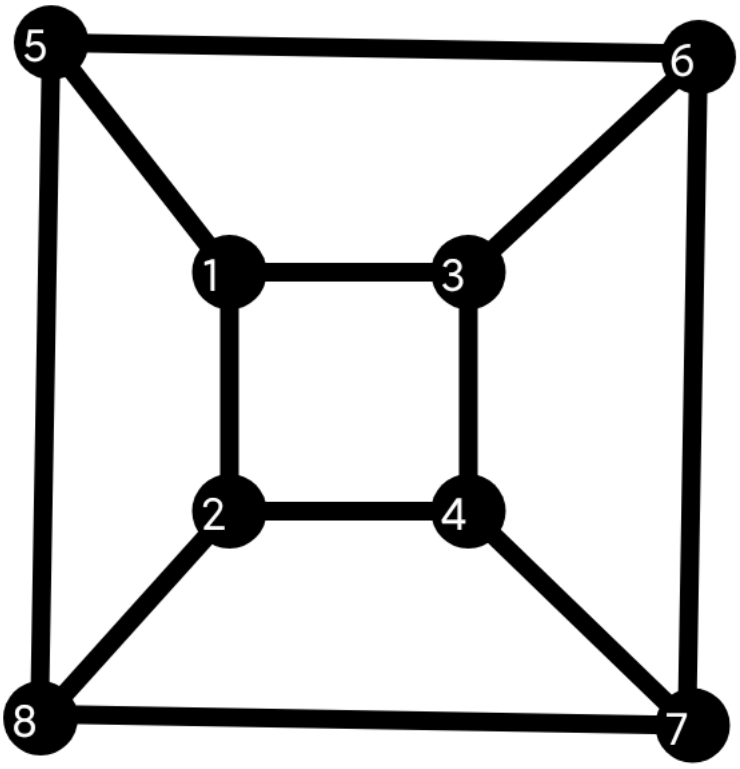
# Print calculated values

*Report generated by:root, 18.02.2020 - 21:11:11*

## The following determinant is calculated:

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| -x | 1.0 | 1.0 | 0.0 | 1.0 | 0.0 | 0.0 | 0.0 |
| 1.0 | -x | 0.0 | 1.0 | 0.0 | 0.0 | 0.0 | 1.0 |
| 1.0 | 0.0 | -x | 1.0 | 0.0 | 1.0 | 0.0 | 0.0 |
| 0.0 | 1.0 | 1.0 | -x | 0.0 | 0.0 | 1.0 | 0.0 |
| 1.0 | 0.0 | 0.0 | 0.0 | -x | 1.0 | 0.0 | 1.0 |
| 0.0 | 0.0 | 1.0 | 0.0 | 1.0 | -x | 1.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 1.0 | 0.0 | 1.0 | -x | 1.0 |
| 0.0 | 1.0 | 0.0 | 0.0 | 1.0 | 0.0 | 1.0 | -x |

