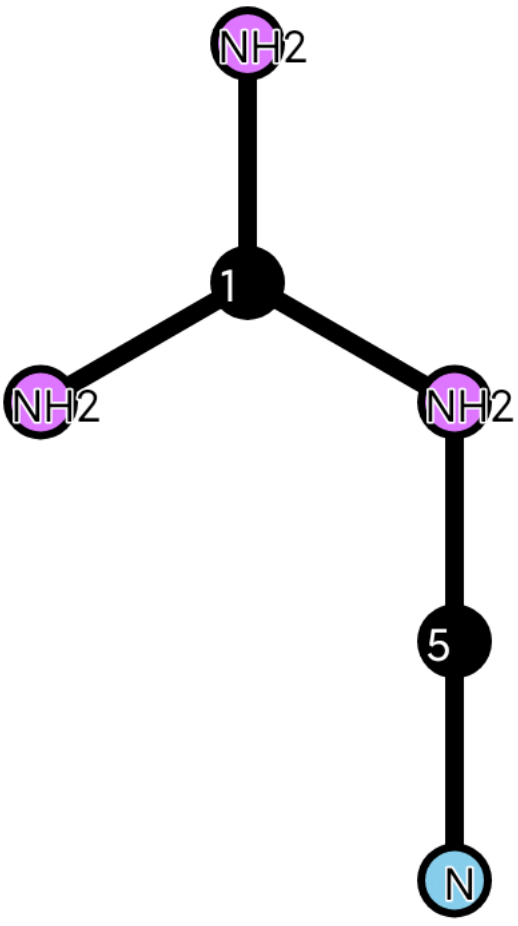
Print calculated values

Report generated by:root, 24.03.2020 - 20:52:42

The following determinant is calculated:

-x	1.3	1.3	1.3	0.0	0.0
1.3	-x+1.47	0.0	0.0	1.3	0.0
1.3	0.0	-x+1.47	0.0	0.0	0.0
1.3	0.0	0.0	-x+1.47	0.0	0.0
0.0	1.3	0.0	0.0	-x	1.66
0.0	0.0	0.0	0.0	1.66	-x+1.47

It is about this molecule:

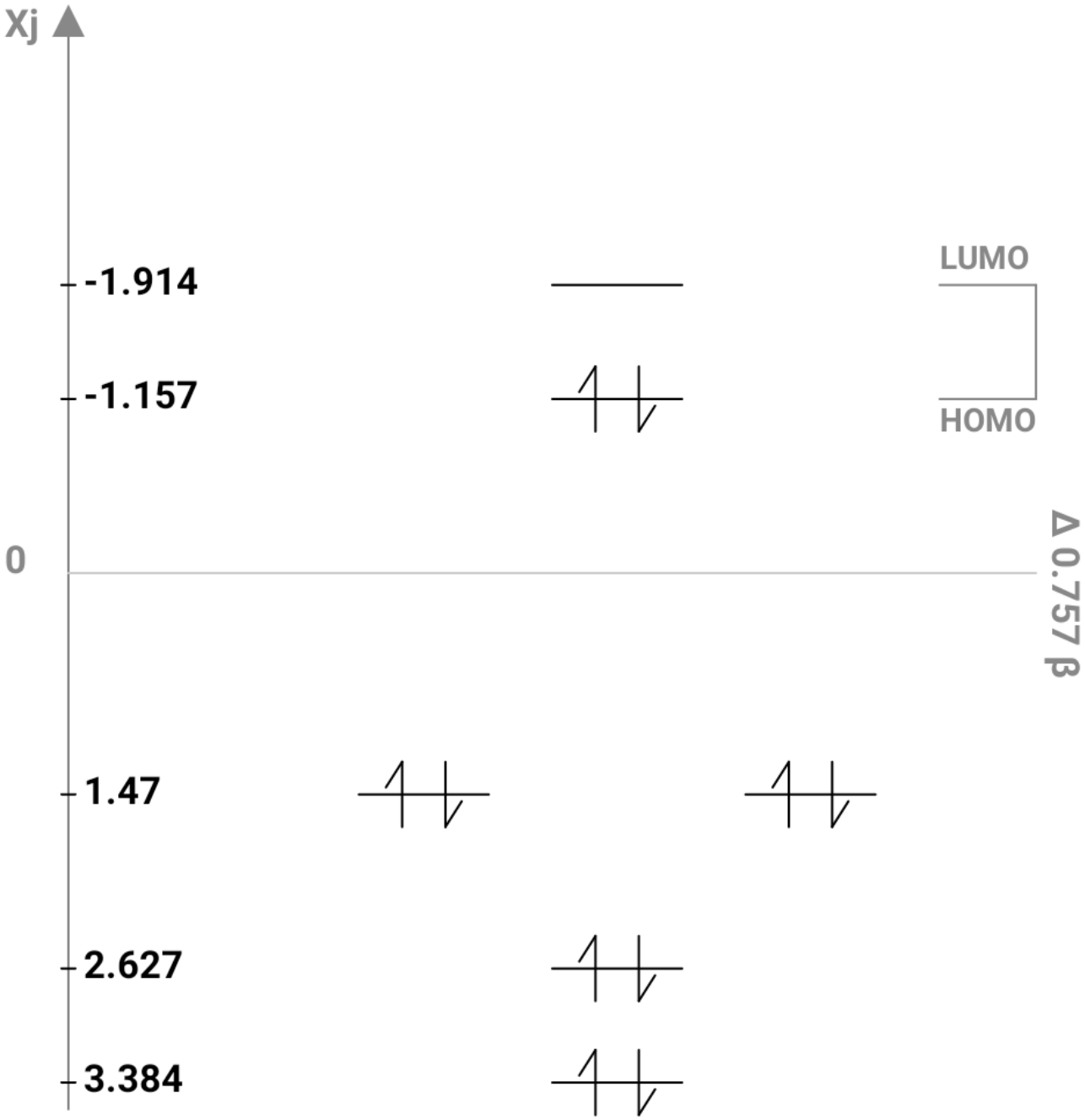


HMO-Energies

x1 = 3.384; x2 = 2.627; x3 = 1.47; x4 = 1.47; x5 = -1.157; x6 = -1.914;

1. Energy-eigenvalues

1.1. Calculated values:



total Power Eπ: 6α + 15.588β -

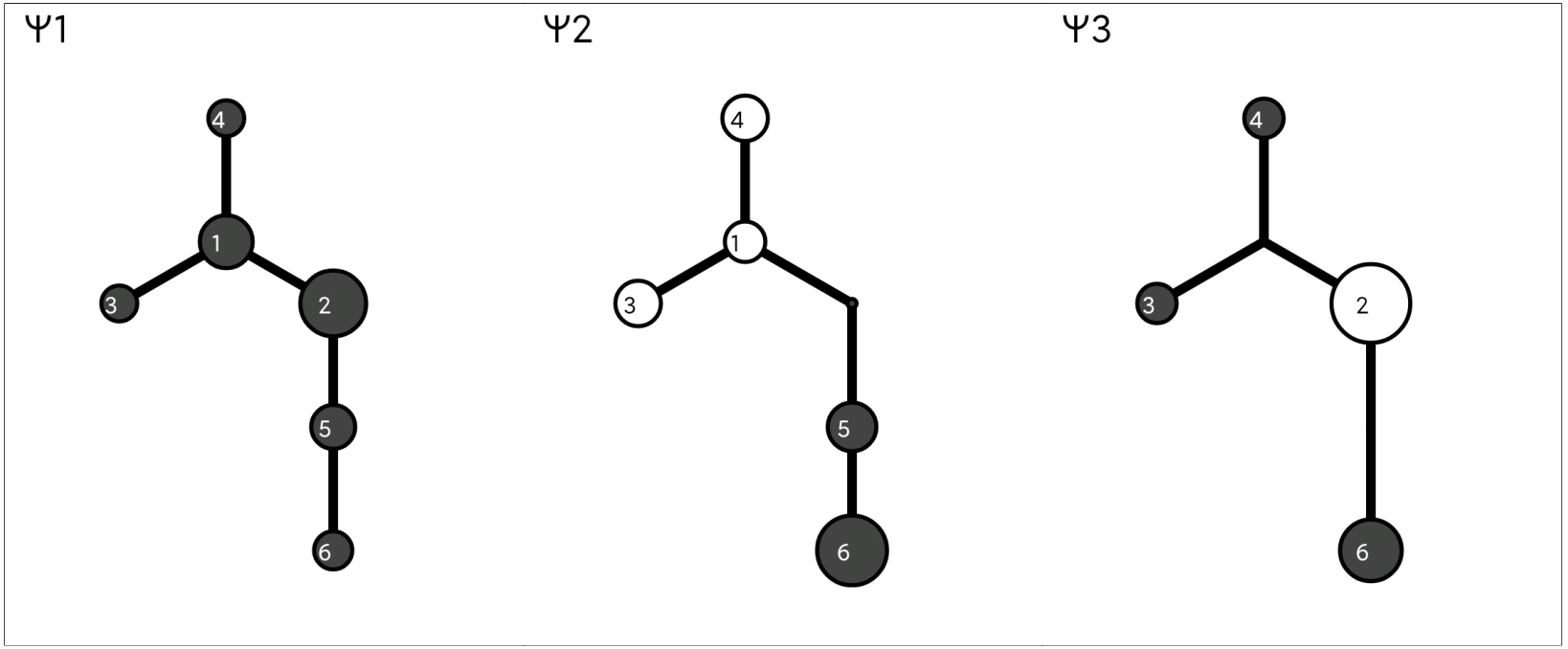
this corresponds to one πelectron: 1.559β

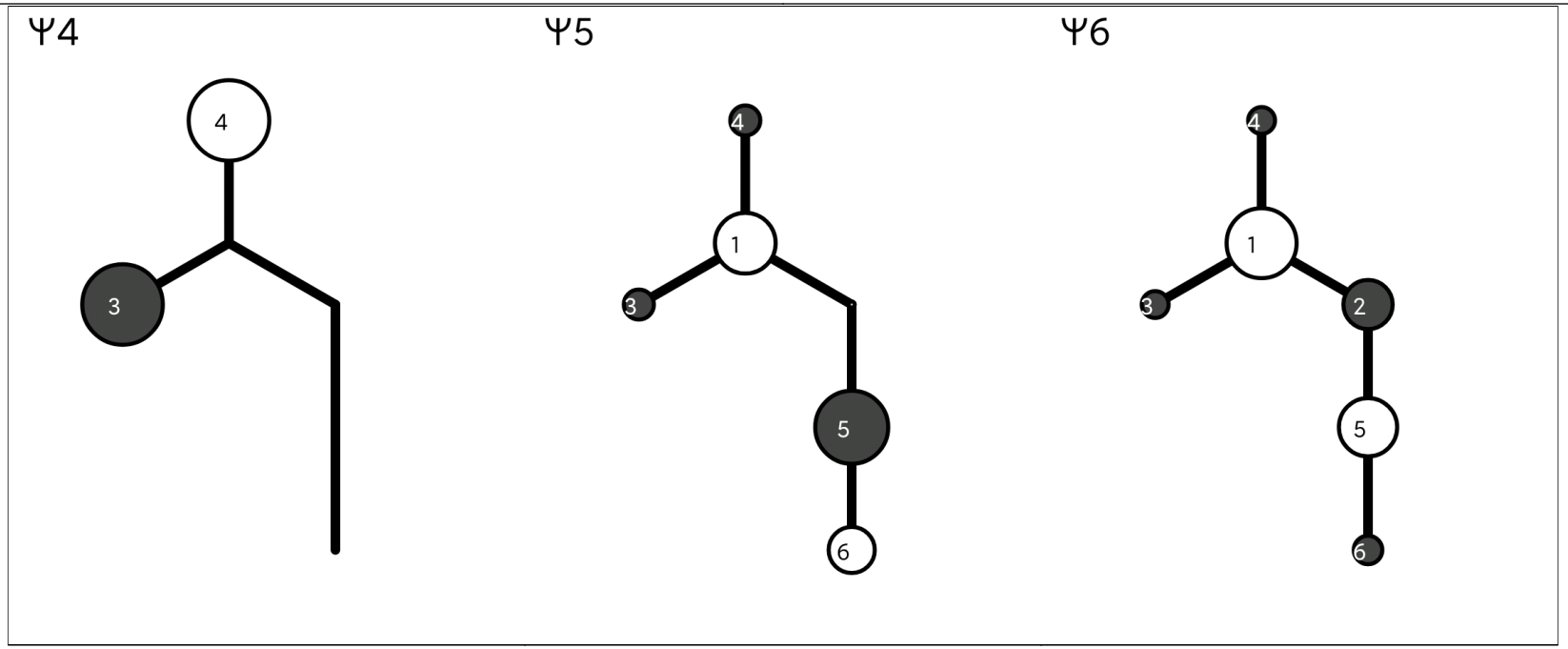
2. Hueckel-coefficient

2.1. Calculated values:

	Psi 1	Psi 2	Psi 3	Psi 4	Psi 5	Psi 6
	x1= 3.384	x2= 2.627	x3= 1.47	x4= 1.47	x5= -1.157	x6= -1.914
1	-0.462	0.354	0.0	0.0	0.533	0.614
2	-0.575	-0.08	0.688	0.0	0.053	-0.432
3	-0.314	0.397	-0.344	-0.707	-0.264	-0.236
4	-0.314	0.397	-0.344	0.707	-0.264	-0.236
5	-0.384	-0.425	0.0	0.0	-0.64	0.511
6	-0.333	-0.61	-0.539	0.0	0.405	-0.251

2.2. Molecule orbital presentation:



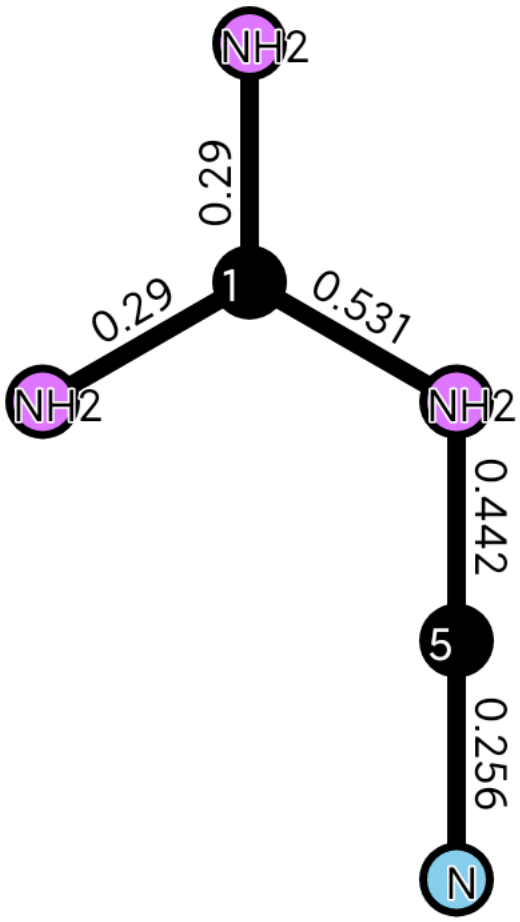

Ψ4
4
3
Ψ5
4
1
3
5
6
Ψ6
4
1
3
2
5
6

3. Bond Order

3.1. Calculated values:

	1	2	3	4	5	6
1	1.245					
2	0.531	1.626				
3	0.29	-0.204	1.889			
4	0.29	-0.204	-0.111	1.889		
5	-0.628	0.442	0.241	0.241	1.477	
6	0.308	-0.217	-0.118	-0.118	0.256	1.874

3.2. Presentation of bond order:

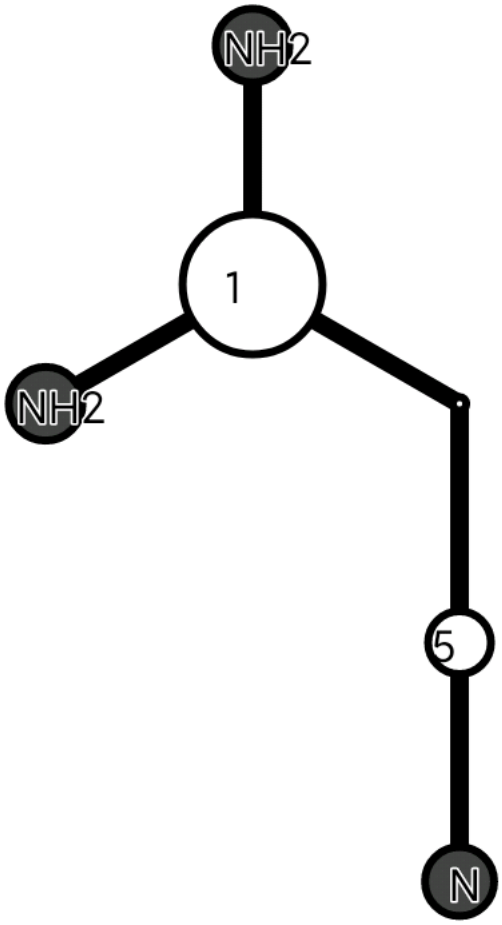


4. Net Charge

4.1. Calculated values:

	1	2	3	4	5	6
1	0.421					
2		0.041				
3			-0.222			
4				-0.222		
5					0.189	
6						-0.208

4.2. Presentation of molecule:

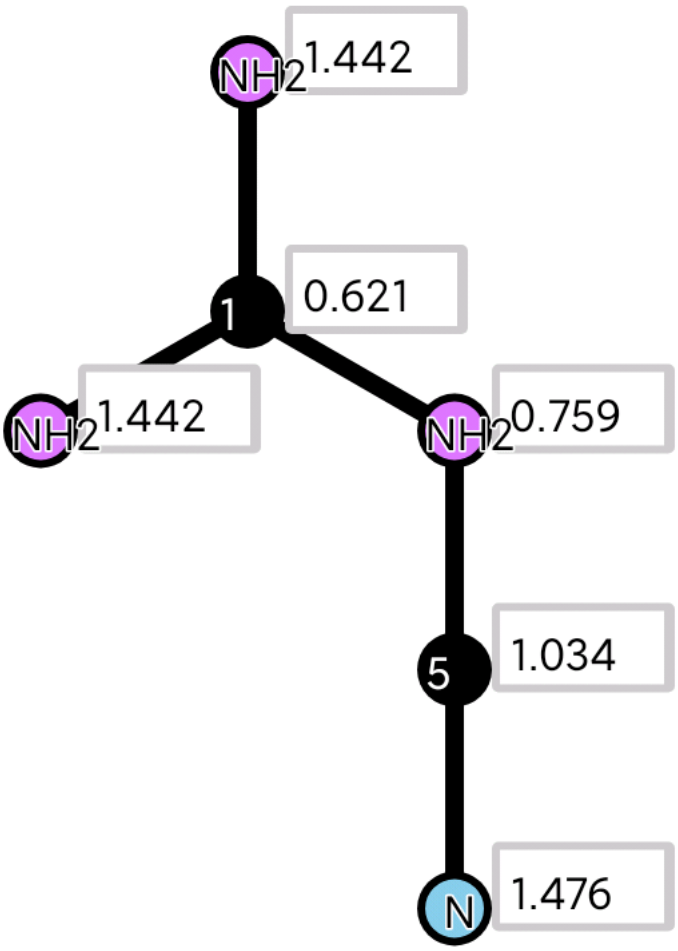


5. Free valences

5.1. Calculated values:

1	2	3	4	5	6
0.621	0.759	1.442	1.442	1.034	1.476

5.2. Presentation of molecule:

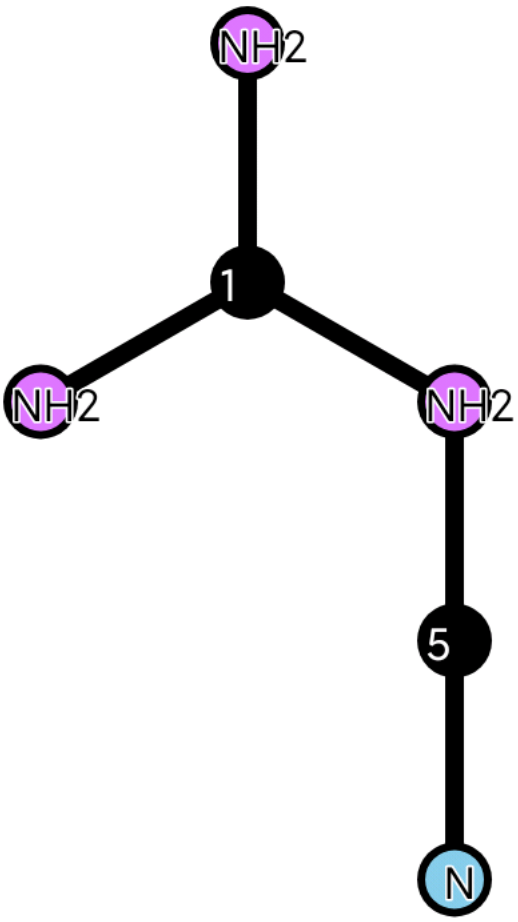


6. Atom-Atom-Polarizability

6.1. Calculated values:

	1	2	3	4	5	6
1	0.669					
2	-0.086	0.155				
3	0.074	-0.025	0.073			
4	0.074	-0.025	0.007	0.073		
5	-0.566	-0.004	-0.101	-0.101	0.637	
6	-0.164	-0.015	-0.028	-0.028	0.134	0.102

6.2. Presentation of molecule:

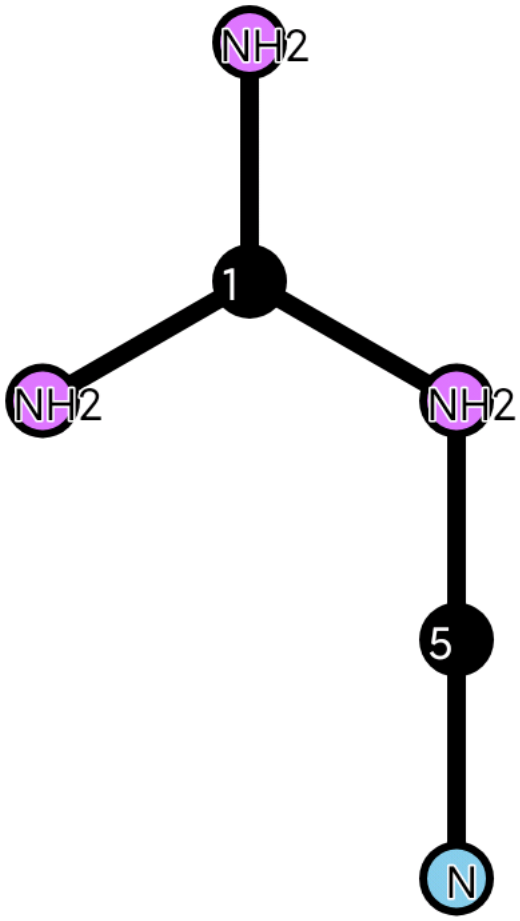


7. Bond-Atom-Polarizability

7.1. Calculated values:

	1	2	3	4	5	6
1 2	-0.174	-0.08	-0.008	-0.008	0.202	0.068
1 3	-0.225	0.049	-0.109	-0.024	0.24	0.068
1 4	-0.225	0.049	-0.024	-0.109	0.24	0.068
2 5	0.29	-0.09	0.057	0.057	-0.267	-0.048
5 6	0.306	0.016	0.054	0.054	-0.293	-0.137

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

	1 2	1 3	1 4	2 5	5 6
1 2	0.236				
1 3	0.088	0.371			
1 4	0.088	0.148	0.371		
2 5	-0.076	-0.261	-0.261	0.333	
5 6	-0.238	-0.257	-0.257	0.229	0.422

8.2. Presentation of molecule: