Print calculated values

Report generated by:root, 20.01.2020 - 21:05:27

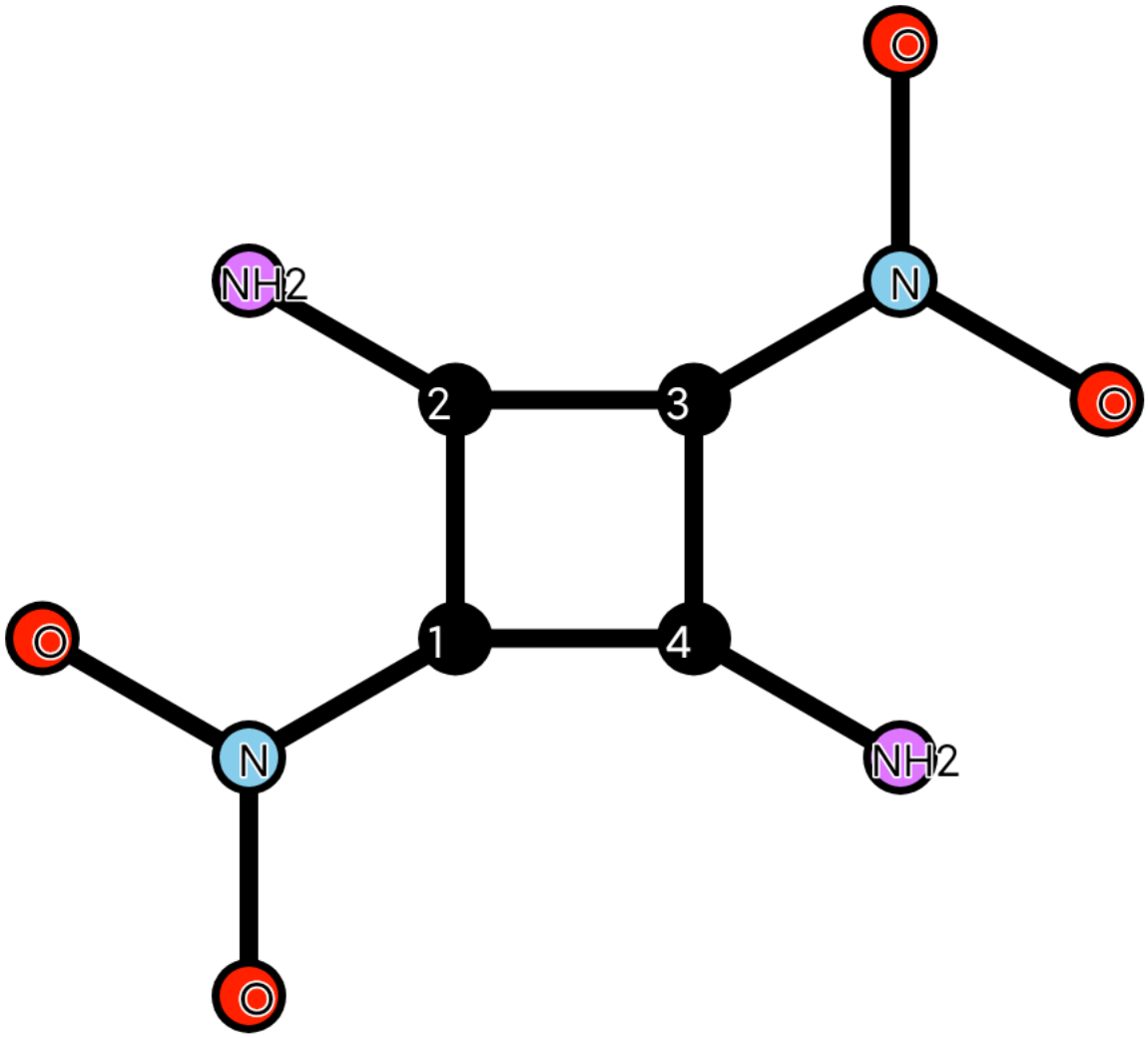
The following determinant is calculated:

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

It is about this molecule:

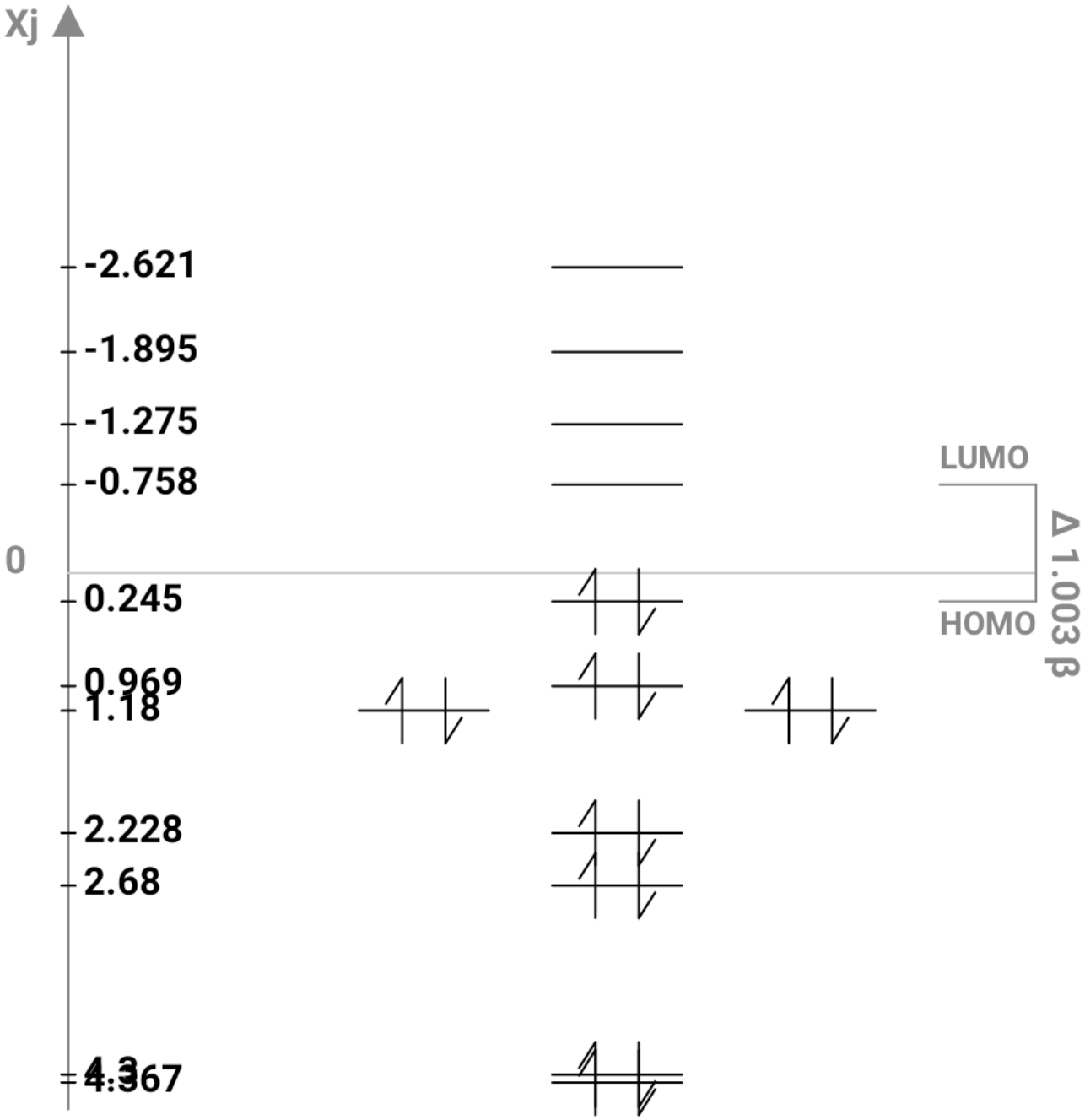
HMO-Energies

x1 = 4.367; x2 = 4.3; x3 = 2.68; x4 = 2.228; x5 = 1.18; x6 = 1.18; x7 = 0.969; x8 = 0.245;
x9 = -0.758; x10 = -1.275; x11 = -1.895; x12 = -2.621;


O
NH2
N
2
3
O
O
1
4
N
NH2
O

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 12α + 34.298β -

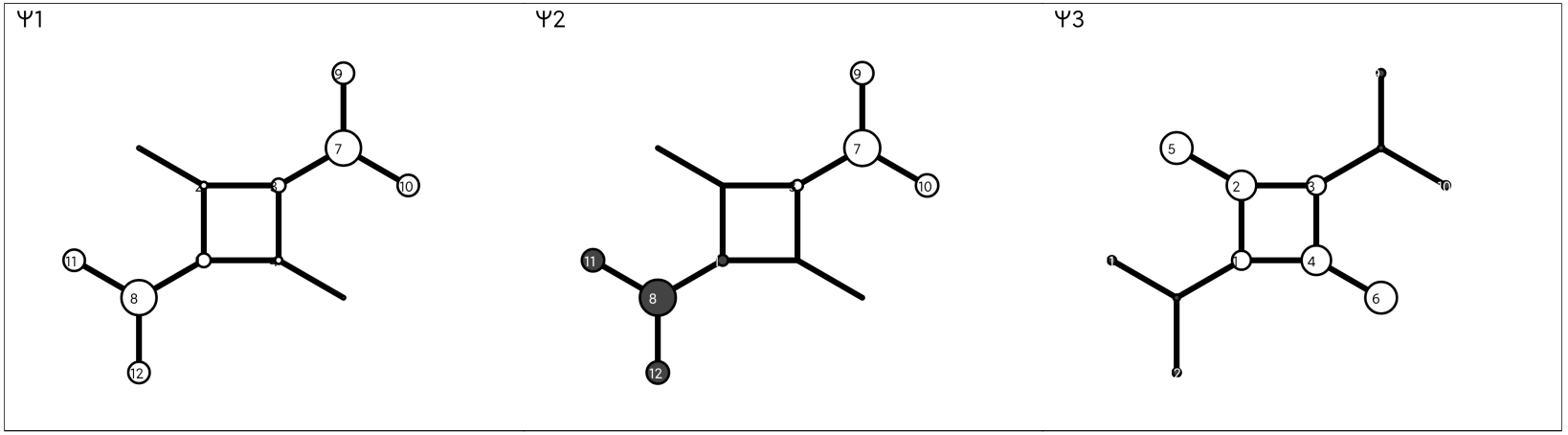
this corresponds to one πelectron: 2.144β

2. Hueckel-coefficient

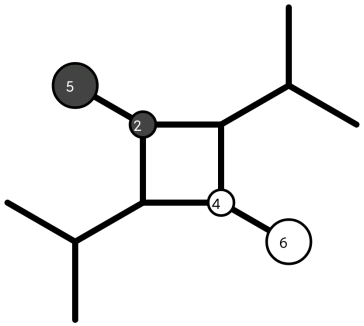
2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6	Psi 7	Psi 8	Psi 9	Psi 10	Psi 11	Psi 12
	x1= 4.367	x2= 4.3	x3= 2.68	x4= 2.228	x5= 1.18	x6= 1.18	x7= 0.969	x8= 0.245	x9= -0.758	x10= -1.275	x11= -1.895	x12= -2.621
1	0.199	-0.156	0.273	0.0	0.0	0.0	-0.417	0.61	0.0	-0.108	-0.322	-0.448
2	0.105	0.0	0.425	-0.356	0.0	0.0	-0.192	0.0	0.611	0.327	0.0	0.406
3	0.199	0.156	0.273	0.0	0.0	0.0	-0.417	-0.61	0.0	-0.108	0.322	-0.448
4	0.105	0.0	0.425	0.356	0.0	0.0	-0.192	0.0	-0.611	0.327	0.0	0.406
5	0.047	0.0	0.456	-0.611	0.0	0.0	0.499	0.0	-0.356	-0.155	0.0	-0.129
6	0.047	0.0	0.456	0.611	0.0	0.0	0.499	0.0	0.356	-0.155	0.0	-0.129
7	0.506	0.517	-0.092	0.0	0.0	0.0	-0.015	-0.115	0.0	-0.397	-0.469	0.279
8	0.506	-0.517	-0.092	0.0	0.0	0.0	-0.015	0.115	0.0	-0.397	0.469	0.279
9	0.309	0.323	-0.119	0.0	-0.704	-0.063	0.141	0.239	0.0	0.316	0.297	-0.143
10	0.309	0.323	-0.119	0.0	0.704	0.063	0.141	0.239	0.0	0.316	0.297	-0.143
11	0.309	-0.323	-0.119	0.0	0.063	-0.704	0.141	-0.239	0.0	0.316	-0.297	-0.143
12	0.309	-0.323	-0.119	0.0	-0.063	0.704	0.141	-0.239	0.0	0.316	-0.297	-0.143

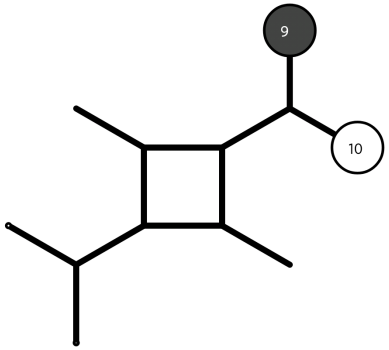
2.2. Molecule orbital presentation:



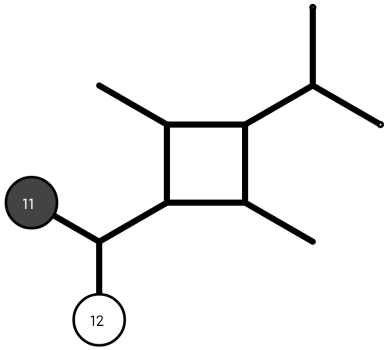
Ψ4



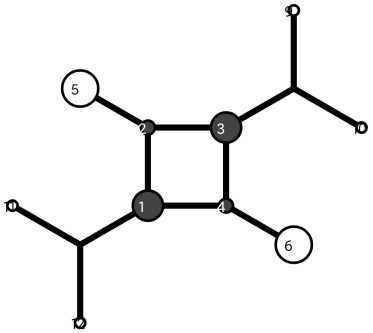
Ψ5



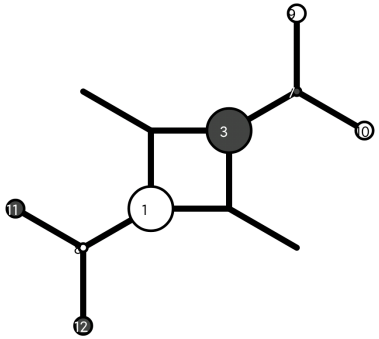
Ψ6



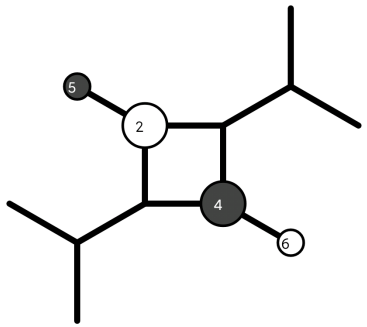
Ψ7



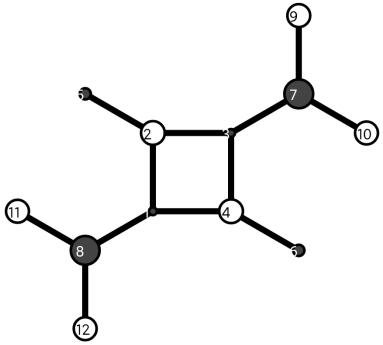
Ψ8



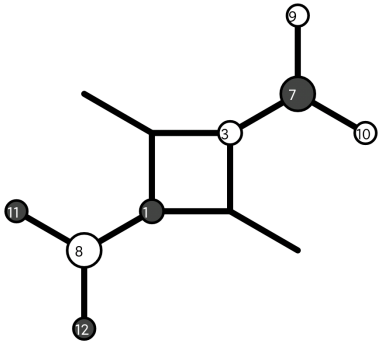
Ψ9



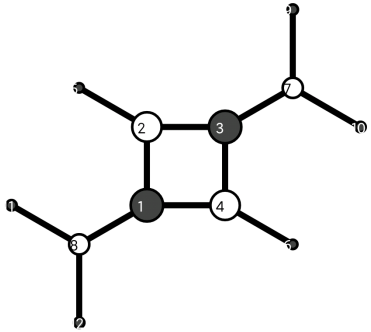
Ψ10



Ψ11



Ψ12

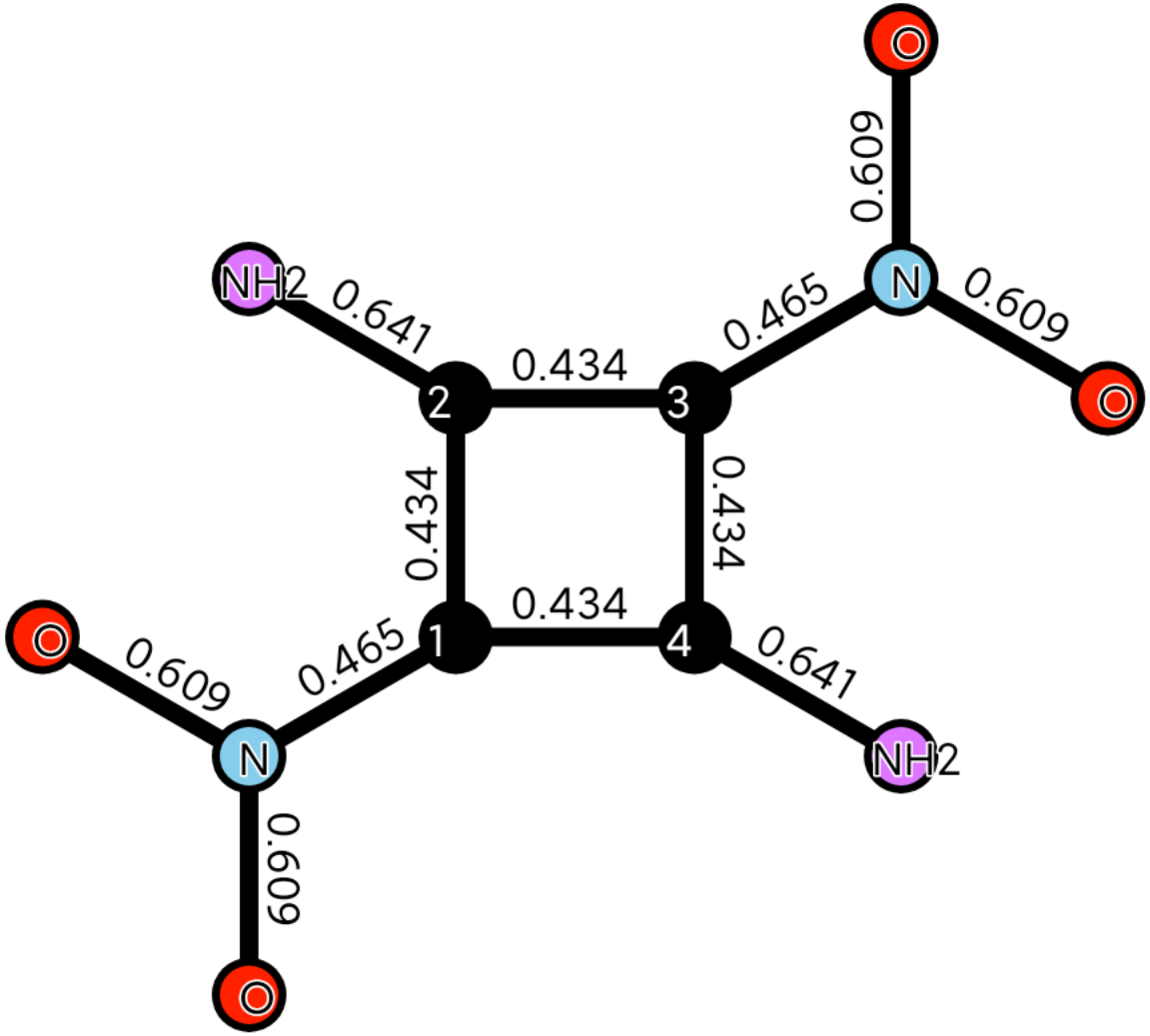


3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.369											
2	0.434	0.711										
3	-0.217	0.434	1.369									
4	0.434	0.203	0.434	0.711								
5	-0.149	0.641	-0.149	-0.229	1.665							
6	-0.149	-0.229	-0.149	0.641	0.173	1.665						
7	-0.138	0.034	0.465	0.034	-0.051	-0.051	1.089					
8	0.465	0.034	-0.138	0.034	-0.051	-0.051	-0.032	1.089				
9	0.131	-0.091	-0.251	-0.091	0.061	0.061	0.609	0.052	1.583			
10	0.131	-0.091	-0.251	-0.091	0.061	0.061	0.609	0.052	-0.417	1.583		
11	-0.251	-0.091	0.131	-0.091	0.061	0.061	0.052	0.609	-0.063	-0.063	1.583	
12	-0.251	-0.091	0.131	-0.091	0.061	0.061	0.052	0.609	-0.063	-0.063	-0.417	1.583

3.2. Presentation of bond order:

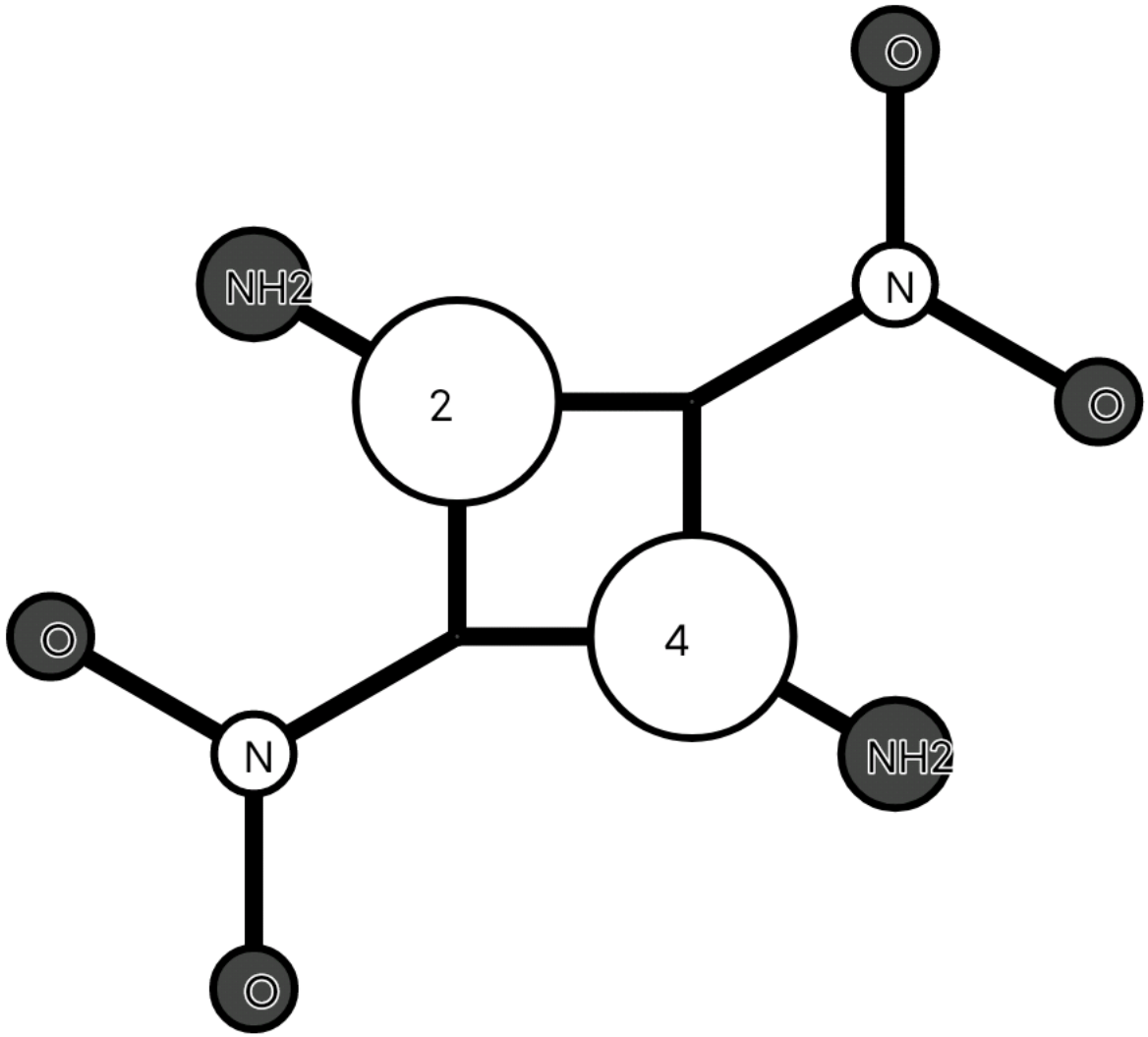

O
0.609
NH2
0.641
0.434
N
0.465
0.609
O
2
3
0.434
0.434
0.434
O
0.609
0.465
1
4
0.641
N
NH2
0.609
O

4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1	-0.036											
2		0.622										
3			-0.036									
4				0.622								
5					-0.332							
6						-0.332						
7							0.244					
8								0.244				
9									-0.25			
10										-0.25		
11											-0.25	
12												-0.25

4.2. Presentation of molecule:

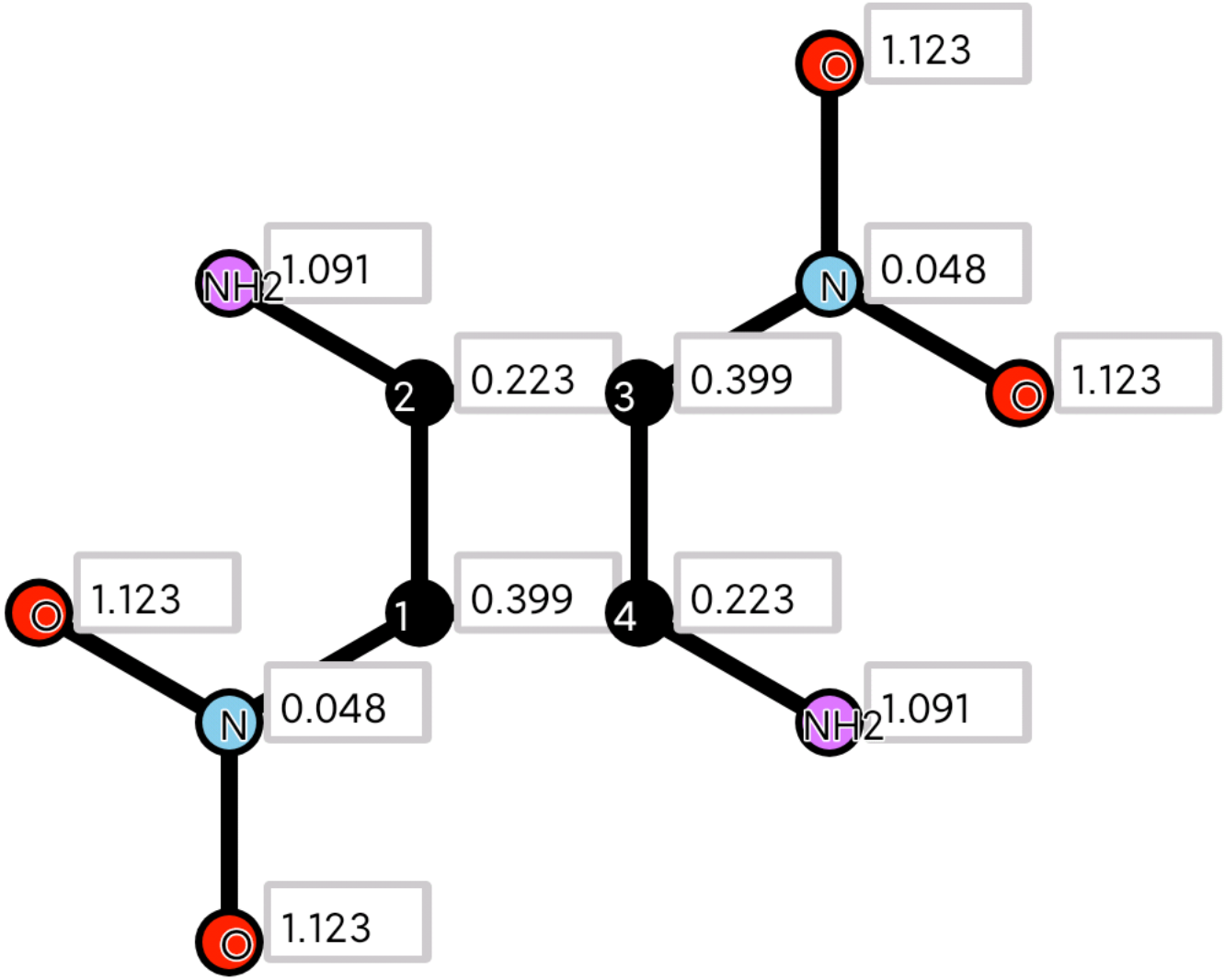

O
NH2
N
2
O
4
O
NH2
N
O

5. Free valences

5.1. Calculated values:

1	2	3	4	5	6	7	8	9	10	11	12
0.399	0.223	0.399	0.223	1.091	1.091	0.048	0.048	1.123	1.123	1.123	1.123

5.2. Presentation of molecule:

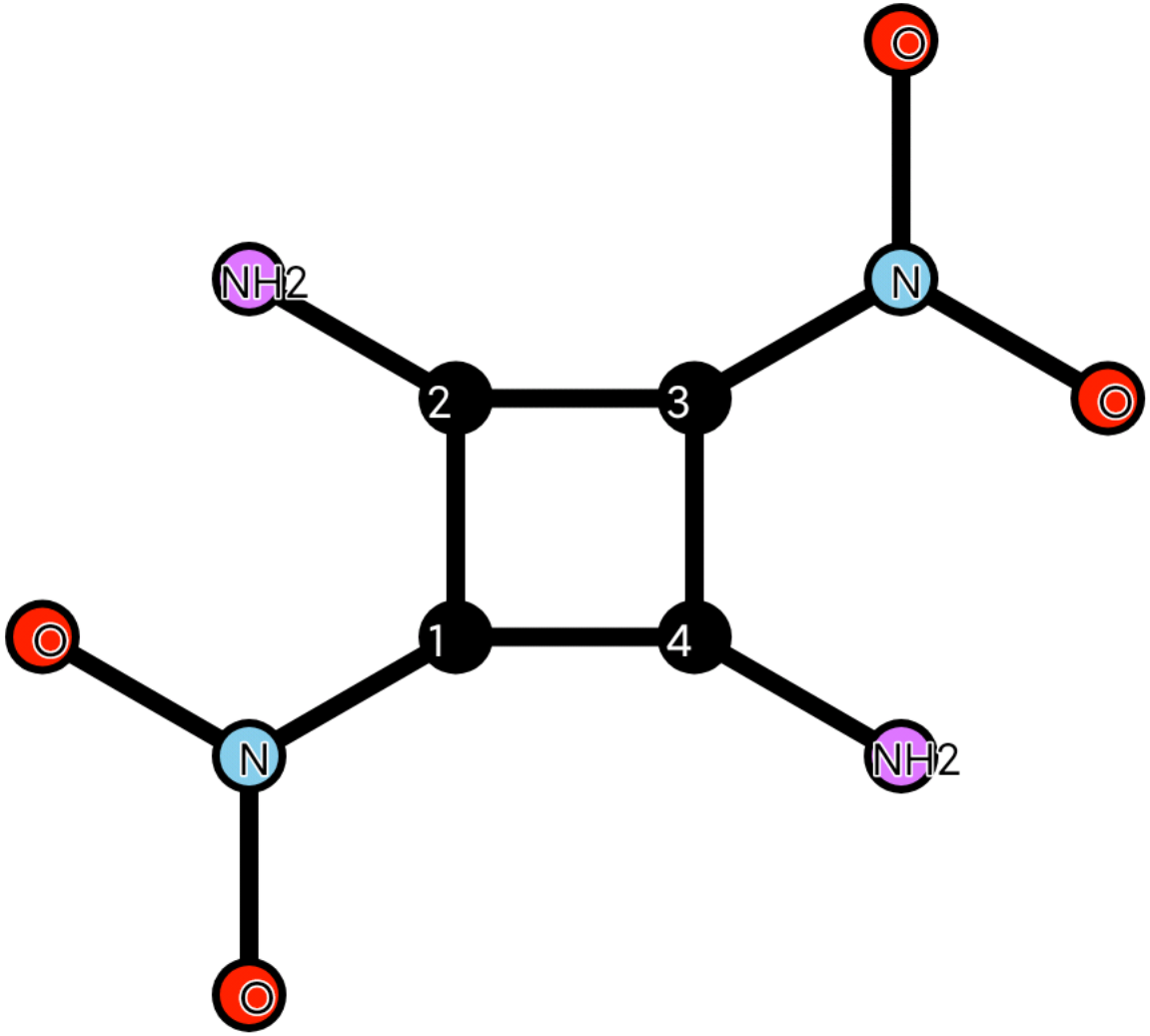

1.123
NH2
1.091
N
0.048
2
0.223
3
0.399
1.123
1.123
1
0.399
4
0.223
N
0.048
NH2
1.091
1.123

6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1	0.286											
2	-0.044	0.267										
3	-0.02	-0.044	0.286									
4	-0.044	-0.025	-0.044	0.267								
5	-0.012	-0.091	-0.012	-0.044	0.206							
6	-0.012	-0.044	-0.012	-0.091	-0.033	0.206						
7	-0.016	0.0	-0.046	0.0	-0.001	-0.001	0.172					
8	-0.046	0.0	-0.016	0.0	-0.001	-0.001	-0.002	0.172				
9	-0.017	-0.005	-0.029	-0.005	-0.003	-0.003	-0.05	-0.003	0.213			
10	-0.017	-0.005	-0.029	-0.005	-0.003	-0.003	-0.05	-0.003	-0.086	0.213		
11	-0.029	-0.005	-0.017	-0.005	-0.003	-0.003	-0.003	-0.05	-0.005	-0.005	0.213	
12	-0.029	-0.005	-0.017	-0.005	-0.003	-0.003	-0.003	-0.05	-0.005	-0.005	-0.086	0.213

6.2. Presentation of molecule:

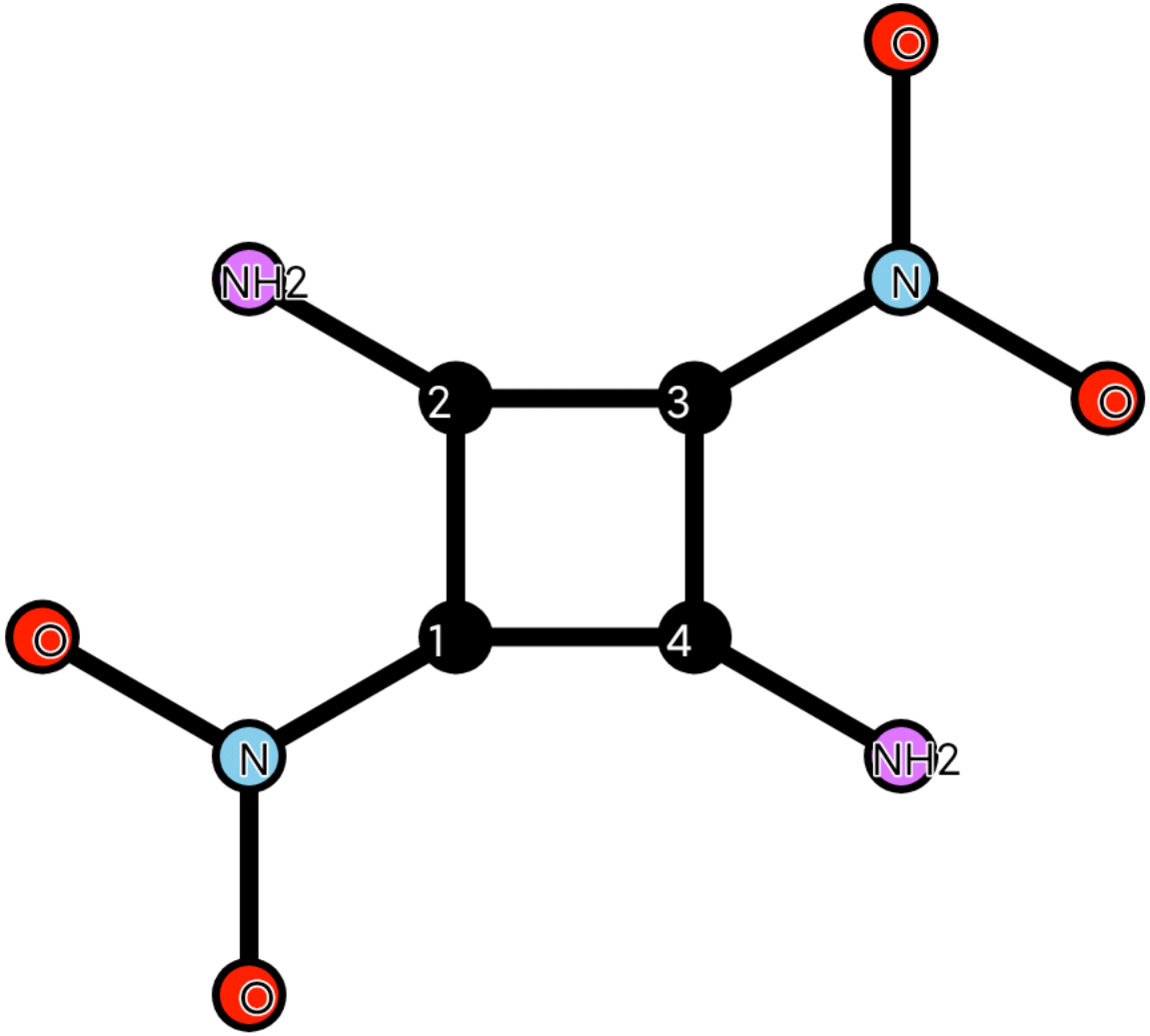

O
NH2
N
2
3
O
O
1
4
N
NH2
O

7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6	7	8	9	10	11	12
1 2	-0.066	0.06	0.043	-0.042	0.054	-0.032	0.007	-0.009	0.012	0.012	-0.019	-0.019
1 4	-0.066	-0.042	0.043	0.06	-0.032	0.054	0.007	-0.009	0.012	0.012	-0.019	-0.019
1 8	-0.066	-0.008	-0.029	-0.008	-0.006	-0.006	-0.005	0.018	-0.009	-0.009	0.064	0.064
2 3	0.043	0.06	-0.066	-0.042	0.054	-0.032	-0.009	0.007	-0.019	-0.019	0.012	0.012
2 5	0.024	0.02	0.024	0.04	-0.166	0.04	0.001	0.001	0.004	0.004	0.004	0.004
3 4	0.043	-0.042	-0.066	0.06	-0.032	0.054	-0.009	0.007	-0.019	-0.019	0.012	0.012
3 7	-0.029	-0.008	-0.066	-0.008	-0.006	-0.006	0.018	-0.005	0.064	0.064	-0.009	-0.009
4 6	0.024	0.04	0.024	0.02	0.04	-0.166	0.001	0.001	0.004	0.004	0.004	0.004
7 9	0.017	0.002	0.041	0.002	0.002	0.002	-0.021	0.002	-0.135	0.079	0.004	0.004
7 10	0.017	0.002	0.041	0.002	0.002	0.002	-0.021	0.002	0.079	-0.135	0.004	0.004
8 11	0.041	0.002	0.017	0.002	0.002	0.002	0.002	-0.021	0.004	0.004	-0.135	0.079
8 12	0.041	0.002	0.017	0.002	0.002	0.002	0.002	-0.021	0.004	0.004	0.079	-0.135

7.2. Presentation of molecule:

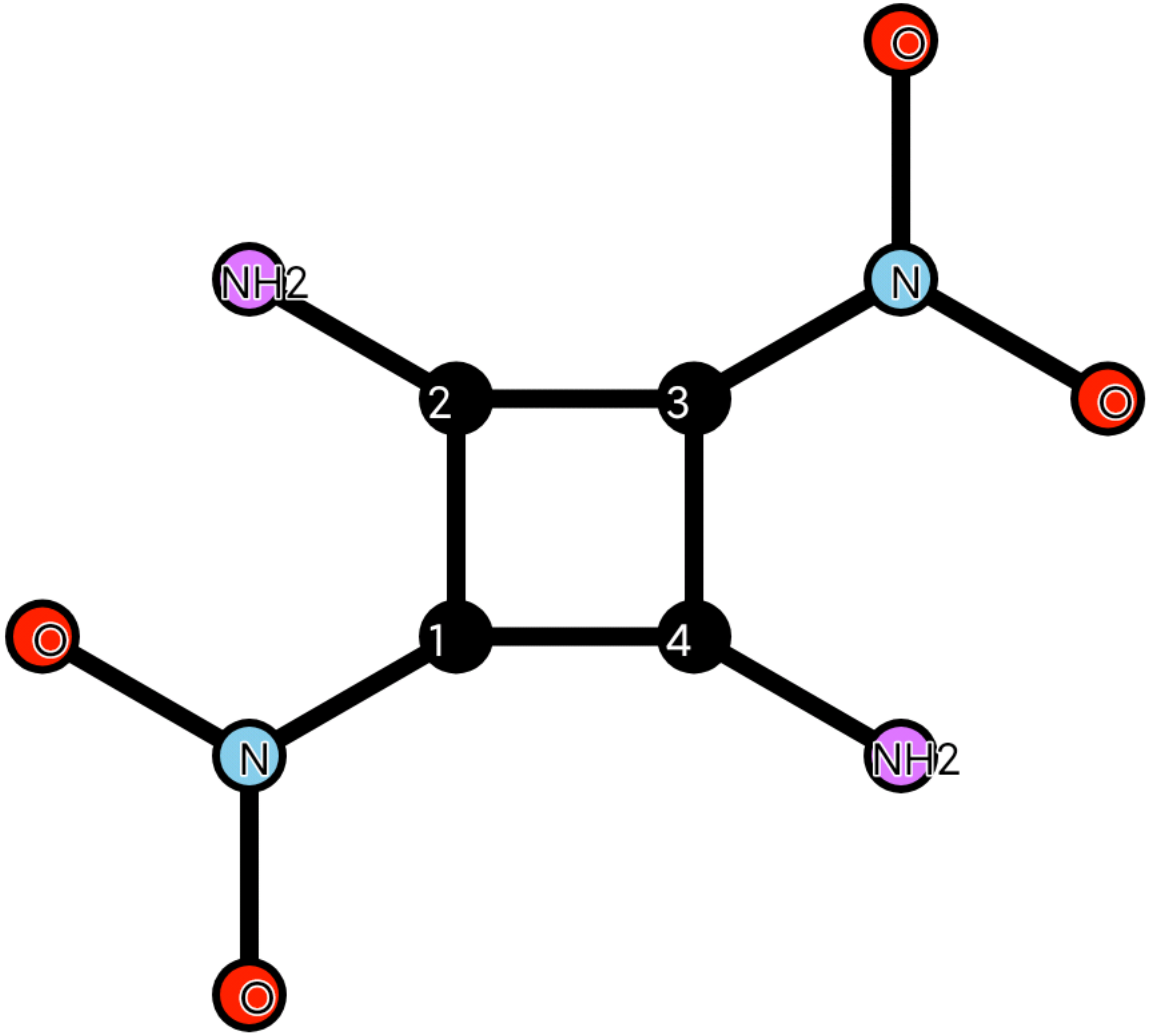

O
NH2
N
2
3
O
O
1
4
N
NH2
O

8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 4	1 8	2 3	2 5	3 4	3 7	4 6	7 9	7 10	8 11	8 12
1 2	0.524											
1 4	-0.266	0.524										
1 8	-0.091	-0.091	0.265									
2 3	-0.266	0.09	0.047	0.524								
2 5	-0.147	0.082	0.016	-0.147	0.312							
3 4	0.09	-0.266	0.047	-0.266	0.082	0.524						
3 7	0.047	0.047	-0.031	-0.091	0.016	-0.091	0.265					
4 6	0.082	-0.147	0.016	0.082	-0.087	-0.147	0.016	0.312				
7 9	-0.02	-0.02	0.015	0.032	-0.005	0.032	-0.114	-0.005	0.213			
7 10	-0.02	-0.02	0.015	0.032	-0.005	0.032	-0.114	-0.005	-0.099	0.213		
8 11	0.032	0.032	-0.114	-0.02	-0.005	-0.02	0.015	-0.005	-0.007	-0.007	0.213	
8 12	0.032	0.032	-0.114	-0.02	-0.005	-0.02	0.015	-0.005	-0.007	-0.007	-0.099	0.213

8.2. Presentation of molecule:


O
NH2
N
2
3
O
O
1
4
N
NH2
O