## It is about this molecule:

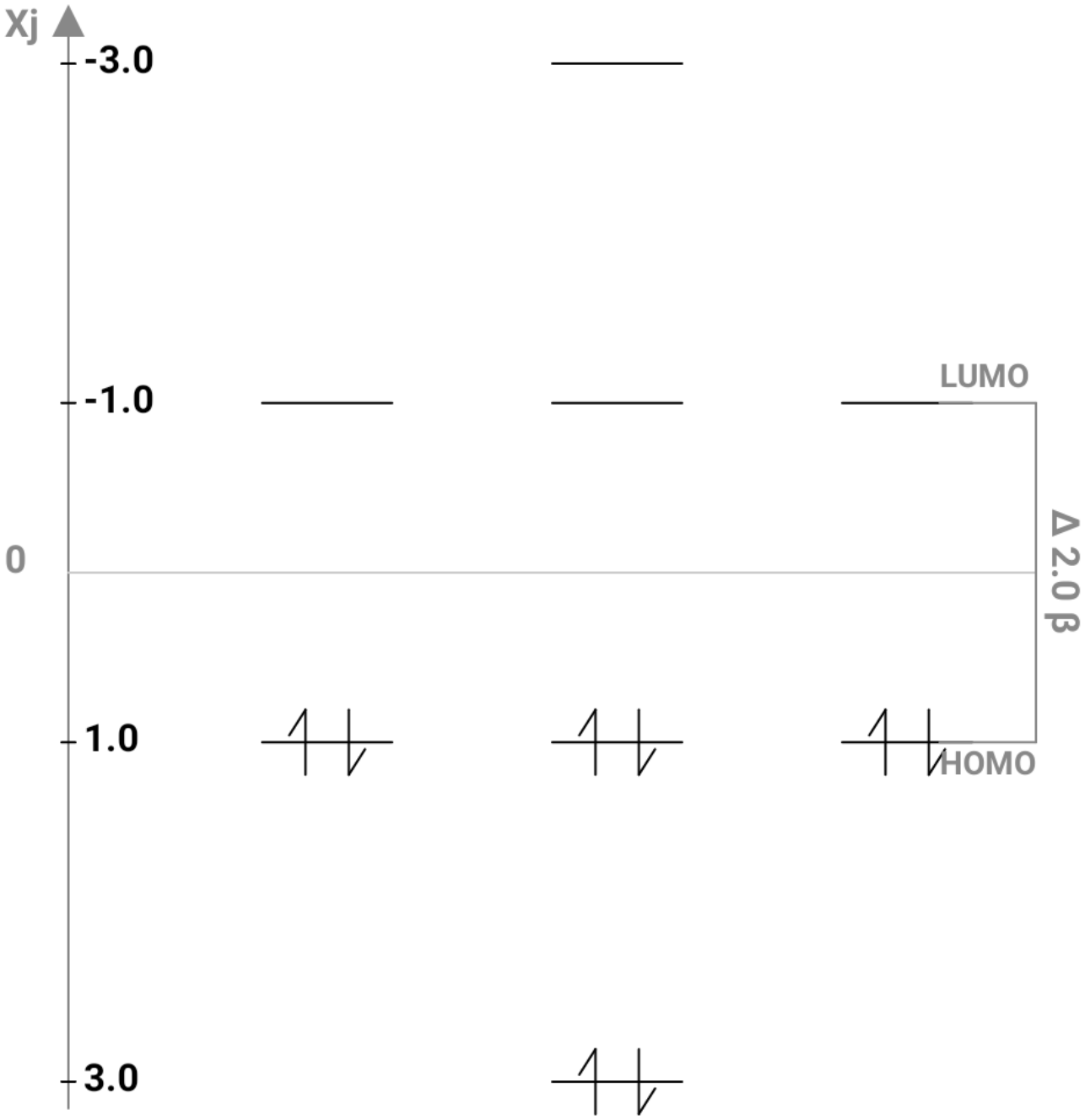



## HMO-Energies

**x1 = 3.0; x2 = 1.0; x3 = 1.0; x4 = 1.0; x5 = -1.0; x6 = -1.0; x7 = -1.0; x8 = -3.0;**

# 1. Energy-eigenvalues

## 1.1. Calculated values:




**total Power Eπ: 8α + 12.0β -**

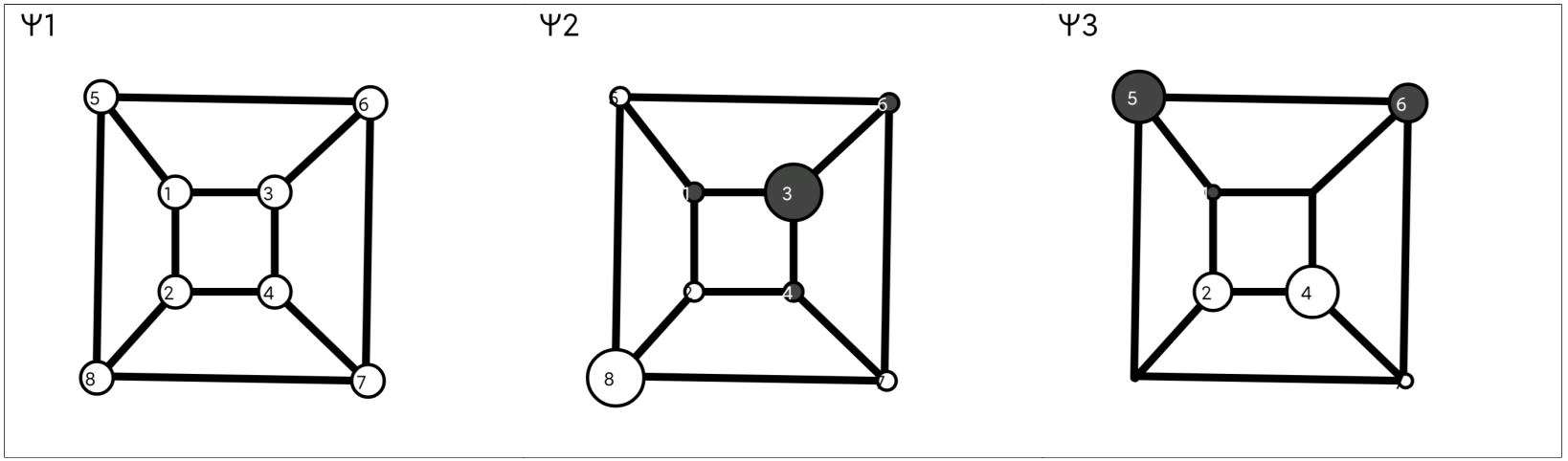
**this corresponds to one πelectron: 1.5β**

# 2. Hueckel-coefficient

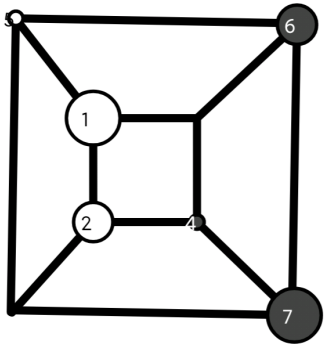
## 2.1. Calculated values:

| | Psi 1 | Psi 2 | Psi 3 | Psi 4 | Psi 5 | Psi 6 | Psi 7 | Psi 8 |
|---|---|---|---|---|---|---|---|---|
| | x1= 3.0 | x2= 1.0 | x3= 1.0 | x4= 1.0 | x5= -1.0 | x6= -1.0 | x7= -1.0 | x8= -3.0 |
| **1** | 0.354 | -0.204 | -0.149 | 0.558 | 0.149 | -0.558 | -0.204 | 0.354 |
| **2** | 0.354 | 0.204 | 0.408 | 0.408 | 0.408 | 0.408 | -0.204 | -0.354 |
| **3** | 0.354 | -0.612 | 0.0 | 0.0 | 0.0 | 0.0 | 0.612 | -0.354 |
| **4** | 0.354 | -0.204 | 0.558 | -0.149 | -0.558 | 0.149 | -0.204 | 0.354 |
| **5** | 0.354 | 0.204 | -0.558 | 0.149 | -0.558 | 0.149 | -0.204 | -0.354 |
| **6** | 0.354 | -0.204 | -0.408 | -0.408 | 0.408 | 0.408 | -0.204 | 0.354 |
| **7** | 0.354 | 0.204 | 0.149 | -0.558 | 0.149 | -0.558 | -0.204 | -0.354 |
| **8** | 0.354 | 0.612 | 0.0 | 0.0 | 0.0 | 0.0 | 0.612 | 0.354 |

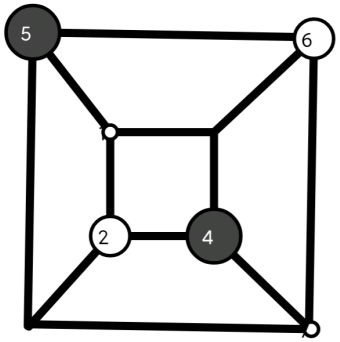
## 2.2. Molecule orbital presentation:



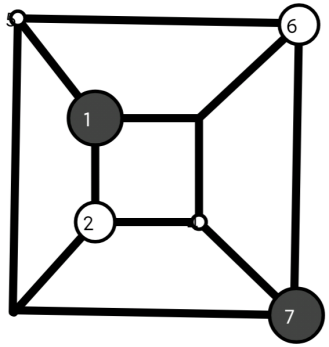
Ψ4



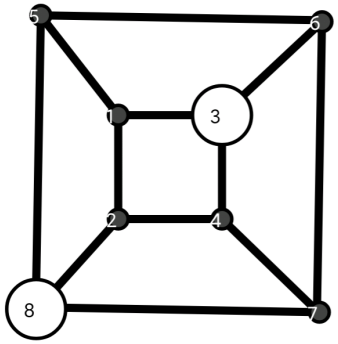

Ψ5



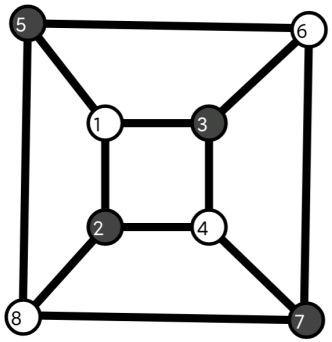

Ψ6




Ψ7




Ψ8

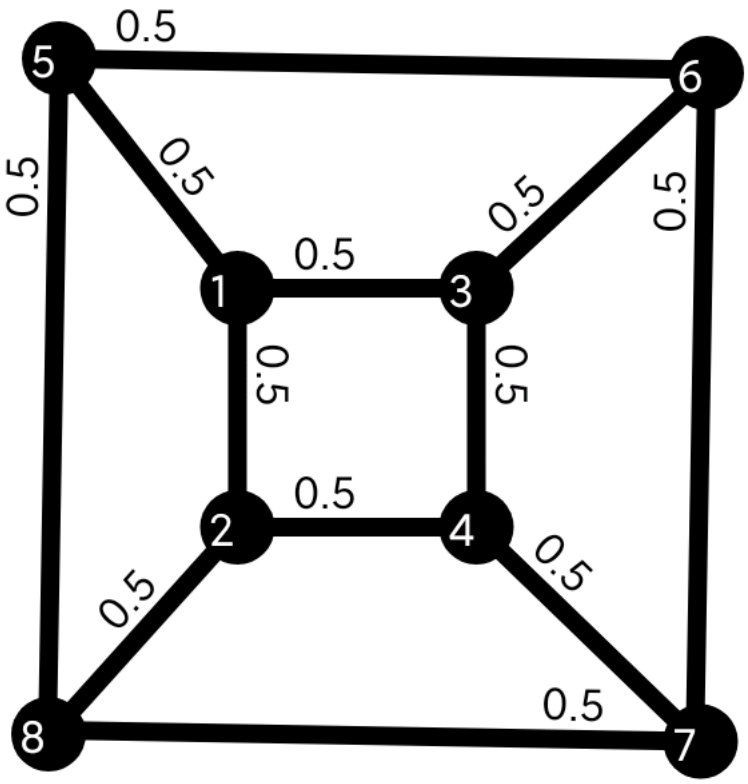


# 3. Bond Order

## 3.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| **1** | 1.0 | | | | | | | |
| **2** | 0.5 | 1.0 | | | | | | |
| **3** | 0.5 | 0.0 | 1.0 | | | | | |
| **4** | 0.0 | 0.5 | 0.5 | 1.0 | | | | |
| **5** | 0.5 | 0.0 | 0.0 | -0.5 | 1.0 | | | |
| **6** | 0.0 | -0.5 | 0.5 | 0.0 | 0.5 | 1.0 | | |
| **7** | -0.5 | 0.0 | 0.0 | 0.5 | 0.0 | 0.5 | 1.0 | |
| **8** | 0.0 | 0.5 | -0.5 | 0.0 | 0.5 | 0.0 | 0.5 | 1.0 |

## 3.2. Presentation of bond order:

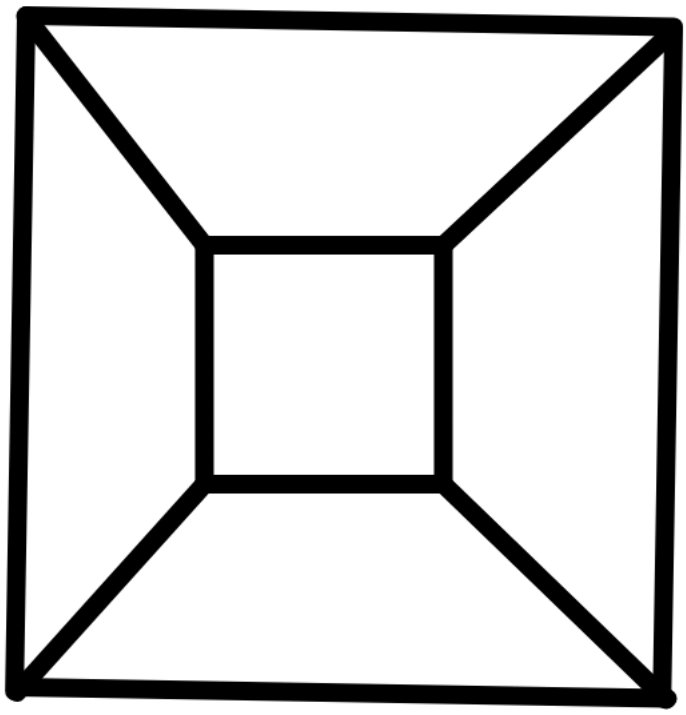


# 4. Net Charge

## 4.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| **1** | 0.0 | | | | | | | |
| **2** | | 0.0 | | | | | | |
| **3** | | | 0.0 | | | | | |
| **4** | | | | 0.0 | | | | |
| **5** | | | | | 0.0 | | | |
| **6** | | | | | | 0.0 | | |
| **7** | | | | | | | 0.0 | |
| **8** | | | | | | | | 0.0 |

## 4.2. Presentation of molecule:

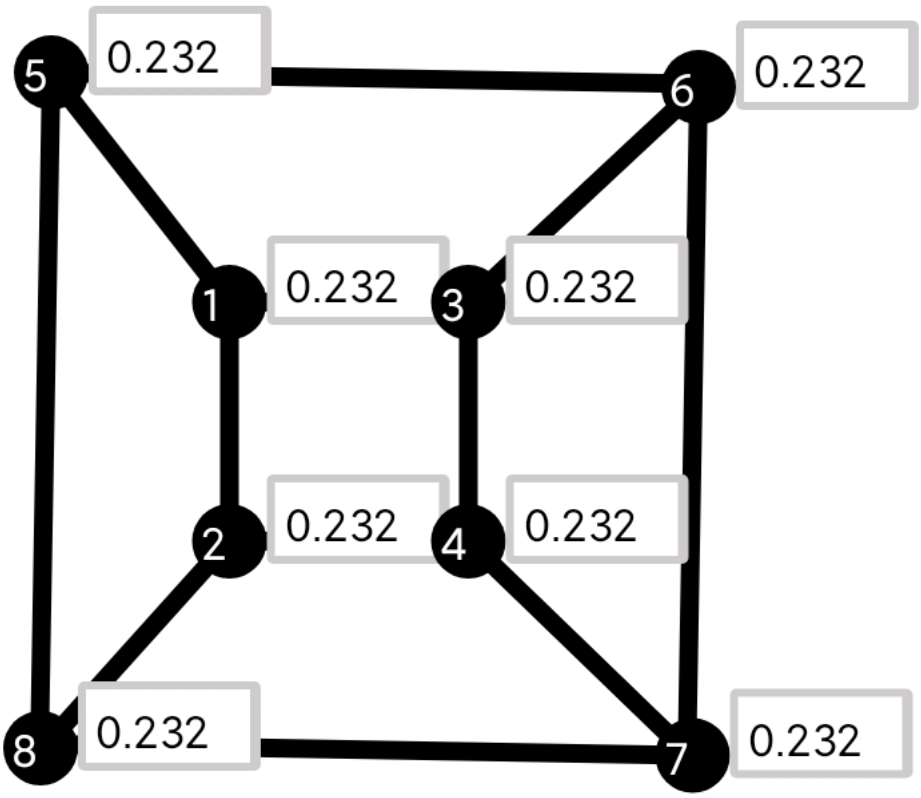


# 5. Free valences

## 5.1. Calculated values:

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|
| 0.232 | 0.232 | 0.232 | 0.232 | 0.232 | 0.232 | 0.232 | 0.232 |

## 5.2. Presentation of molecule:

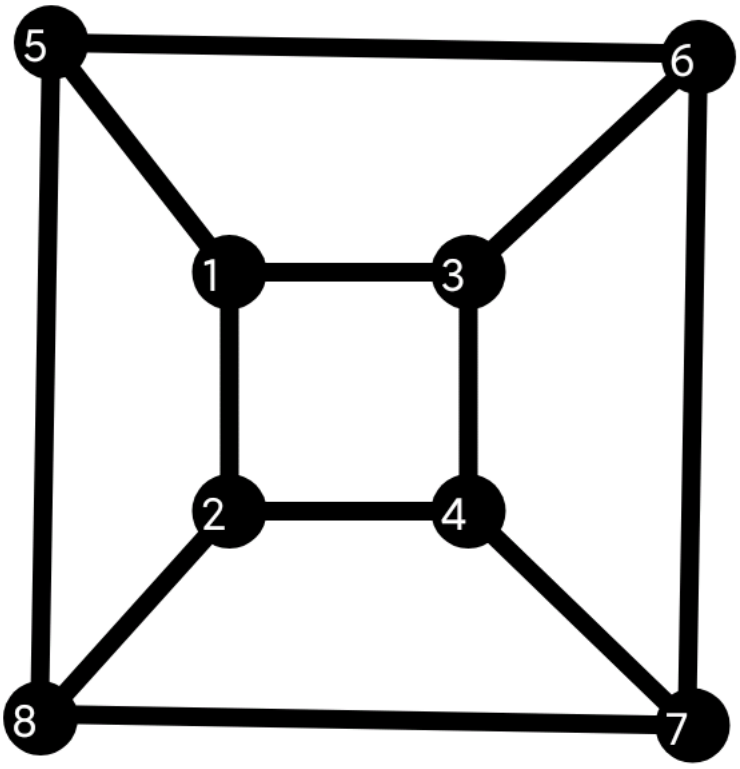


# 6. Atom-Atom-Polarizability

## 6.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| **1** | 0.385 | | | | | | | |
| **2** | -0.073 | 0.385 | | | | | | |
| **3** | -0.073 | 0.01 | 0.385 | | | | | |
| **4** | 0.01 | -0.073 | -0.073 | 0.385 | | | | |
| **5** | -0.073 | 0.01 | 0.01 | -0.198 | 0.385 | | | |
| **6** | 0.01 | -0.198 | -0.073 | 0.01 | -0.073 | 0.385 | | |
| **7** | -0.198 | 0.01 | 0.01 | -0.073 | 0.01 | -0.073 | 0.385 | |
| **8** | 0.01 | -0.073 | -0.198 | 0.01 | -0.073 | 0.01 | -0.073 | 0.385 |

## 6.2. Presentation of molecule:

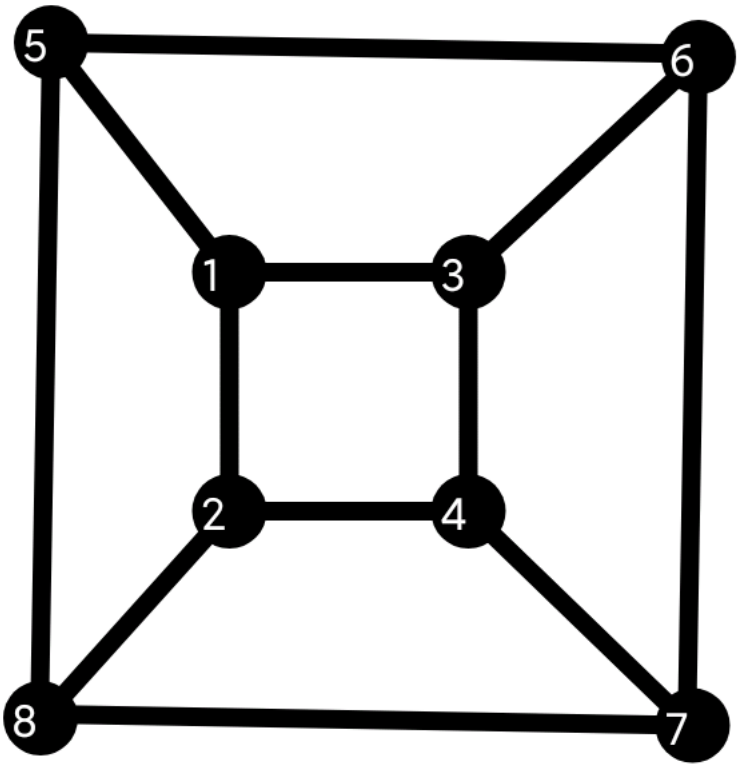


# 7. Bond-Atom-Polarizability

## 7.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| **1 2** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **1 3** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **1 5** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **2 4** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **2 8** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **3 4** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **3 6** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **4 7** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **5 6** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **5 8** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **6 7** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **7 8** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

## 7.2. Presentation of molecule:



# 8. Bond-Bond-Polarizability

## 8.1. Calculated values:

| | 1 2 | 1 3 | 1 5 | 2 4 | 2 8 | 3 4 | 3 6 | 4 7 | 5 6 | 5 8 | 6 7 | 7 8 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1 2** | 0.312 | | | | | | | | | | | |
| **1 3** | -0.125 | 0.312 | | | | | | | | | | |
| **1 5** | -0.125 | -0.125 | 0.312 | | | | | | | | | |
| **2 4** | -0.125 | -0.063 | 0.125 | 0.312 | | | | | | | | |
| **2 8** | -0.125 | 0.125 | -0.063 | -0.125 | 0.312 | | | | | | | |
| **3 4** | -0.062 | -0.125 | 0.125 | -0.125 | 0.125 | 0.312 | | | | | | |
| **3 6** | 0.125 | -0.125 | -0.062 | 0.125 | -0.187 | -0.125 | 0.312 | | | | | |
| **4 7** | 0.125 | 0.125 | -0.187 | -0.125 | -0.062 | -0.125 | -0.063 | 0.312 | | | | |
| **5 6** | 0.125 | -0.062 | -0.125 | -0.188 | 0.125 | 0.125 | -0.125 | 0.125 | 0.313 | | | |
| **5 8** | -0.062 | 0.125 | -0.125 | 0.125 | -0.125 | -0.187 | 0.125 | 0.125 | -0.125 | 0.312 | | |
| **6 7** | -0.187 | 0.125 | 0.125 | 0.125 | 0.125 | -0.063 | -0.125 | -0.125 | -0.125 | -0.062 | 0.313 | |
| **7 8** | 0.125 | -0.187 | 0.125 | -0.062 | -0.125 | 0.125 | 0.125 | -0.125 | -0.062 | -0.125 | -0.125 | 0.312 |

## 8.2. Presentation of molecule: