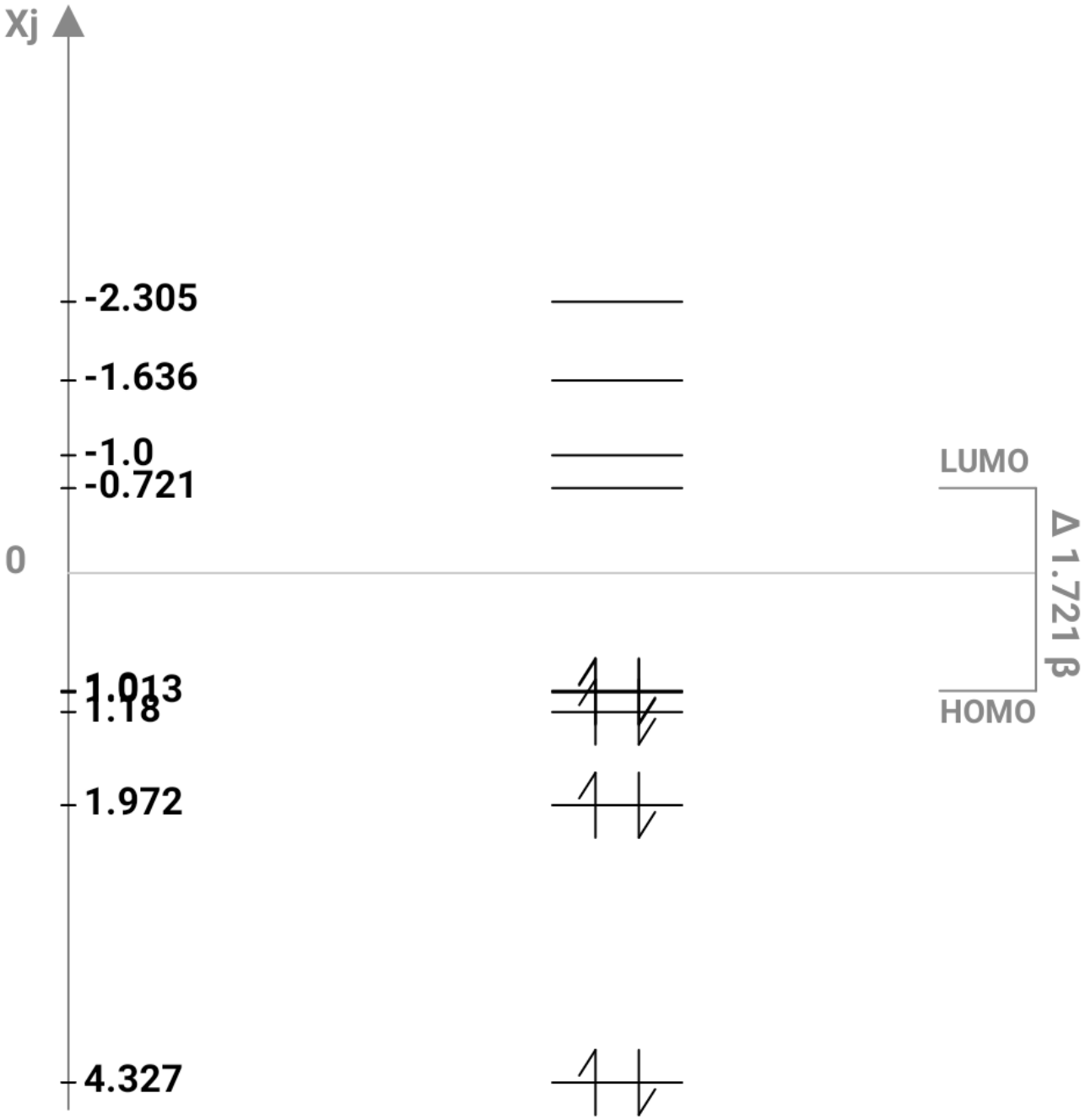
HMO-Energies

x1 = 4.327; x2 = 1.972; x3 = 1.18; x4 = 1.013; x5 = 1.0; x6 = -0.721; x7 = -1.0; x8 = -1.636; x9 = -2.305;


O
O
N
1
2
6
3
5
4

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 9α + 18.984β -

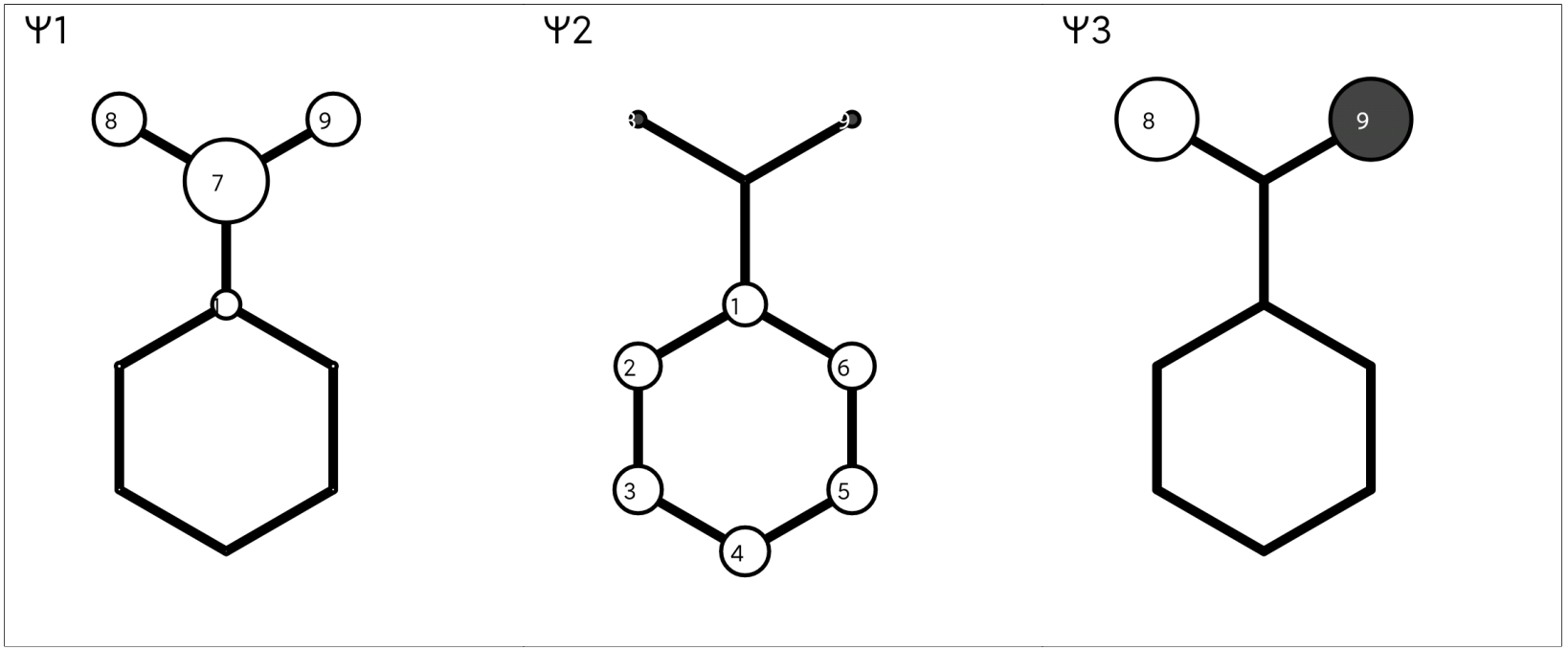
this corresponds to one πelectron: 1.898β

2. Hueckel-coefficient

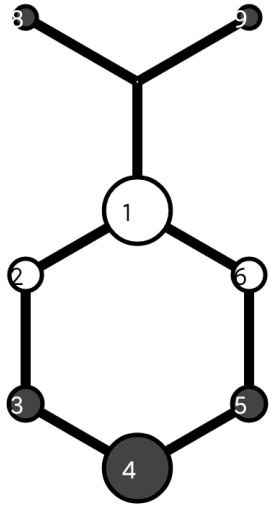
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9
	x1= 4.327	x2= 1.972	x3= 1.18	x4= 1.013	x5= 1.0	x6= -0.721	x7= -1.0	x8= -1.636	x9= -2.305
1	0.246	0.367	0.0	0.558	0.0	-0.425	0.0	-0.132	0.545
2	0.06	0.395	0.0	0.272	-0.5	0.351	0.5	-0.167	-0.339
3	0.016	0.413	0.0	-0.282	-0.5	0.171	-0.5	0.406	0.236
4	0.007	0.419	0.0	-0.558	0.0	-0.475	0.0	-0.496	-0.204
5	0.016	0.413	0.0	-0.282	0.5	0.171	0.5	0.406	0.236
6	0.06	0.395	0.0	0.272	0.5	0.351	-0.5	-0.167	-0.339
7	0.726	-0.052	0.0	0.016	0.0	-0.305	0.0	0.423	-0.445
8	0.45	-0.129	0.707	-0.188	0.0	0.313	0.0	-0.293	0.249
9	0.45	-0.129	-0.707	-0.188	0.0	0.313	0.0	-0.293	0.249

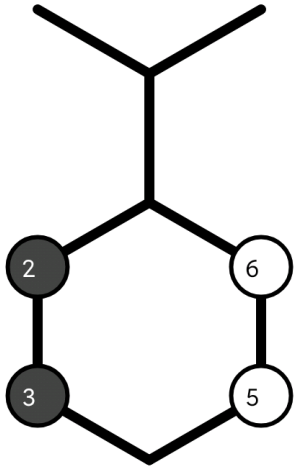
2.2. Molecule orbital presentation:



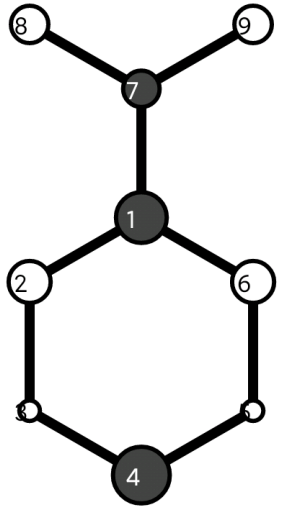
Ψ4



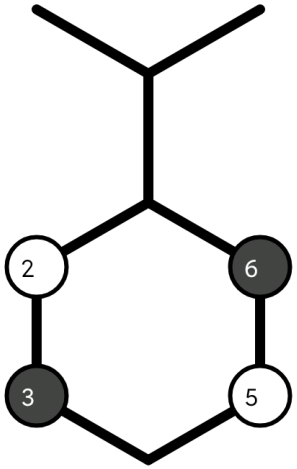
Ψ5



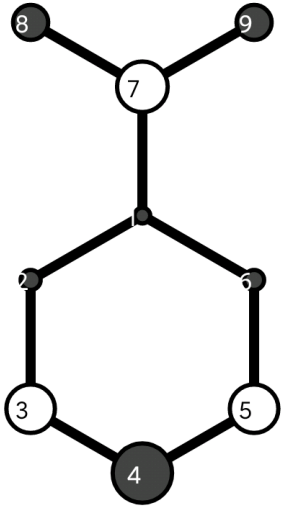
Ψ6



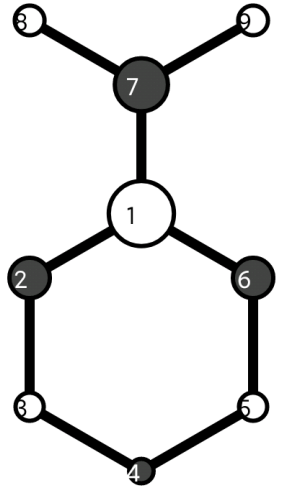
Ψ7



Ψ8



Ψ9

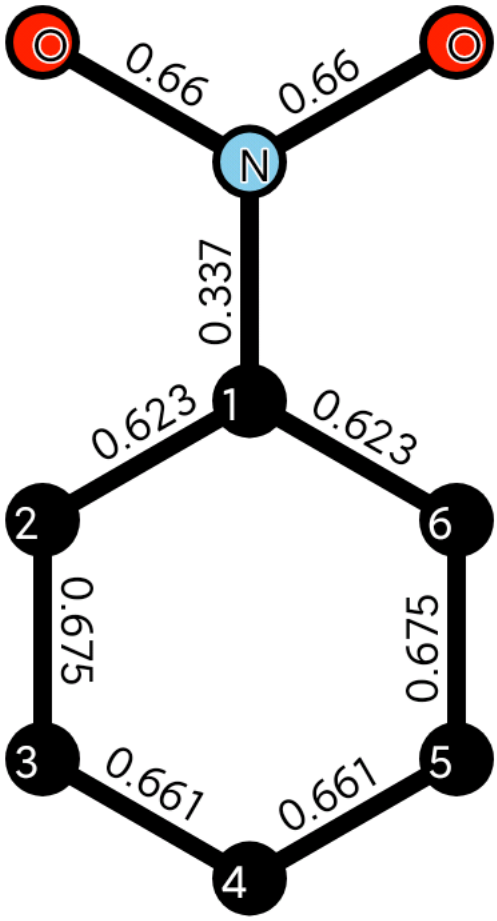


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	1.012								
2	0.623	0.968							
3	-0.004	0.675	1.001						
4	-0.311	0.029	0.661	0.973					
5	-0.004	-0.325	0.001	0.661	1.001				
6	0.623	-0.032	-0.325	0.029	0.675	0.968			
7	0.337	0.055	-0.03	-0.051	-0.03	0.055	1.06		
8	-0.083	-0.15	0.014	0.108	0.014	-0.15	0.66	1.508	
9	-0.083	-0.15	0.014	0.108	0.014	-0.15	0.66	-0.492	1.508

3.2. Presentation of bond order:

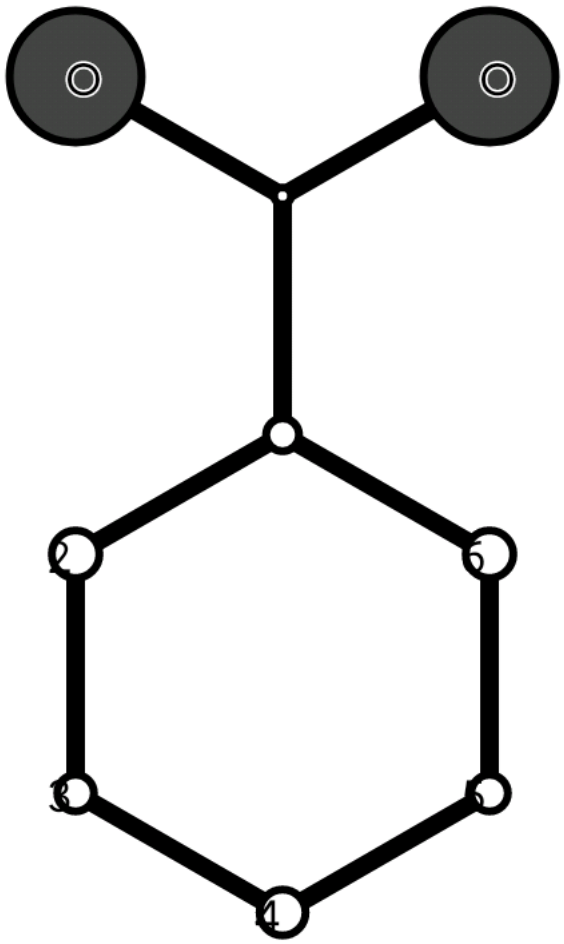


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.099								
2		0.143							
3			0.11						
4				0.138					
5					0.11				
6						0.143			
7							0.051		
8								-0.397	
9									-0.397

4.2. Presentation of molecule:

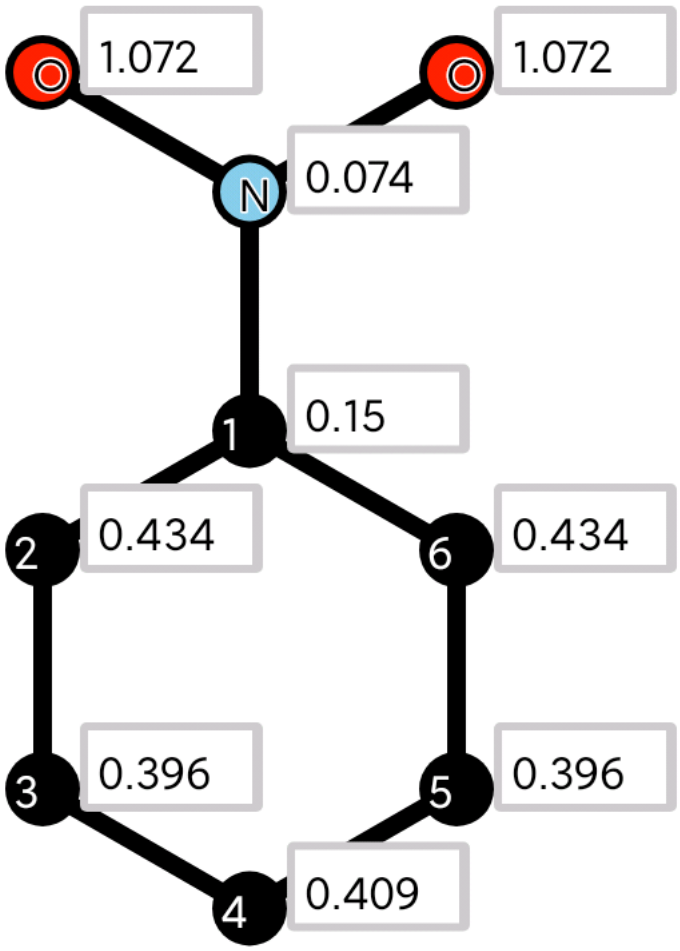


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9
0.15	0.434	0.396	0.409	0.396	0.434	0.074	1.072	1.072

5.2. Presentation of molecule:

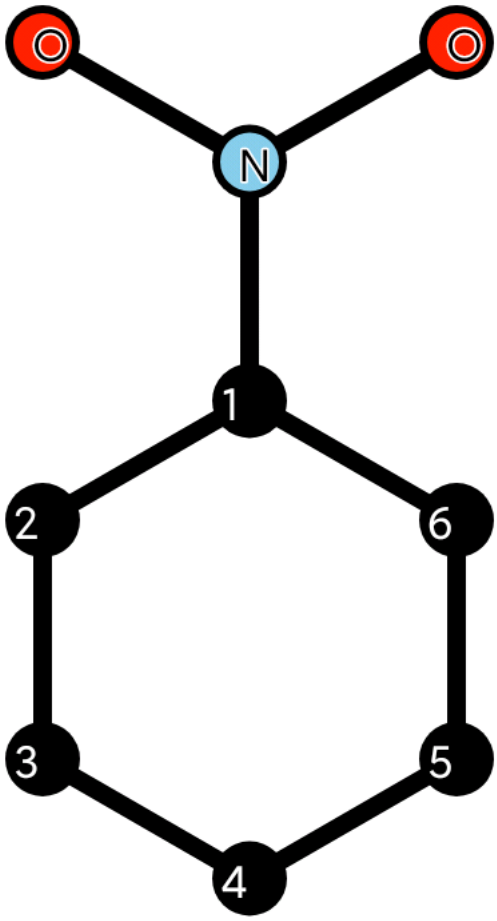


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1	0.345								
2	-0.138	0.417							
3	0.008	-0.162	0.396						
4	-0.092	0.012	-0.154	0.407					
5	0.008	-0.098	0.01	-0.154	0.396				
6	-0.138	0.003	-0.098	0.012	-0.162	0.417			
7	-0.013	-0.001	0.0	-0.002	0.0	-0.001	0.167		
8	0.01	-0.017	0.001	-0.014	0.001	-0.017	-0.075	0.255	
9	0.01	-0.017	0.001	-0.014	0.001	-0.017	-0.075	-0.145	0.255

6.2. Presentation of molecule:

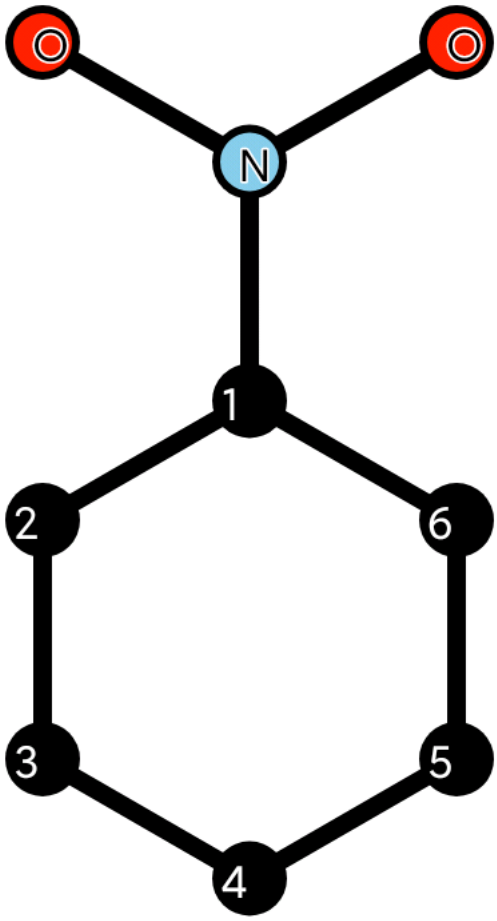


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9
1 2	-0.01	0.007	0.001	0.01	-0.002	0.015	-0.005	-0.008	-0.008
1 6	-0.01	0.015	-0.002	0.01	0.001	0.007	-0.005	-0.008	-0.008
1 7	0.007	-0.023	0.001	-0.019	0.001	-0.023	0.005	0.025	0.025
2 3	0.003	0.016	0.001	-0.012	0.0	-0.013	0.001	0.002	0.002
3 4	-0.002	-0.014	-0.002	0.011	0.0	0.011	-0.001	-0.002	-0.002
4 5	-0.002	0.011	0.0	0.011	-0.002	-0.014	-0.001	-0.002	-0.002
5 6	0.003	-0.013	0.0	-0.012	0.001	0.016	0.001	0.002	0.002
7 8	0.002	0.007	0.0	0.007	0.0	0.007	-0.008	-0.133	0.119
7 9	0.002	0.007	0.0	0.007	0.0	0.007	-0.008	0.119	-0.133

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 6	1 7	2 3	3 4	4 5	5 6	7 8	7 9
1 2	0.242								
1 6	-0.17	0.242							
1 7	-0.063	-0.063	0.232						
2 3	-0.194	0.117	0.012	0.245					
3 4	0.126	-0.085	-0.008	-0.211	0.248				
4 5	-0.085	0.126	-0.008	0.128	-0.202	0.248			
5 6	0.117	-0.194	0.012	-0.091	0.128	-0.211	0.245		
7 8	0.018	0.018	-0.065	-0.004	0.003	0.003	-0.004	0.189	
7 9	0.018	0.018	-0.065	-0.004	0.003	0.003	-0.004	-0.149	0.189

8.2. Presentation of molecule: