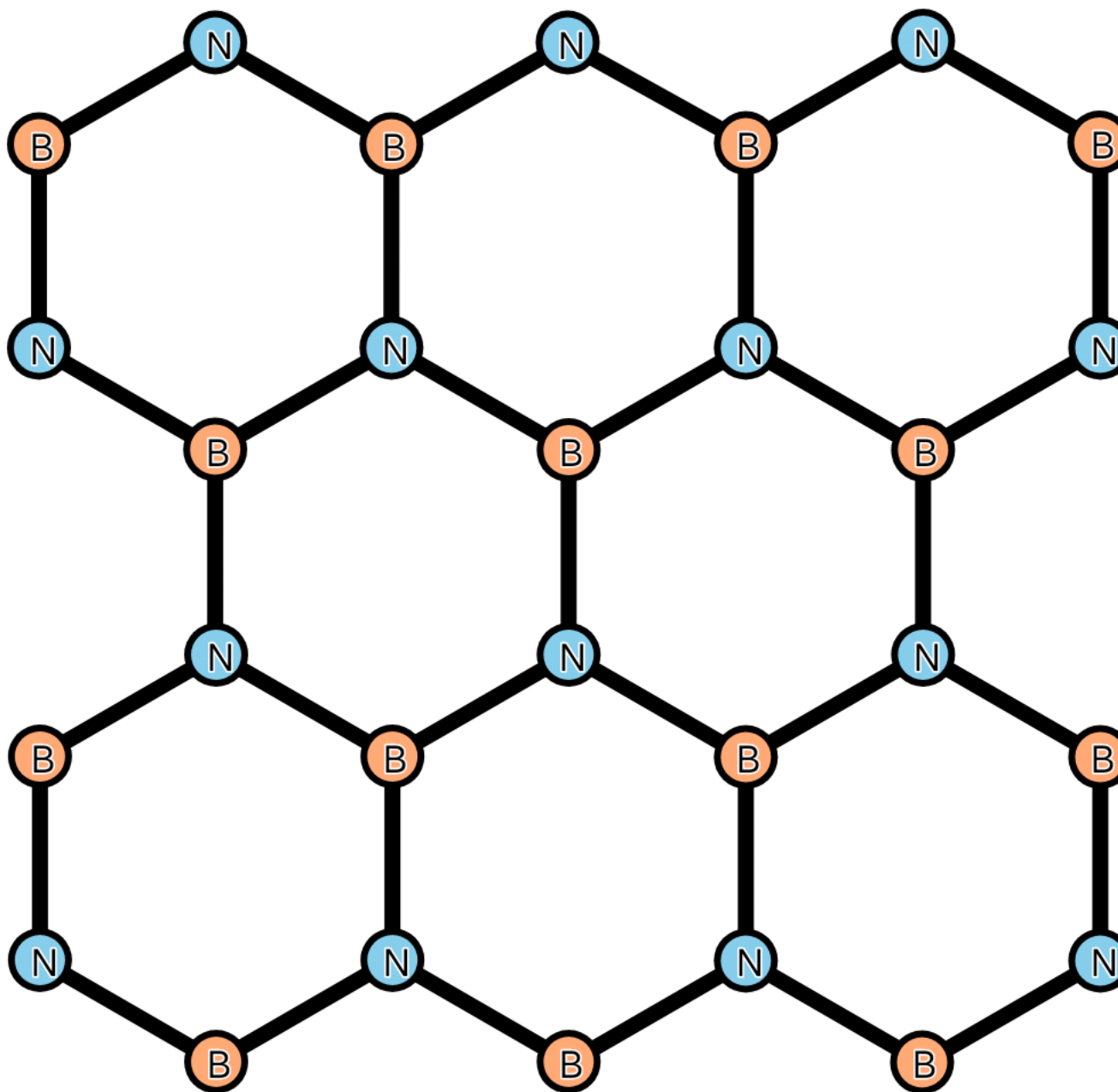


Report generated by:root, 20.01.2020 - 18:00:45

[illegible]

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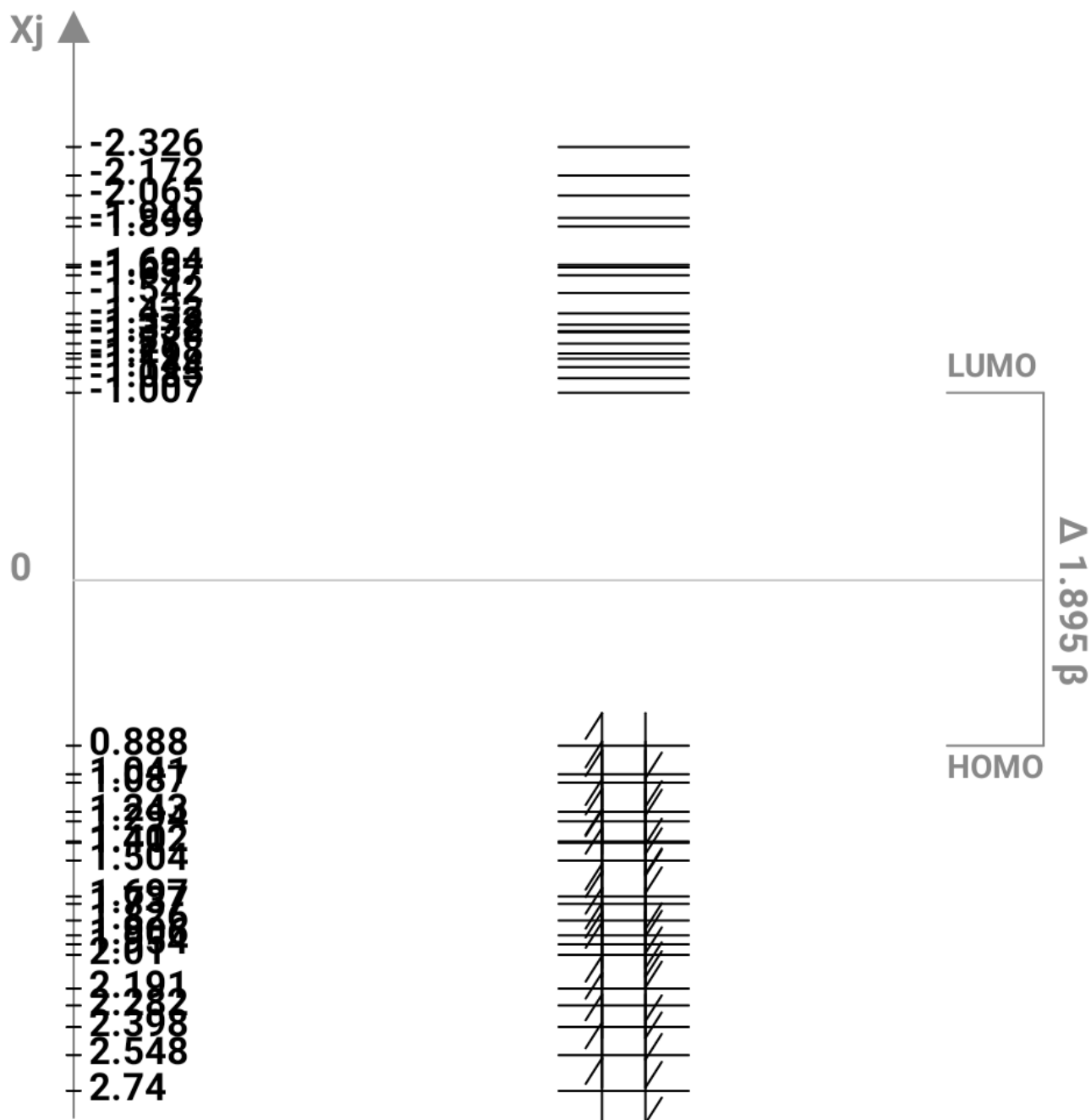
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$x_1 = 2.74$; $x_2 = 2.548$; $x_3 = 2.398$; $x_4 = 2.282$; $x_5 = 2.191$; $x_6 = 2.01$; $x_7 = 1.954$; $x_8 = 1.906$;
 $x_9 = 1.826$; $x_{10} = 1.737$; $x_{11} = 1.697$; $x_{12} = 1.504$; $x_{13} = 1.41$; $x_{14} = 1.402$; $x_{15} = 1.294$; $x_{16} = 1.243$;
 $x_{17} = 1.087$; $x_{18} = 1.041$; $x_{19} = 0.888$; $x_{20} = -1.007$; $x_{21} = -1.085$; $x_{22} = -1.144$; $x_{23} = -1.19$; $x_{24} = -1.218$;
 $x_{25} = -1.27$; $x_{26} = -1.332$; $x_{27} = -1.338$; $x_{28} = -1.372$; $x_{29} = -1.432$; $x_{30} = -1.542$; $x_{31} = -1.637$; $x_{32} = -1.68$;
 $x_{33} = -1.694$; $x_{34} = -1.899$; $x_{35} = -1.944$; $x_{36} = -2.065$; $x_{37} = -2.172$; $x_{38} = -2.326$;

1. Energy-eigenvalues

1.1. Calculated values:



total Power E_π : $38\alpha + 66.316\beta$ -

this corresponds to one π electron: 1.745β

2. Hueckel-coefficient

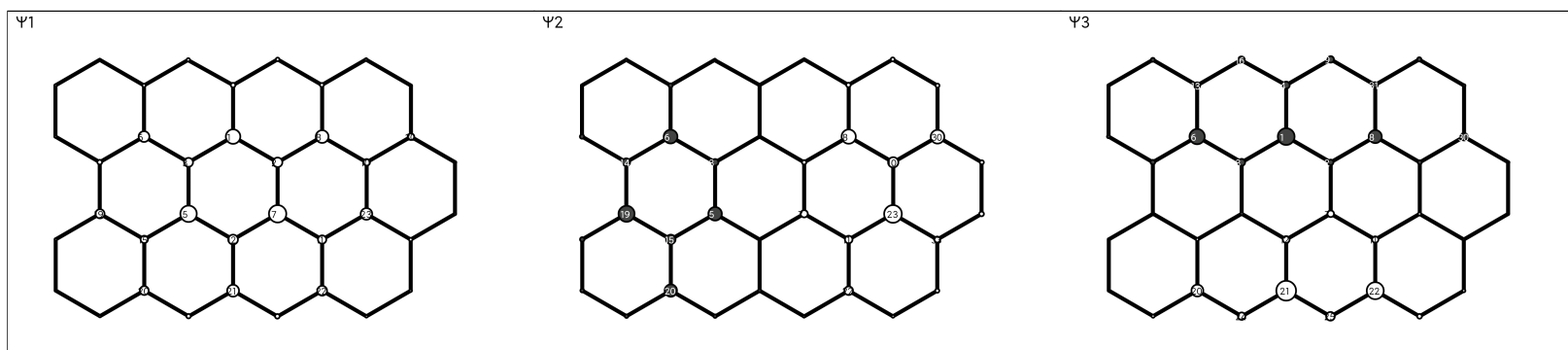
2.1. Calculated values:

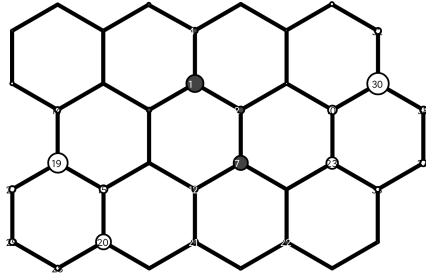
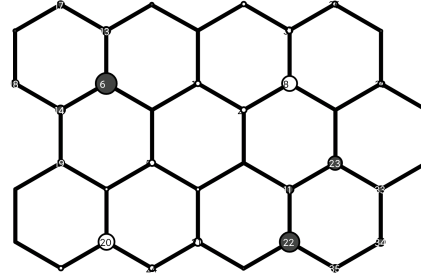
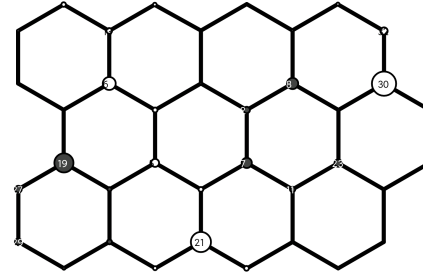
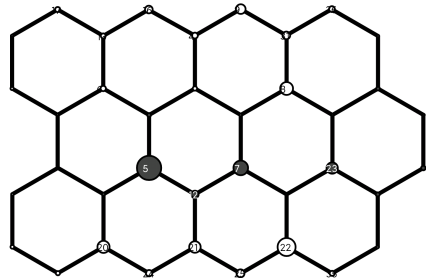
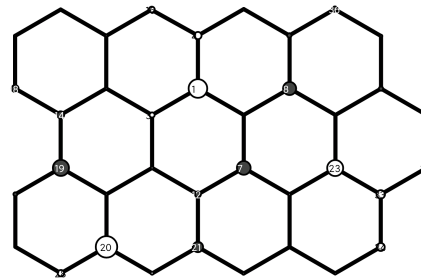
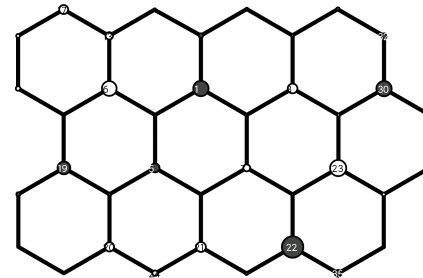
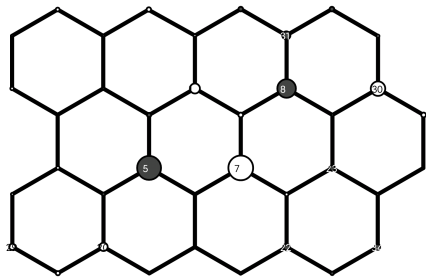
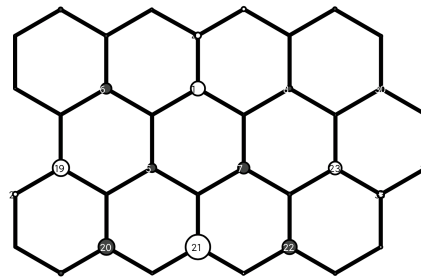
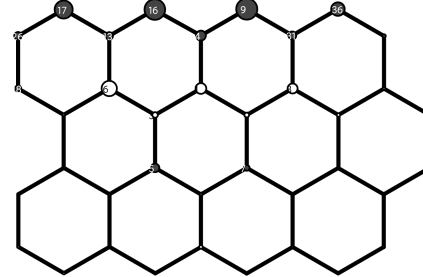
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|----|---------|----------|----------|----------|----------|---------|----------|----------|----------|-----------|-----------|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|----------|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|
| | x1=2.74 | x2=2.548 | x3=2.398 | x4=2.282 | x5=2.191 | x6=2.01 | x7=1.954 | x8=1.906 | x9=1.826 | x10=1.737 | x11=1.697 | x12=1.504 | x13=1.41 | x14=1.402 | x15=1.294 | x16=1.243 | x17=1.087 | x18=1.041 | x19=0.888 | x20=1.007 | x21=1.085 | x22=1.144 | x23=1.19 | x24=1.218 | x25=1.27 | x26=1.332 | x27=1.338 | x28=1.372 | x29=1.432 | x30=1.542 | x31=1.637 | x32=1.68 | x33=1.694 | x34=1.899 | x35=1.944 | x36=2.065 | x37=2.172 | x38=2.326 |
| 1 | 0.304 | -0.043 | -0.352 | -0.348 | 0.11 | -0.052 | 0.089 | 0.379 | -0.313 | 0.204 | 0.299 | 0.219 | -0.045 | 0.168 | 0.132 | 0.103 | -0.115 | 0.105 | 0.017 | -0.003 | -0.078 | -0.022 | -0.025 | -0.026 | 0.079 | 0.129 | 0.05 | -0.082 | 0.009 | -0.007 | -0.044 | -0.162 | 0.045 | -0.074 | -0.118 | 0.119 | 0.041 | 0.183 |
| 2 | 0.2 | 0.092 | -0.115 | -0.141 | 0.114 | -0.13 | 0.015 | -0.046 | 0.007 | 0.097 | -0.017 | 0.098 | -0.094 | 0.026 | -0.011 | -0.013 | -0.036 | 0.025 | -0.014 | -0.137 | 0.187 | -0.061 | -0.404 | -0.223 | -0.037 | -0.243 | -0.265 | 0.176 | 0.166 | 0.219 | 0.3 | 0.144 | 0.182 | 0.077 | 0.271 | -0.111 | 0.108 | -0.316 |
| 3 | 0.187 | -0.139 | -0.145 | -0.096 | -0.048 | 0.099 | -0.084 | 0.104 | -0.055 | 0.088 | -0.028 | 0.114 | 0.021 | -0.011 | 0.023 | 0.065 | -0.006 | 0.022 | 0.026 | 0.186 | 0.137 | 0.173 | 0.33 | 0.263 | 0.051 | -0.253 | -0.257 | -0.152 | -0.192 | -0.212 | -0.111 | 0.411 | 0.105 | 0.121 | 0.074 | -0.06 | -0.227 | -0.301 |
| 4 | 0.096 | -0.012 | -0.148 | -0.115 | 0.032 | -0.005 | 0.129 | 0.149 | -0.092 | 0.059 | 0.127 | -0.202 | 0.076 | -0.029 | -0.041 | 0.082 | 0.097 | -0.103 | -0.024 | -0.04 | -0.074 | -0.218 | 0.156 | 0.047 | -0.285 | 0.042 | 0.342 | 0.273 | -0.008 | 0.02 | -0.018 | 0.083 | -0.466 | 0.115 | 0.16 | -0.356 | -0.07 | -0.253 |
| 5 | 0.344 | -0.284 | 0.054 | -0.048 | 0.127 | 0.163 | -0.495 | 0.054 | -0.181 | -0.487 | -0.173 | -0.175 | -0.018 | 0.111 | -0.092 | 0.073 | 0.058 | -0.028 | -0.043 | 0.012 | 0.029 | -0.036 | -0.108 | 0.037 | 0.043 | -0.099 | 0.049 | 0.089 | -0.011 | 0.094 | 0.104 | -0.139 | -0.074 | 0.007 | -0.091 | -0.115 | 0.115 | 0.167 |
| 6 | 0.225 | -0.288 | -0.32 | 0.002 | -0.427 | 0.263 | 0.109 | -0.054 | 0.3 | -0.016 | -0.214 | 0.311 | 0.126 | -0.313 | 0.026 | 0.007 | 0.041 | -0.02 | 0.087 | -0.01 | 0.035 | -0.028 | 0.054 | -0.082 | -0.139 | 0.074 | 0.017 | 0.067 | 0.106 | 0.056 | 0.028 | -0.048 | -0.062 | -0.069 | 0.122 | 0.072 | 0.176 | 0.148 |
| 7 | 0.365 | 0.152 | 0.139 | -0.289 | 0.04 | -0.208 | -0.298 | -0.28 | 0.141 | 0.504 | -0.233 | -0.117 | -0.048 | -0.189 | 0.032 | -0.043 | -0.007 | 0.05 | 0.023 | -0.009 | 0.041 | 0.028 | 0.108 | -0.029 | 0.019 | 0.054 | 0.07 | -0.075 | 0.012 | 0.092 | -0.089 | 0.001 | -0.122 | -0.111 | 0.123 | -0.087 | -0.07 | 0.177 |
| 8 | 0.266 | 0.298 | -0.274 | 0.057 | 0.306 | -0.228 | 0.267 | -0.267 | 0.198 | -0.378 | -0.113 | 0.203 | -0.191 | 0.097 | -0.196 | -0.096 | 0.027 | 0.009 | -0.073 | 0.013 | 0.018 | -0.05 | 0.012 | 0.116 | -0.085 | 0.102 | 0.008 | 0.07 | -0.084 | -0.046 | -0.106 | 0.038 | -0.082 | 0.099 | -0.079 | 0.115 | -0.133 | 0.163 |
| 9 | 0.076 | 0.039 | -0.135 | -0.052 | 0.094 | -0.04 | 0.197 | 0.042 | -0.058 | -0.094 | 0.091 | -0.43 | 0.161 | -0.249 | 0.126 | -0.018 | 0.393 | -0.263 | 0.493 | -0.028 | 0.059 | -0.056 | -0.059 | -0.043 | 0.012 | -0.068 | -0.098 | -0.047 | -0.082 | 0.099 | -0.021 | 0.071 | 0.176 | 0.049 | -0.1 | 0.187 | -0.025 | 0.12 |
| 10 | 0.138 | 0.215 | -0.085 | 0.178 | 0.034 | 0.03 | -0.012 | -0.008 | 0.061 | -0.057 | 0.014 | 0.072 | 0.068 | 0.116 | -0.06 | -0.032 | -0.006 | 0.008 | -0.006 | -0.176 | -0.133 | 0.37 | -0.228 | 0.075 | -0.257 | 0.313 | -0.282 | -0.102 | 0.279 | 0.028 | 0.013 | 0.232 | -0.213 | -0.121 | -0.078 | 0.327 | -0.237 | |
| 11 | 0.174 | 0.159 | 0.132 | -0.04 | -0.16 | -0.107 | -0.044 | 0.013 | 0.01 | 0.075 | -0.078 | -0.033 | 0.115 | 0.023 | 0.033 | 0.001 | 0.036 | 0.036 | 0.003 | 0.211 | 0.059 | 0.179 | -0.128 | 0.418 | -0.228 | 0.288 | 0.166 | -0.106 | -0.233 | 0.135 | 0.289 | -0.139 | 0.072 | 0.252 | -0.025 | 0.217 | 0.247 | -0.25 |
| 12 | 0.205 | -0.046 | 0.143 | -0.112 | 0.082 | 0.097 | -0.151 | -0.12 | 0.046 | -0.003 | 0.028 | -0.069 | -0.018 | -0.039 | -0.029 | 0.024 | 0.004 | -0.034 | -0.005 | -0.048 | 0.376 | 0.211 | -0.096 | 0.2 | 0.418 | -0.091 | 0.178 | 0.122 | -0.005 | -0.243 | -0.011 | 0.227 | 0.14 | 0.278 | 0.277 | -0.039 | -0.274 | |
| 13 | 0.071 | -0.088 | 0.128 | -0.017 | -0.164 | 0.114 | 0.1 | 0.01 | 0.151 | 0.045 | -0.075 | -0.152 | 0.006 | 0.025 | -0.177 | -0.085 | -0.105 | 0.075 | -0.017 | -0.031 | 0.009 | 0.062 | -0.273 | -0.191 | 0.271 | 0.171 | -0.081 | -0.279 | -0.209 | 0.294 | -0.227 | -0.146 | 0.111 | 0.241 | -0.261 | -0.256 | -0.204 | |
| 14 | 0.1 | -0.161 | -0.097 | 0.115 | -0.177 | -0.036 | 0.04 | -0.144 | 0.038 | 0.037 | 0.043 | 0.052 | -0.037 | 0.013 | 0.148 | 0.012 | 0.091 | -0.087 | -0.072 | -0.123 | -0.258 | -0.145 | -0.237 | 0.204 | 0.154 | -0.185 | 0.279 | 0.199 | 0.017 | -0.293 | 0.228 | -0.076 | -0.252 | -0.332 | -0.006 | -0.318 | -0.197 | |

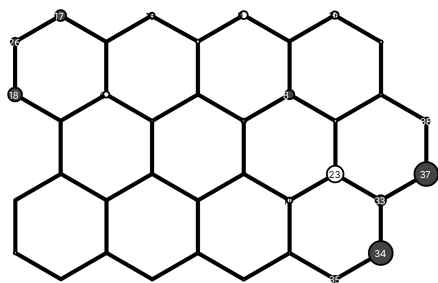
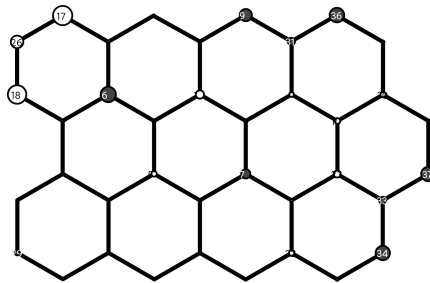
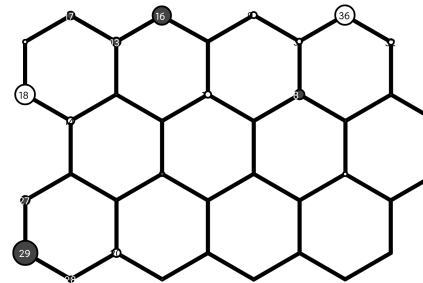
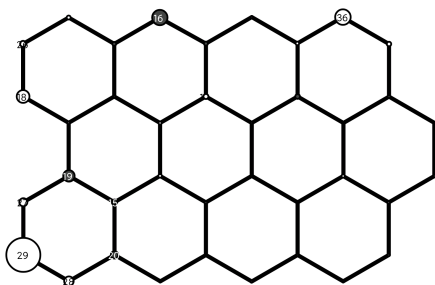
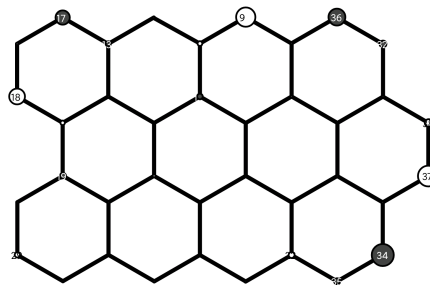
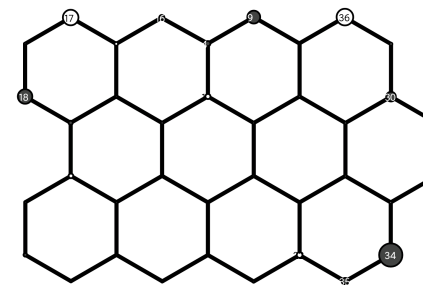
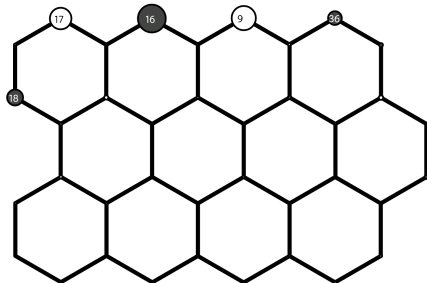
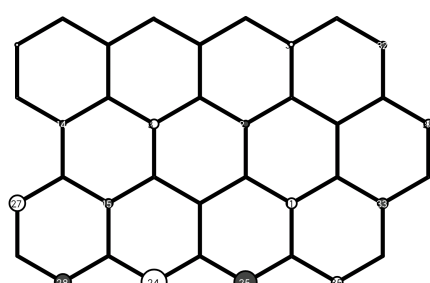
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|----|-----------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 15 | 0.15 4 | - 0.19 8 | 0.06 5 | 0.16 | 0.08 | - 0.08 7 | - 0.06 8 | 0.04 5 | - 0.07 2 | - 0.07 2 | - 0.04 9 | - 0.05 2 | - 0.00 2 | 0.03 2 | 0.02 6 | - 0.11 1 | - 0.02 5 | 0.02 8 | 0.01 1 | - 0.17 4 | 0.14 7 | 0.15 5 | - 0.14 4 | - 0.29 1 | - 0.39 8 | 0.18 5 | 0.20 5 | - 0.33 6 | 0.11 1 | - 0.13 8 | - 0.05 | 0.14 8 | - 0.03 8 | - 0.29 | 0.03 5 | 0.27 1 | - 0.25 6 | - 0.21 8 |
| 16 | 0.07 | - 0.04 6 | - 0.14 1 | - 0.07 3 | - 0.07 5 | 0.07 4 | 0.15 6 | 0.11 8 | 0.04 7 | 0.09 2 | 0.04 9 | - 0.42 | 0.11 4 | - 0.00 5 | 0.37 5 | - 0.31 3 | - 0.02 5 | - 0.10 5 | - 0.56 6 | 0.03 1 | 0.02 7 | 0.06 3 | 0.04 7 | 0.05 6 | 0.00 5 | - 0.07 8 | - 0.09 6 | 0.00 2 | 0.07 7 | - 0.10 6 | 0.07 9 | 0.02 3 | 0.18 3 | - 0.10 4 | 0.02 9 | 0.16 7 | 0.08 7 | 0.11 6 |
| 17 | 0.03 8 | - 0.05 7 | - 0.08 4 | 0.0 | - 0.13 5 | 0.09 3 | 0.10 4 | - 0.02 7 | 0.18 4 | 0.07 8 | - 0.08 7 | - 0.36 8 | - 0.22 1 | 0.39 3 | - 0.15 8 | 0.08 2 | - 0.29 1 | 0.31 8 | 0.43 9 | - 0.02 | - 0.06 3 | - 0.04 7 | - 0.03 6 | 0.07 8 | 0.04 2 | - 0.06 7 | 0.11 4 | 0.06 1 | - 0.07 | - 0.14 9 | 0.07 3 | 0.15 2 | - 0.02 5 | - 0.09 7 | 0.15 7 | 0.09 4 | 0.11 2 | 0.07 4 |
| 18 | 0.05 | - 0.09 1 | - 0.06 8 | 0.07 3 | - 0.14 5 | - 0.00 9 | 0.06 6 | - 0.14 2 | 0.09 4 | 0.07 1 | 0.02 2 | - 0.12 5 | - 0.28 1 | 0.37 6 | 0.40 2 | 0.26 | 0.32 1 | - 0.29 6 | - 0.32 4 | 0.02 | 0.04 8 | 0.03 7 | - 0.05 | - 0.07 5 | 0.08 7 | 0.06 3 | - 0.01 8 | - 0.11 3 | - 0.15 | 0.04 9 | - 0.07 5 | 0.13 | - 0.13 9 | - 0.00 6 | 0.17 8 | 0.02 7 | 0.12 9 | 0.07 3 |
| 19 | 0.19 1 | - 0.33 6 | - 0.02 6 | 0.39 7 | - 0.13 3 | - 0.38 9 | 0.00 4 | 0.32 8 | - 0.26 | 0.07 2 | 0.33 6 | - 0.02 4 | 0.04 4 | - 0.02 4 | 0.00 3 | 0.23 3 | - 0.12 4 | 0.09 5 | 0.06 7 | - 0.00 8 | - 0.05 6 | 0.01 7 | 0.05 2 | 0.10 2 | 0.0 | - 0.06 2 | - 0.11 5 | - 0.04 7 | 0.03 5 | 0.09 4 | - 0.13 5 | - 0.01 7 | - 0.01 6 | 0.15 5 | 0.09 3 | - 0.09 1 | 0.16 2 | 0.10 7 |
| 20 | 0.18 7 | - 0.25 9 | 0.24 8 | 0.30 6 | 0.32 6 | - 0.09 9 | 0.24 7 | 0.43 7 | 0.18 8 | 0.16 9 | - 0.32 8 | 0.03 6 | - 0.03 2 | 0.00 9 | 0.16 9 | - 0.15 1 | 0.0 | 0.00 4 | 0.00 1 | - 0.00 2 | 0.01 2 | - 0.00 9 | 0.09 | - 0.06 | 0.09 1 | 0.08 7 | - 0.01 1 | 0.11 4 | - 0.08 3 | - 0.09 5 | 0.07 1 | 0.03 1 | 0.12 3 | 0.16 3 | - 0.04 4 | - 0.16 | 0.09 9 | 0.08 8 |
| 21 | 0.24 9 | - 0.07 | 0.41 4 | - 0.12 3 | 0.15 9 | 0.41 4 | 0.23 4 | - 0.21 | 0.20 2 | - 0.02 8 | 0.50 2 | 0.07 4 | 0.01 3 | - 0.01 2 | - 0.02 3 | 0.03 8 | - 0.04 1 | - 0.01 | 0.00 8 | - 0.00 3 | - 0.02 9 | 0.04 5 | - 0.04 1 | 0.01 9 | - 0.12 9 | 0.05 6 | - 0.05 5 | - 0.10 2 | - 0.03 9 | 0.00 1 | 0.17 8 | 0.14 7 | - 0.00 1 | - 0.05 3 | - 0.11 4 | - 0.17 2 | 0.01 2 | 0.11 |
| 22 | 0.20 6 | 0.18 1 | 0.35 6 | - 0.11 1 | 0.39 9 | - 0.04 5 | 0.36 7 | 0.00 2 | - 0.43 7 | - 0.13 4 | - 0.29 2 | 0.04 3 | 0.05 6 | 0.10 8 | - 0.02 5 | - 0.02 3 | 0.12 2 | 0.11 6 | - 0.01 8 | 0.00 7 | - 0.00 3 | - 0.09 3 | 0.00 1 | 0.01 4 | 0.08 5 | 0.05 7 | 0.00 1 | 0.00 4 | 0.15 1 | 0.09 2 | - 0.07 | 0.15 8 | 0.07 2 | - 0.15 | 0.02 5 | - 0.14 | - 0.10 1 | 0.10 1 |
| 23 | 0.24 3 | 0.37 1 | 0.06 7 | 0.23 7 | - 0.27 9 | - 0.15 1 | - 0.23 1 | 0.32 6 | 0.33 | - 0.11 4 | 0.26 4 | - 0.03 | 0.33 9 | 0.14 2 | 0.08 7 | 0.06 7 | - 0.02 3 | 0.02 5 | 0.00 1 | 0.0 | - 0.04 4 | 0.03 3 | - 0.07 9 | - 0.09 8 | - 0.02 3 | - 0.04 3 | - 0.12 6 | 0.11 5 | - 0.01 | - 0.09 | - 0.07 1 | - 0.04 1 | - 0.01 3 | - 0.02 2 | 0.12 7 | - 0.06 2 | - 0.19 1 | 0.13 7 |
| 24 | 0.09 3 | - 0.07 4 | 0.15 6 | 0.04 4 | 0.12 2 | 0.08 3 | 0.13 | 0.06 3 | 0.11 1 | 0.04 1 | 0.05 2 | 0.03 5 | - 0.00 6 | - 0.00 1 | 0.05 1 | - 0.04 | - 0.01 6 | - 0.00 2 | 0.00 4 | 0.51 4 | 0.16 6 | - 0.20 3 | - 0.20 4 | 0.15 3 | 0.11 2 | - 0.34 3 | 0.15 7 | - 0.02 8 | 0.22 7 | 0.13 7 | - 0.31 4 | - 0.20 9 | - 0.14 1 | - 0.09 9 | 0.13 4 | 0.25 | - 0.07 5 | - 0.11 9 |
| 25 | 0.09 7 | 0.02 5 | 0.18 2 | - 0.05 7 | - 0.06 | 0.09 7 | 0.16 3 | - 0.05 7 | - 0.06 6 | - 0.04 8 | 0.06 2 | 0.03 7 | 0.02 3 | 0.03 2 | - 0.01 7 | 0.00 5 | 0.03 1 | 0.04 2 | - 0.00 4 | - 0.45 8 | 0.30 4 | 0.26 6 | 0.16 8 | - 0.11 9 | 0.12 9 | - 0.27 1 | 0.12 8 | 0.21 | - 0.20 7 | - 0.13 8 | - 0.13 6 | - 0.35 8 | - 0.08 2 | 0.18 6 | 0.07 5 | 0.23 1 | 0.06 1 | - 0.12 7 |
| 26 | 0.01 9 | - 0.03 3 | - 0.03 6 | 0.01 8 | - 0.07 | 0.02 2 | 0.04 6 | - 0.04 6 | 0.07 9 | 0.04 4 | - 0.01 9 | - 0.15 8 | - 0.16 6 | 0.25 6 | 0.08 5 | 0.12 2 | 0.01 2 | 0.00 8 | 0.04 9 | 0.07 8 | 0.14 3 | 0.05 3 | 0.36 4 | - 0.01 1 | - 0.38 1 | 0.01 7 | - 0.22 7 | 0.11 1 | 0.40 6 | 0.14 9 | 0.00 2 | - 0.33 1 | 0.18 9 | 0.09 1 | - 0.28 4 | - 0.09 1 | - 0.16 4 | - 0.08 9 |
| 27 | 0.05 | - 0.09 4 | 0.00 2 | 0.12 8 | - 0.02 3 | - 0.14 | 0.02 | - 0.08 | - 0.08 2 | 0.05 9 | 0.10 1 | - 0.00 1 | 0.03 6 | - 0.04 3 | - 0.17 3 | 0.16 4 | - 0.00 7 | 0.00 8 | 0.01 3 | 0.32 2 | 0.29 | - 0.06 4 | 0.20 6 | - 0.25 7 | 0.24 2 | 0.21 7 | - 0.07 6 | 0.30 3 | - 0.25 4 | 0.07 9 | 0.34 7 | - 0.00 4 | - 0.14 8 | - 0.29 3 | 0.09 8 | 0.13 5 | - 0.16 1 | - 0.09 |
| 28 | 0.04 9 | - 0.07 6 | 0.06 7 | 0.10 6 | 0.09 2 | - 0.06 3 | 0.08 7 | 0.13 1 | 0.04 5 | 0.08 7 | - 0.09 6 | 0.01 8 | 0.01 1 | - 0.03 2 | - 0.11 4 | 0.19 4 | 0.04 1 | - 0.02 8 | - 0.01 5 | - 0.33 3 | - 0.35 1 | 0.07 7 | 0.05 | 0.34 | - 0.02 7 | - 0.14 1 | - 0.32 3 | - 0.04 3 | - 0.03 6 | 0.35 6 | 0.08 8 | - 0.06 | - 0.30 9 | - 0.3 | 0.01 7 | 0.18 7 | - 0.11 8 | - 0.07 9 |
| 29 | 0.04 1 | - 0.07 9 | 0.03 5 | 0.12 9 | 0.04 | - 0.13 8 | 0.07 6 | 0.03 8 | - 0.03 | 0.12 9 | 0.00 5 | 0.02 | 0.06 4 | - 0.10 4 | - 0.49 5 | 0.69 4 | 0.10 7 | - 0.07 5 | - 0.03 7 | 0.00 5 | 0.02 5 | - 0.00 5 | - 0.10 1 | - 0.03 2 | - 0.08 2 | - 0.02 8 | 0.14 7 | - 0.09 4 | 0.10 3 | - 0.14 7 | - 0.14 1 | 0.02 5 | 0.14 4 | 0.17 4 | 0.02 3 | - 0.08 9 | 0.07 4 | 0.04 3 |
| 30 | 0.13 8 | 0.28 6 | - 0.15 6 | 0.43 8 | 0.11 1 | 0.49 4 | - 0.07 7 | - 0.08 8 | - 0.31 1 | 0.29 5 | - 0.10 3 | 0.05 1 | 0.05 7 | 0.10 8 | - 0.06 3 | - 0.06 | - 0.01 9 | - 0.19 7 | 0.09 1 | - 0.01 3 | 0.04 5 | 0.04 1 | - 0.02 1 | 0.04 4 | 0.08 7 | 0.04 8 | - 0.01 4 | - 0.05 4 | 0.14 8 | - 0.04 9 | 0.15 4 | - 0.00 8 | - 0.10 6 | 0.16 2 | 0.09 4 | 0.05 | - 0.14 7 | 0.09 2 |
| 31 | 0.08 4 | 0.09 5 | - 0.11 7 | 0.02 1 | 0.12 7 | - 0.05 5 | 0.15 7 | - 0.09 2 | 0.01 9 | - 0.16 5 | - 0.02 9 | - 0.16 1 | 0.04 | - 0.14 9 | 0.11 4 | 0.07 2 | 0.02 9 | 0.03 4 | 0.06 3 | 0.10 3 | - 0.06 8 | 0.35 6 | - 0.00 7 | 0.06 2 | 0.25 4 | 0.14 4 | - 0.07 5 | - 0.14 3 | 0.23 9 | - 0.31 4 | 0.08 2 | - 0.30 7 | - 0.09 1 | - 0.28 2 | 0.18 5 | - 0.32 1 | 0.16 6 | - 0.22 1 |

| | 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 | Psi 14 | Psi 15 | Psi 16 | Psi 17 | Psi 18 | Psi 19 | Psi 20 | Psi 21 | Psi 22 | Psi 23 | Psi 24 | Psi 25 | Psi 26 | Psi 27 | Psi 28 | Psi 29 | Psi 30 | Psi 31 | Psi 32 | Psi 33 | Psi 34 | Psi 35 | Psi 36 | Psi 37 | Psi 38 |
|----|-------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 32 | 0.041 | 0.083 | -0.058 | 0.127 | 0.055 | 0.148 | 0.011 | -0.054 | -0.108 | 0.059 | -0.053 | -0.072 | 0.069 | -0.063 | 0.117 | 0.091 | -0.139 | 0.056 | -0.085 | -0.135 | 0.234 | -0.459 | -0.115 | 0.169 | -0.222 | 0.108 | -0.256 | 0.023 | -0.342 | -0.166 | -0.271 | -0.169 | 0.141 | -0.295 | -0.045 | -0.132 | -0.166 | -0.106 |
| 33 | 0.074 | 0.125 | 0.03 | 0.102 | -0.126 | 0.025 | -0.084 | 0.172 | 0.076 | -0.056 | 0.138 | 0.04 | 0.209 | -0.148 | 0.008 | 0.012 | -0.019 | 0.015 | -0.011 | 0.205 | 0.258 | -0.152 | 0.021 | 0.146 | 0.248 | 0.128 | -0.043 | -0.023 | 0.37 | -0.073 | -0.042 | 0.288 | -0.252 | 0.054 | -0.398 | 0.134 | 0.303 | -0.162 |
| 34 | 0.054 | 0.087 | 0.066 | 0.047 | -0.156 | -0.031 | 0.014 | 0.162 | -0.05 | -0.113 | 0.066 | -0.05 | -0.485 | 0.293 | -0.004 | 0.025 | -0.449 | -0.474 | 0.053 | -0.009 | 0.04 | 0.118 | 0.009 | 0.08 | -0.02 | 0.035 | 0.121 | 0.05 | -0.093 | 0.14 | -0.025 | -0.052 | 0.167 | -0.074 | 0.16 | -0.084 | -0.121 | 0.067 |
| 35 | 0.056 | 0.06 | 0.1 | -0.015 | -0.139 | -0.02 | 0.103 | 0.045 | -0.138 | -0.072 | -0.067 | -0.002 | 0.143 | -0.061 | -0.01 | 0.001 | -0.125 | -0.14 | 0.015 | 0.225 | -0.355 | -0.14 | -0.044 | -0.345 | -0.194 | -0.209 | -0.3 | -0.118 | -0.107 | -0.342 | 0.119 | -0.124 | -0.276 | 0.2 | -0.157 | 0.168 | 0.152 | -0.101 |
| 36 | 0.052 | 0.083 | -0.089 | 0.081 | 0.107 | 0.063 | 0.12 | -0.108 | -0.071 | -0.094 | -0.076 | 0.276 | 0.15 | -0.297 | 0.397 | 0.317 | -0.344 | 0.34 | -0.279 | 0.014 | -0.07 | 0.042 | 0.048 | -0.09 | -0.012 | -0.093 | 0.122 | 0.044 | 0.036 | 0.162 | 0.061 | 0.152 | -0.016 | 0.169 | -0.045 | 0.125 | -0.087 | 0.083 |
| 37 | 0.047 | 0.099 | -0.004 | 0.133 | -0.068 | 0.088 | -0.092 | 0.138 | -0.013 | 0.037 | 0.137 | -0.045 | -0.484 | 0.293 | -0.06 | -0.058 | 0.423 | 0.487 | -0.079 | 0.011 | -0.024 | -0.124 | 0.065 | -0.02 | -0.036 | 0.04 | 0.017 | -0.156 | -0.097 | 0.0 | 0.129 | -0.151 | 0.064 | 0.036 | 0.182 | -0.034 | -0.131 | 0.065 |
| 38 | 0.04 | 0.087 | -0.038 | 0.139 | 0.011 | 0.155 | -0.046 | 0.014 | -0.092 | 0.097 | 0.01 | 0.002 | -0.142 | -0.062 | -0.043 | -0.042 | 0.155 | 0.114 | 0.005 | 0.18 | -0.202 | 0.457 | -0.185 | 0.089 | -0.151 | -0.021 | -0.007 | 0.452 | -0.095 | 0.074 | -0.356 | 0.188 | 0.048 | -0.176 | -0.234 | -0.012 | 0.19 | -0.095 |

2.2. Molecule orbital presentation:



Ψ_4  Ψ_5  Ψ_6  Ψ_7  Ψ_8  Ψ_9  Ψ_{10}  Ψ_{11}  Ψ_{12} 

Ψ_{13}  Ψ_{14}  Ψ_{15}  Ψ_{16}  Ψ_{17}  Ψ_{18}  Ψ_{19}  Ψ_{20} 

The picture export was cancelled, more than 20 pictures are not possible.

3. Bond Order

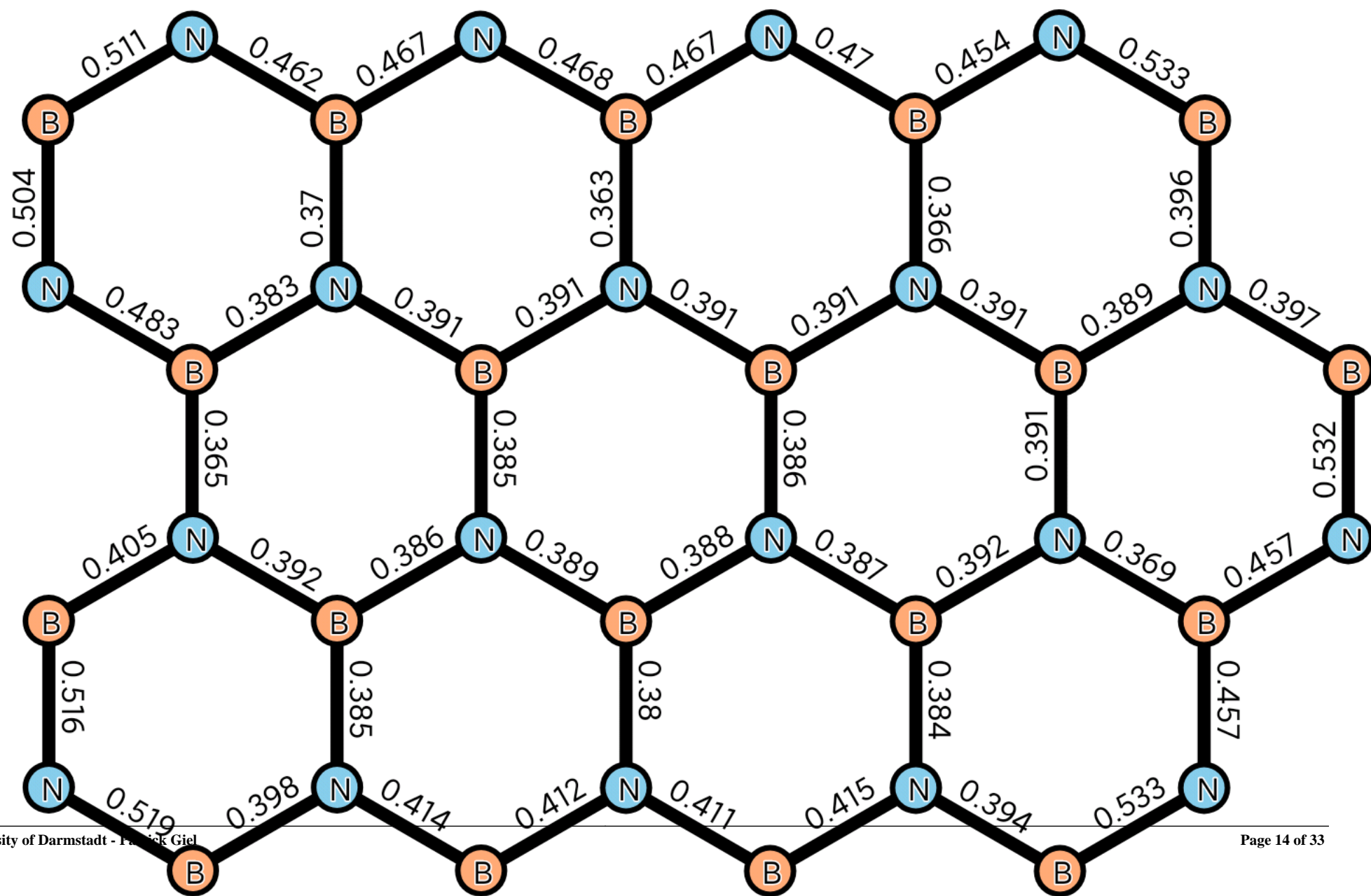
3.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------|----------------|-----------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | 1.72 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | 0.39 1 | 0.29 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | 0.39 1 | 0.06 1 | 0.29 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | 0.36 3 | 0.04 3 | 0.04 3 | 0.37 3 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | - 0.05 9 | - 0.06 6 | 0.38 5 | - 0.02 5 | 1.71 5 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | - 0.05 8 | - 0.02 6 | 0.39 1 | - 0.07 1 | - 0.06 | 1.72 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | - 0.05 9 | 0.38 6 | - 0.06 6 | - 0.02 1 | - 0.05 9 | 0.01 7 | 1.71 4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | - 0.05 9 | 0.39 1 | - 0.02 6 | - 0.07 | 0.01 7 | 0.00 2 | - 0.05 9 | 1.71 9 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | - 0.06 9 | - 0.09 | - 0.02 8 | 0.46 7 | 0.00 3 | 0.02 8 | 0.02 2 | - 0.07 1 | 1.71 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 10 | - 0.02 6 | 0.06 | - 0.00 5 | - 0.01 5 | 0.01 2 | 0.0 | - 0.06 7 | 0.39 1 | - 0.02 7 | 0.29 3 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 11 | - 0.02 5 | 0.05 7 | - 0.01 6 | - 0.00 2 | - 0.02 5 | 0.00 7 | 0.38 7 | - 0.06 8 | 0.01 6 | 0.06 | 0.28 8 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12 | - 0.06 7 | 0.05 8 | 0.05 8 | - 0.01 2 | 0.38 9 | - 0.02 6 | 0.38 8 | - 0.02 5 | 0.01 5 | - 0.01 7 | 0.05 8 | 0.28 4 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 13 | - 0.07 | - 0.01 6 | 0.04 6 | 0.08 5 | - 0.02 3 | 0.37 | 0.01 1 | 0.01 6 | - 0.05 8 | 0.00 4 | 0.00 2 | - 0.00 3 | 0.37 4 | | | | | | | | | | | | | | | | | | | | | | | | | |
| 14 | - 0.02 6 | - 0.00 5 | 0.05 7 | - 0.01 2 | - 0.06 2 | 0.38 3 | 0.01 1 | 0.00 1 | 0.00 9 | 0.0 | 0.00 3 | - 0.01 5 | 0.02 7 | 0.33 2 | | | | | | | | | | | | | | | | | | | | | | | | |
| 15 | - 0.02 5 | - 0.01 6 | 0.05 8 | - 0.00 3 | 0.38 6 | - 0.06 5 | - 0.02 5 | 0.00 7 | 0.0 | 0.00 3 | - 0.00 3 | 0.05 8 | - 0.00 9 | 0.05 2 | 0.28 8 | | | | | | | | | | | | | | | | | | | | | | | |
| 16 | - 0.06 9 | - 0.02 8 | - 0.09 1 | 0.46 8 | 0.02 2 | - 0.07 2 | 0.00 3 | 0.02 8 | - 0.11 4 | 0.01 1 | 0.0 | 0.01 6 | 0.46 7 | - 0.02 | 0.01 4 | 1.71 2 | | | | | | | | | | | | | | | | | | | | | | |
| 17 | 0.02 5 | 0.01 1 | - 0.02 4 | - 0.05 7 | 0.00 1 | - 0.06 | - 0.00 3 | - 0.00 8 | 0.02 3 | - 0.00 3 | - 0.00 1 | - 0.00 1 | 0.46 2 | - 0.11 5 | 0.01 9 | - 0.11 1 | 1.69 2 | | | | | | | | | | | | | | | | | | | | | |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|--------|--------|--------|-------|-------|----|----|----|----|
| 18 | 0.001 | 0.0 | -0.033 | 0.026 | 0.023 | -0.066 | -0.004 | 0.002 | -0.012 | 0.001 | -0.002 | 0.011 | -0.108 | 0.483 | -0.042 | 0.042 | -0.106 | 1.685 | | | | | | | | | | | | | | | | | | | | |
| 19 | 0.017 | 0.012 | -0.064 | 0.008 | -0.061 | -0.055 | 0.005 | -0.003 | -0.003 | -0.002 | 0.001 | -0.027 | -0.013 | 0.365 | 0.392 | 0.0 | 0.028 | -0.084 | 1.714 | | | | | | | | | | | | | | | | | | | |
| 20 | 0.004 | 0.011 | -0.025 | 0.001 | -0.057 | 0.014 | 0.016 | -0.003 | 0.001 | -0.003 | 0.013 | -0.067 | 0.004 | -0.018 | 0.385 | -0.003 | -0.004 | 0.007 | -0.051 | 1.701 | | | | | | | | | | | | | | | | | | |
| 21 | 0.016 | -0.024 | -0.023 | 0.005 | -0.056 | 0.004 | -0.056 | 0.004 | -0.003 | 0.011 | -0.067 | 0.381 | 0.009 | 0.009 | -0.067 | -0.004 | 0.001 | -0.005 | 0.015 | -0.063 | 1.699 | | | | | | | | | | | | | | | | | |
| 22 | 0.004 | -0.024 | 0.011 | 0.0 | 0.016 | -0.003 | -0.057 | 0.016 | -0.004 | -0.024 | 0.384 | -0.068 | -0.001 | -0.003 | 0.013 | 0.001 | 0.0 | 0.001 | -0.003 | 0.007 | -0.063 | 1.702 | | | | | | | | | | | | | | | | |
| 23 | 0.017 | -0.067 | 0.012 | 0.011 | 0.004 | -0.003 | -0.061 | -0.061 | 0.004 | 0.391 | 0.392 | -0.026 | -0.004 | -0.002 | 0.001 | -0.004 | 0.002 | 0.0 | 0.0 | -0.003 | 0.016 | -0.054 | 1.717 | | | | | | | | | | | | | | | |
| 24 | 0.013 | -0.004 | -0.019 | 0.002 | -0.073 | 0.012 | -0.026 | 0.001 | -0.002 | 0.003 | -0.021 | 0.064 | 0.002 | -0.002 | 0.068 | -0.005 | -0.002 | 0.002 | -0.023 | 0.414 | 0.412 | -0.037 | 0.008 | 0.211 | | | | | | | | | | | | | | |
| 25 | 0.013 | -0.018 | -0.004 | 0.002 | -0.026 | 0.001 | -0.073 | 0.013 | -0.005 | -0.004 | 0.067 | 0.064 | 0.0 | 0.003 | -0.021 | -0.002 | 0.001 | -0.002 | 0.008 | -0.036 | 0.411 | 0.415 | -0.024 | 0.089 | 0.211 | | | | | | | | | | | | | |
| 26 | 0.02 | 0.005 | -0.024 | -0.016 | 0.017 | -0.094 | -0.005 | -0.004 | 0.011 | -0.001 | -0.001 | 0.005 | 0.089 | 0.099 | -0.01 | -0.062 | 0.511 | 0.504 | -0.042 | 0.002 | -0.002 | 0.001 | 0.001 | 0.0 | -0.001 | 0.328 | | | | | | | | | | | | |
| 27 | 0.008 | 0.003 | -0.016 | 0.002 | -0.023 | -0.03 | 0.0 | -0.001 | -0.002 | 0.0 | -0.001 | -0.001 | -0.002 | 0.063 | 0.051 | 0.001 | 0.017 | -0.051 | 0.405 | -0.089 | 0.016 | -0.003 | 0.001 | -0.032 | 0.007 | -0.015 | 0.271 | | | | | | | | | | | |
| 28 | -0.001 | 0.002 | 0.0 | -0.001 | -0.021 | 0.014 | 0.007 | -0.001 | 0.001 | -0.001 | 0.004 | -0.017 | 0.002 | -0.024 | 0.047 | -0.001 | -0.008 | 0.018 | -0.092 | 0.398 | -0.035 | 0.004 | -0.002 | 0.082 | -0.012 | 0.006 | 0.131 | 0.269 | | | | | | | | | | |
| 29 | -0.005 | -0.005 | 0.018 | -0.002 | 0.023 | 0.007 | -0.005 | 0.001 | 0.001 | 0.001 | -0.003 | 0.019 | 0.001 | -0.041 | -0.1 | 0.001 | -0.006 | 0.016 | -0.078 | -0.075 | 0.009 | -0.001 | 0.001 | -0.051 | 0.006 | 0.008 | 0.516 | 0.519 | 1.661 | | | | | | | | | |
| 30 | 0.002 | -0.025 | 0.0 | 0.017 | -0.003 | 0.002 | 0.016 | -0.056 | 0.03 | 0.389 | -0.025 | 0.007 | -0.004 | 0.001 | -0.001 | -0.009 | 0.002 | -0.001 | 0.0 | 0.001 | -0.002 | 0.001 | -0.055 | -0.001 | -0.001 | 0.001 | 0.0 | 0.0 | 0.0 | 1.706 | | | | | | | | |
| 31 | -0.07 | 0.045 | -0.016 | 0.087 | 0.017 | 0.017 | -0.021 | 0.366 | 0.47 | 0.041 | -0.012 | -0.002 | -0.016 | 0.003 | 0.003 | -0.059 | 0.011 | -0.006 | -0.003 | -0.001 | 0.0 | 0.006 | -0.022 | -0.001 | 0.003 | 0.003 | -0.001 | 0.0 | 0.001 | -0.076 | 0.369 | | | | | | | |
| 32 | 0.02 | -0.02 | 0.006 | -0.02 | -0.004 | -0.005 | 0.012 | -0.083 | -0.071 | 0.052 | -0.002 | 0.003 | 0.004 | -0.001 | -0.001 | 0.013 | -0.003 | 0.002 | 0.001 | 0.001 | -0.001 | -0.002 | 0.0 | -0.002 | -0.001 | 0.0 | 0.0 | -0.001 | 0.396 | 0.106 | 0.277 | | | | | | | |
| 33 | 0.006 | -0.012 | 0.002 | 0.001 | 0.0 | -0.001 | -0.021 | -0.022 | -0.002 | 0.042 | 0.043 | -0.001 | 0.0 | 0.0 | -0.001 | -0.001 | 0.0 | 0.0 | 0.0 | -0.002 | 0.014 | -0.075 | 0.369 | 0.005 | -0.026 | 0.0 | 0.001 | -0.001 | 0.0 | -0.077 | 0.002 | -0.022 | 0.364 | | | | | |
| 34 | -0.004 | 0.015 | -0.005 | -0.001 | -0.005 | 0.001 | 0.022 | 0.003 | 0.002 | -0.025 | -0.095 | 0.021 | 0.001 | 0.001 | -0.004 | 0.0 | 0.0 | -0.001 | 0.001 | -0.001 | 0.011 | -0.081 | -0.065 | 0.007 | -0.055 | -0.001 | 0.001 | -0.001 | 0.0 | 0.028 | -0.002 | 0.015 | 0.457 | 1.683 | | | | |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|-------|--------|--------|--------|--------|-------|--------|--------|--------|-------|-------|
| 35 | 0.0 | -0.002 | 0.002 | 0.0 | 0.007 | -0.001 | -0.021 | 0.013 | -0.001 | -0.019 | 0.049 | -0.017 | 0.0 | -0.001 | 0.004 | 0.001 | 0.0 | 0.001 | -0.002 | 0.004 | -0.034 | 0.394 | -0.083 | -0.012 | 0.08 | 0.0 | -0.001 | 0.002 | -0.001 | 0.022 | 0.001 | 0.007 | 0.107 | 0.533 | 0.275 | | | |
| 36 | 0.025 | -0.026 | 0.011 | -0.055 | -0.004 | 0.008 | 0.003 | -0.063 | -0.108 | -0.095 | 0.015 | 0.0 | 0.012 | -0.002 | -0.001 | 0.022 | -0.005 | 0.003 | 0.001 | 0.0 | 0.001 | -0.003 | 0.021 | 0.001 | -0.001 | -0.002 | 0.001 | 0.0 | 0.0 | -0.083 | 0.454 | 0.533 | 0.021 | -0.008 | -0.008 | 1.685 | | |
| 37 | -0.003 | 0.015 | -0.002 | -0.007 | 0.001 | 0.0 | 0.003 | 0.022 | -0.009 | -0.095 | -0.025 | -0.001 | 0.002 | 0.0 | 0.001 | 0.003 | -0.001 | 0.0 | 0.0 | 0.001 | -0.005 | 0.027 | -0.064 | -0.003 | 0.017 | 0.0 | 0.0 | 0.0 | 0.0 | -0.082 | 0.021 | -0.051 | 0.457 | -0.102 | -0.068 | 0.015 | 1.683 | |
| 38 | -0.001 | -0.002 | -0.001 | 0.005 | -0.001 | 0.001 | 0.012 | -0.02 | 0.016 | 0.052 | -0.02 | 0.002 | -0.001 | 0.0 | 0.0 | -0.004 | 0.001 | -0.001 | 0.0 | 0.001 | -0.005 | 0.021 | -0.084 | -0.002 | 0.009 | 0.0 | 0.0 | 0.0 | 0.0 | 0.397 | -0.022 | 0.071 | 0.107 | -0.068 | -0.026 | -0.051 | 0.532 | 0.277 |

3.2. Presentation of bond order:



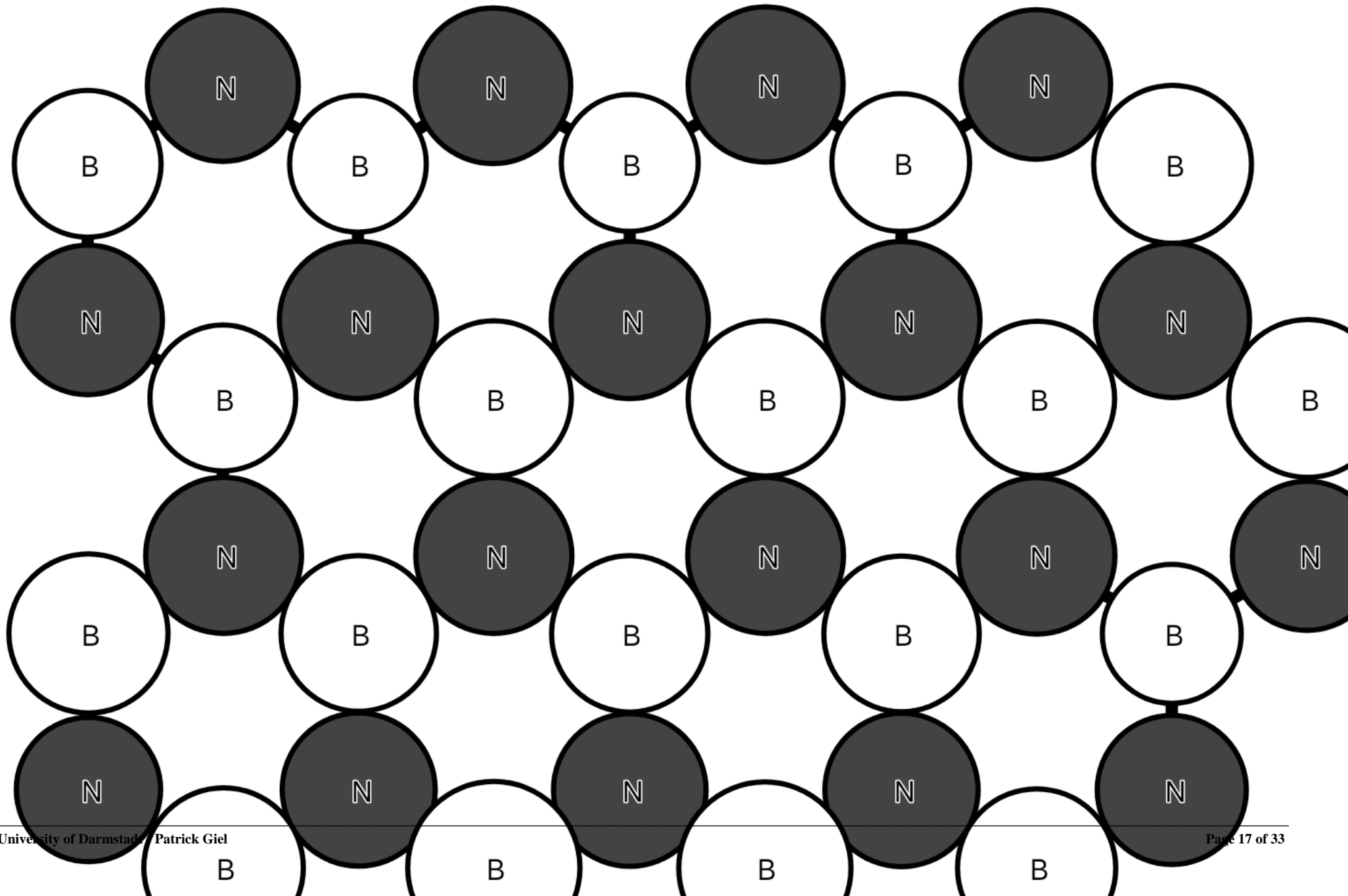
4. Net Charge

4.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|----|-------|------|------|-----------|------------|-------|------------|------------|-------|-----------|-----------|-----------|-----------|-----------|-----------|----|------------|------------|------------|------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | -0.72 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | | 0.71 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | | | 0.71 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | | | | 0.62 7 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | | | | | -0.71 5 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | | | | | | -0.72 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | | | | | | | -0.71 4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | | | | | | | | -0.71 9 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | | | | | | | | | -0.71 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 10 | | | | | | | | | | 0.70 7 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 11 | | | | | | | | | | | 0.71 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12 | | | | | | | | | | | | 0.71 6 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 13 | | | | | | | | | | | | | 0.62 6 | | | | | | | | | | | | | | | | | | | | | | | | | |
| 14 | | | | | | | | | | | | | | 0.66 8 | | | | | | | | | | | | | | | | | | | | | | | | |
| 15 | | | | | | | | | | | | | | | 0.71 2 | | | | | | | | | | | | | | | | | | | | | | | |
| 16 | | | | | | | | | | | | | | | | | -0.71 2 | | | | | | | | | | | | | | | | | | | | | |
| 17 | | | | | | | | | | | | | | | | | | -0.69 2 | | | | | | | | | | | | | | | | | | | | |
| 18 | | | | | | | | | | | | | | | | | | | -0.68 5 | | | | | | | | | | | | | | | | | | | |
| 19 | | | | | | | | | | | | | | | | | | | | -0.71 4 | | | | | | | | | | | | | | | | | | |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|----|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|------------|-----------|-----------|----|----|-----------|-----------|-----------|------------|------------|-----------|-----------|-----------|------------|-----------|------------|------------|----|-----------|
| 20 | | | | | | | | | | | | | | | | | | | | -0.70 1 | | | | | | | | | | | | | | | | | | |
| 21 | | | | | | | | | | | | | | | | | | | | -0.69 9 | | | | | | | | | | | | | | | | | | |
| 22 | | | | | | | | | | | | | | | | | | | | -0.70 2 | | | | | | | | | | | | | | | | | | |
| 23 | | | | | | | | | | | | | | | | | | | | -0.71 7 | | | | | | | | | | | | | | | | | | |
| 24 | | | | | | | | | | | | | | | | | | | | | 0.78 9 | | | | | | | | | | | | | | | | | |
| 25 | | | | | | | | | | | | | | | | | | | | | | 0.78 9 | | | | | | | | | | | | | | | | |
| 26 | | | | | | | | | | | | | | | | | | | | | | | | | 0.67 2 | | | | | | | | | | | | | |
| 27 | | | | | | | | | | | | | | | | | | | | | | | | | | 0.72 9 | | | | | | | | | | | | |
| 28 | | | | | | | | | | | | | | | | | | | | | | | | | | | 0.73 1 | | | | | | | | | | | |
| 29 | | | | | | | | | | | | | | | | | | | | | | | | | | | | -0.66 1 | | | | | | | | | | |
| 30 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | -0.70 6 | | | | | | | | | |
| 31 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 0.63 1 | | | | | | | | |
| 32 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 0.72 3 | | | | | | | |
| 33 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 0.63 6 | | | | | | |
| 34 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | -0.68 3 | | | | | |
| 35 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 0.72 5 | | | | |
| 36 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | -0.68 5 | | | |
| 37 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | -0.68 3 | | |
| 38 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 0.72 3 |

4.2. Presentation of molecule:

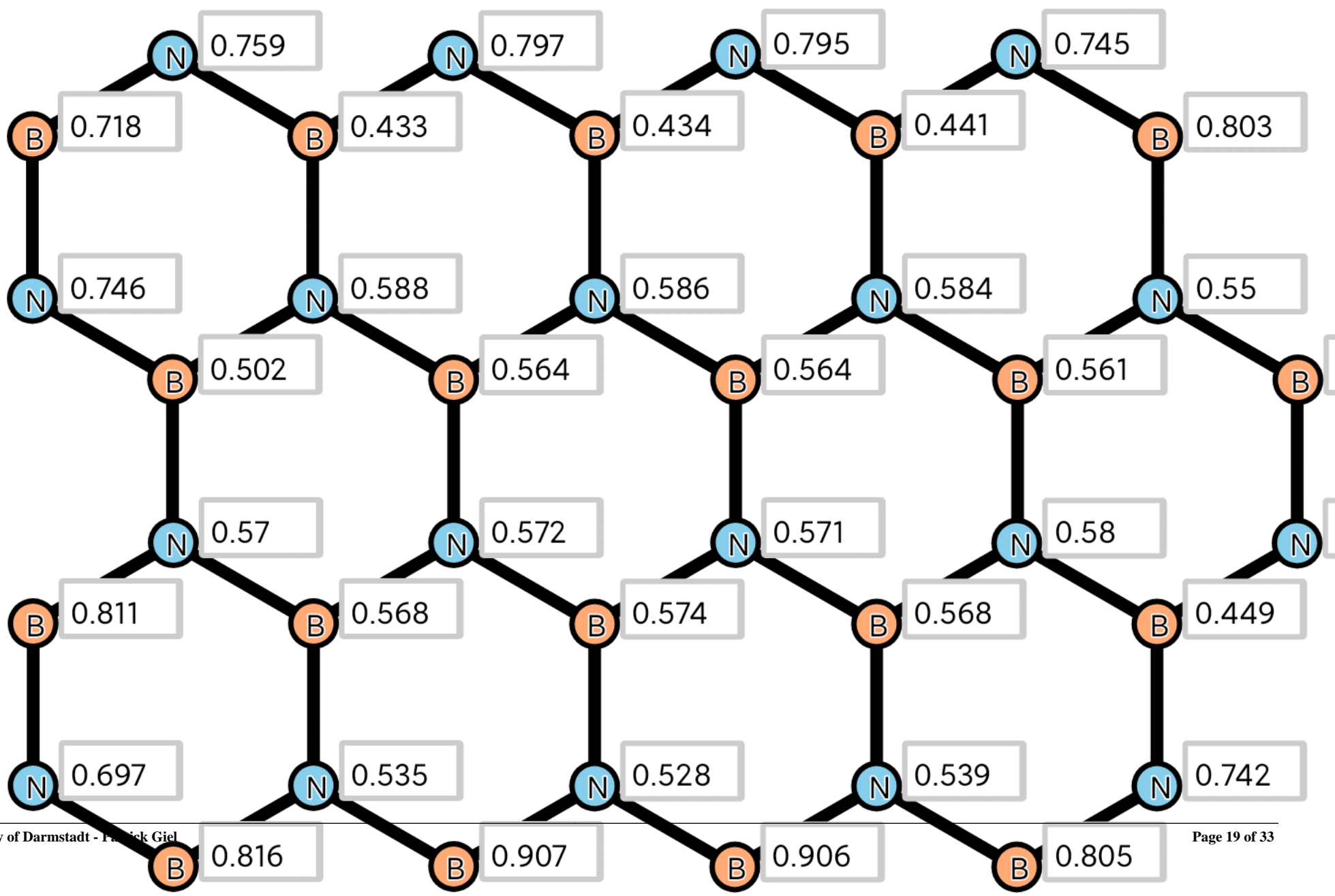


5. Free valences

5.1. Calculated values:

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|------|-----------|-----------|-----------|------|-----------|-----------|-----------|-----------|-----------|-----------|------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 0.58 6 | 0.56 4 | 0.56 4 | 0.43 4 | 0.57 2 | 0.58 8 | 0.57 1 | 0.58 4 | 0.79 5 | 0.56 1 | 0.56 8 | 0.57 4 | 0.43 3 | 0.50 2 | 0.56 8 | 0.79 7 | 0.75 9 | 0.74 6 | 0.57 | 0.53 5 | 0.52 8 | 0.53 9 | 0.58 | 0.90 7 | 0.90 6 | 0.71 8 | 0.81 1 | 0.81 6 | 0.69 7 | 0.55 | 0.44 1 | 0.80 3 | 0.44 9 | 0.74 2 | 0.80 5 | 0.74 5 | 0.74 2 | 0.80 3 |

5.2. Presentation of molecule:



6. Atom-Atom-Polarizability

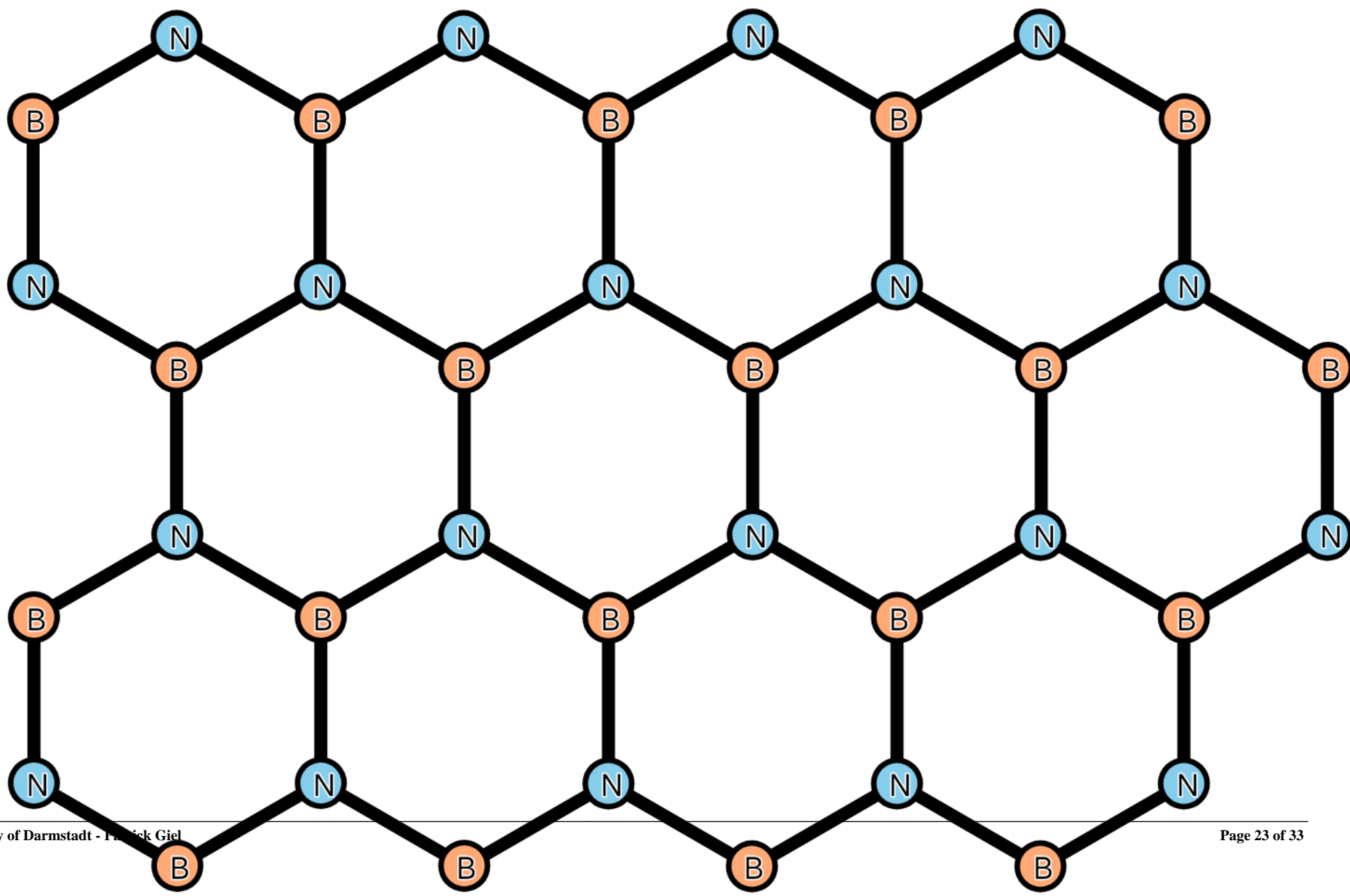
6.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|-------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1 | 0.13 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | -0.038 | 0.135 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | -0.038 | -0.002 | 0.135 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | -0.029 | 0.0 | 0.0 | 0.183 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | -0.001 | -0.003 | -0.036 | 0.0 | 0.132 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | -0.001 | 0.0 | -0.038 | -0.003 | -0.001 | 0.13 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | -0.001 | -0.036 | -0.003 | 0.0 | -0.001 | 0.0 | 0.132 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | -0.001 | -0.038 | 0.0 | -0.003 | 0.0 | 0.0 | -0.001 | 0.131 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | -0.002 | -0.006 | 0.0 | -0.065 | 0.0 | -0.001 | 0.0 | -0.002 | 0.169 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 10 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | -0.038 | 0.0 | 0.137 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 11 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | -0.037 | -0.003 | 0.0 | -0.002 | 0.134 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12 | -0.003 | -0.001 | -0.001 | 0.0 | -0.038 | 0.0 | -0.037 | 0.0 | 0.0 | 0.0 | -0.001 | 0.131 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 13 | -0.003 | 0.0 | 0.0 | -0.004 | 0.0 | -0.031 | 0.0 | 0.0 | -0.003 | 0.0 | 0.0 | 0.0 | 0.184 | | | | | | | | | | | | | | | | | | | | | | | | | |
| 14 | 0.0 | 0.0 | -0.001 | 0.0 | -0.002 | -0.036 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.162 | | | | | | | | | | | | | | | | | | | | | | | | |
| 15 | 0.0 | 0.0 | -0.001 | 0.0 | -0.037 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | -0.001 | 0.135 | | | | | | | | | | | | | | | | | | | | | | | |
| 16 | -0.002 | 0.0 | -0.006 | -0.066 | 0.0 | -0.002 | 0.0 | -0.001 | -0.008 | 0.0 | 0.0 | 0.0 | -0.065 | 0.0 | 0.0 | 0.168 | | | | | | | | | | | | | | | | | | | | | | |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-----|--------|--------|--------|--------|-------|--------|-----|-----|-------|----|----|----|--|
| 17 | -0.001 | 0.0 | 0.0 | -0.003 | 0.0 | -0.001 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | -0.063 | -0.011 | 0.0 | -0.007 | 0.179 | | | | | | | | | | | | | | | | | | | | | | |
| 18 | 0.0 | 0.0 | -0.001 | -0.001 | 0.0 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.009 | -0.073 | -0.001 | -0.002 | -0.006 | 0.182 | | | | | | | | | | | | | | | | | | | | | |
| 19 | 0.0 | 0.0 | -0.003 | 0.0 | -0.002 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.03 | -0.039 | 0.0 | -0.001 | -0.003 | 0.132 | | | | | | | | | | | | | | | | | | | | |
| 20 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.0 | 0.0 | -0.036 | 0.0 | 0.0 | 0.0 | -0.001 | 0.138 | | | | | | | | | | | | | | | | | | | |
| 21 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | -0.003 | -0.035 | 0.0 | 0.0 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | -0.002 | 0.138 | | | | | | | | | | | | | | | | | | |
| 22 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | -0.036 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.002 | 0.137 | | | | | | | | | | | | | | | | | |
| 23 | 0.0 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.002 | 0.0 | -0.038 | -0.039 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.132 | | | | | | | | | | | | | | | | | |
| 24 | 0.0 | 0.0 | 0.0 | 0.0 | -0.004 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.002 | 0.0 | 0.0 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | -0.045 | -0.044 | -0.001 | 0.0 | 0.11 | | | | | | | | | | | | | | | |
| 25 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.004 | 0.0 | 0.0 | 0.0 | 0.0 | -0.002 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.044 | -0.045 | 0.0 | -0.004 | 0.11 | | | | | | | | | | | | | | |
| 26 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.006 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.004 | -0.006 | 0.0 | -0.003 | -0.085 | -0.081 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.188 | | | | | | | | | | | | |
| 27 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | -0.002 | -0.042 | -0.006 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.154 | | | | | | | | | | | | |
| 28 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.006 | -0.039 | -0.001 | 0.0 | 0.0 | -0.003 | 0.0 | 0.0 | -0.002 | 0.152 | | | | | | | | | | | |
| 29 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.008 | 0.0 | 0.0 | 0.0 | -0.003 | -0.002 | 0.0 | 0.0 | 0.0 | -0.002 | 0.0 | 0.0 | -0.008 | -0.089 | 0.194 | | | | | | | | | | |
| 30 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.001 | -0.038 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.135 | | | | | | | | | |
| 31 | -0.003 | 0.0 | 0.0 | -0.004 | 0.0 | 0.0 | 0.0 | -0.03 | -0.067 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.004 | 0.18 | | | | | | | | |
| 32 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.005 | -0.004 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.039 | -0.007 | 0.159 | | | | | | | | |
| 33 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.004 | -0.031 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.004 | 0.0 | 0.0 | 0.177 | | | | |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | | | |
|----|--------|-----|-----|--------|-----|-----|-----|--------|--------|--------|--------|-----|-----|-----|-----|--------|-----|-----|-----|-----|--------|--------|--------|-----|--------|-----|-----|-----|--------|--------|--------|--------|--------|--------|--------|--------|-------|----|--|--|--|
| 34 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.007 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | -0.002 | 0.0 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | -0.061 | 0.184 | | | | | | | |
| 35 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.038 | -0.005 | 0.0 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | -0.007 | -0.098 | 0.158 | | | | | | |
| 36 | -0.001 | 0.0 | 0.0 | -0.002 | 0.0 | 0.0 | 0.0 | -0.001 | -0.007 | -0.007 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | -0.059 | -0.098 | 0.0 | 0.0 | 0.0 | 0.183 | | | | | | |
| 37 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.007 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.0 | -0.002 | -0.061 | -0.005 | -0.004 | 0.0 | 0.184 | | | | |
| 38 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.005 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.039 | 0.0 | -0.002 | -0.007 | -0.004 | -0.001 | -0.002 | -0.097 | 0.159 | | | | |

6.2. Presentation of molecule:



7. Bond-Atom-Polarizability

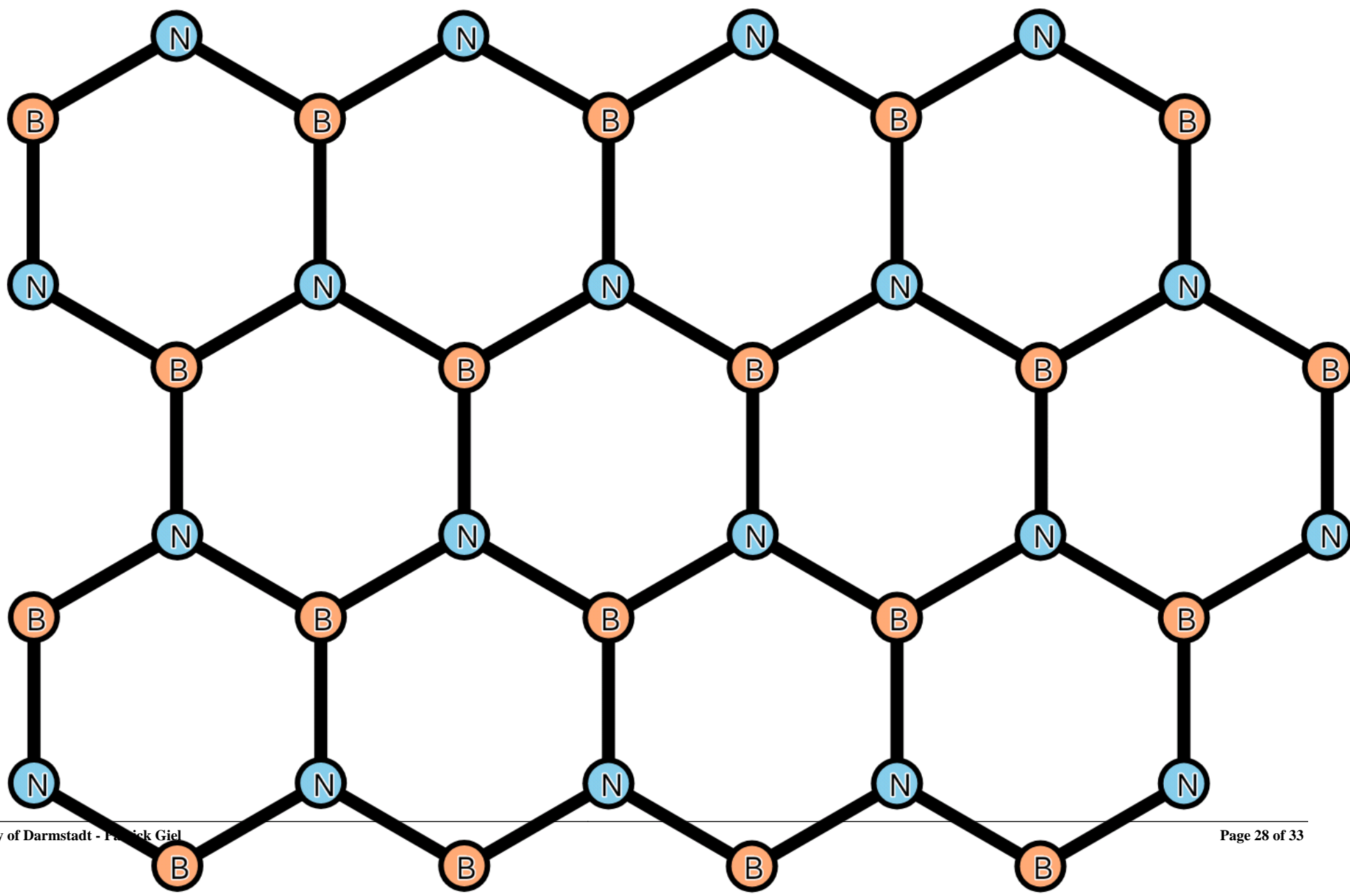
7.1. Calculated values:

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | | | | | |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|--------|-------|-------|--------|--------|--------|-----|-------|-------|--------|-----|-----|-----|-----|-----|-----|-----|
| 12 | -0.077 | 0.076 | -0.009 | -0.005 | -0.003 | -0.001 | 0.009 | 0.009 | -0.005 | 0.001 | 0.001 | 0.003 | -0.001 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | | |
| 13 | -0.077 | -0.009 | 0.076 | -0.005 | 0.009 | 0.009 | -0.003 | -0.001 | -0.001 | 0.0 | 0.0 | 0.003 | 0.002 | 0.001 | 0.001 | -0.005 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | | |
| 14 | -0.076 | -0.006 | -0.006 | 0.051 | -0.001 | -0.003 | -0.001 | -0.003 | 0.014 | 0.0 | 0.0 | -0.001 | 0.004 | 0.0 | 0.0 | 0.014 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.004 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | | | | |
| 27 | 0.009 | 0.073 | 0.003 | 0.0 | -0.003 | 0.0 | -0.074 | 0.009 | 0.002 | 0.003 | -0.008 | -0.009 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.001 | -0.003 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | |
| 28 | 0.009 | 0.075 | 0.001 | 0.002 | 0.001 | 0.0 | 0.009 | -0.076 | -0.005 | -0.009 | 0.003 | 0.001 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.005 | -0.001 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | | | | |
| 35 | 0.009 | 0.003 | 0.073 | 0.0 | -0.074 | 0.009 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | -0.009 | 0.001 | 0.002 | -0.009 | 0.002 | 0.0 | 0.001 | -0.003 | -0.001 | -0.001 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | |
| 36 | 0.009 | 0.001 | 0.076 | 0.002 | 0.009 | -0.077 | 0.001 | 0.0 | 0.001 | 0.0 | 0.0 | 0.001 | -0.006 | -0.008 | 0.003 | -0.005 | -0.001 | -0.001 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | |
| 49 | 0.013 | 0.003 | 0.001 | 0.095 | 0.0 | 0.002 | 0.0 | -0.004 | -0.113 | 0.0 | 0.0 | 0.0 | 0.004 | 0.0 | 0.0 | 0.026 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.019 | -0.002 | 0.0 | 0.0 | 0.0 | -0.005 | 0.0 | 0.0 | 0.0 | | | | |
| 416 | 0.011 | 0.003 | 0.003 | 0.096 | 0.0 | -0.004 | 0.0 | 0.002 | 0.026 | 0.0 | 0.0 | 0.0 | -0.019 | 0.0 | 0.0 | -0.113 | -0.005 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.004 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | | | |
| 512 | -0.003 | 0.003 | -0.008 | 0.0 | -0.075 | -0.001 | 0.009 | 0.0 | 0.0 | 0.0 | 0.001 | 0.075 | 0.0 | -0.001 | -0.008 | 0.0 | 0.0 | 0.0 | -0.001 | -0.003 | 0.008 | 0.001 | 0.0 | 0.003 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | |
| 515 | -0.001 | -0.001 | -0.008 | 0.0 | -0.074 | -0.003 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | -0.009 | 0.0 | 0.002 | 0.073 | 0.0 | 0.0 | 0.001 | 0.009 | 0.008 | -0.002 | 0.0 | 0.0 | 0.003 | 0.0 | 0.0 | 0.001 | 0.0 | 0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |
| 613 | -0.003 | 0.0 | -0.007 | 0.004 | -0.001 | -0.071 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.054 | -0.003 | 0.0 | 0.015 | 0.011 | -0.005 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.006 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |
| 614 | -0.001 | 0.0 | -0.009 | -0.001 | -0.003 | -0.075 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.065 | 0.002 | -0.001 | -0.005 | 0.014 | 0.007 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.007 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |
| 711 | -0.001 | -0.008 | -0.001 | 0.0 | -0.001 | 0.0 | -0.074 | -0.003 | 0.0 | 0.003 | 0.074 | -0.009 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.002 | 0.008 | 0.009 | 0.0 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.002 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | |
| 712 | -0.003 | -0.009 | 0.003 | 0.0 | 0.009 | 0.0 | -0.075 | -0.001 | 0.0 | -0.001 | -0.009 | 0.075 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.008 | -0.003 | -0.001 | 0.001 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 8 10 | -0.001 | -0.009 | 0.0 | -0.001 | 0.0 | 0.0 | -0.003 | -0.076 | -0.001 | 0.075 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.009 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.008 | -0.005 | 0.003 | 0.0 | 0.0 | 0.0 | -0.004 | 0.002 | 0.0 |
| 8 31 | -0.003 | -0.007 | 0.0 | 0.004 | 0.0 | 0.0 | -0.001 | -0.075 | 0.015 | -0.006 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.053 | 0.006 | 0.0 | 0.0 | 0.0 | 0.012 | 0.0 | 0.0 |
| 9 31 | -0.004 | 0.003 | 0.0 | -0.019 | 0.0 | -0.001 | 0.0 | 0.01 | -0.114 | 0.001 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | -0.006 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.002 | 0.098 | 0.007 | 0.0 | 0.0 | 0.0 | 0.023 | 0.0 | 0.0 |
| 10 23 | 0.0 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | 0.009 | 0.0 | 0.075 | -0.009 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | -0.076 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.008 | 0.0 | 0.0 | -0.005 | -0.001 | -0.001 | 0.002 | -0.005 | 0.003 |
| 10 30 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.008 | 0.001 | 0.075 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.008 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.073 | 0.002 | -0.007 | 0.002 | 0.0 | -0.006 | -0.006 | -0.007 | |
| 11 22 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.008 | 0.001 | 0.0 | 0.001 | 0.074 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | -0.071 | 0.008 | -0.001 | -0.011 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.002 | -0.006 | -0.007 | 0.0 | 0.0 | 0.0 |
| 11 23 | 0.0 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.009 | -0.003 | 0.0 | -0.009 | 0.076 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | 0.008 | -0.076 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | -0.005 | -0.005 | 0.003 | 0.0 | -0.001 | -0.001 |
| 12 21 | 0.001 | 0.001 | 0.001 | 0.0 | 0.008 | 0.0 | 0.008 | 0.0 | 0.0 | 0.0 | 0.003 | 0.072 | 0.0 | 0.0 | 0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.003 | -0.07 | -0.003 | 0.0 | -0.011 | -0.011 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13 16 | -0.004 | 0.0 | 0.003 | -0.019 | 0.0 | 0.011 | 0.0 | 0.0 | -0.006 | 0.0 | 0.0 | 0.0 | 0.095 | 0.0 | 0.0 | -0.113 | 0.025 | 0.004 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.005 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |
| 13 17 | 0.002 | 0.0 | 0.001 | 0.004 | 0.0 | 0.009 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | 0.0 | 0.094 | 0.002 | 0.0 | 0.025 | -0.106 | -0.01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.023 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |
| 14 18 | 0.0 | 0.0 | 0.001 | 0.0 | 0.001 | 0.011 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.002 | 0.112 | 0.002 | 0.001 | -0.011 | -0.111 | 0.012 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.025 | 0.003 | 0.001 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 14 19 | 0.0 | 0.0 | 0.002 | 0.0 | -0.003 | 0.008 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.058 | -0.008 | 0.0 | 0.003 | 0.008 | -0.068 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.003 | -0.01 | -0.002 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 19 | 0.0 | 0.0 | 0.002 | 0.0 | 0.009 | -0.002 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | -0.006 | 0.076 | 0.0 | -0.001 | -0.003 | -0.076 | 0.007 | 0.001 | 0.0 | 0.0 | 0.0 | 0.001 | 0.0 | 0.0 | -0.008 | 0.003 | -0.006 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 20 | 0.0 | 0.0 | 0.001 | 0.0 | 0.008 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.003 | 0.0 | 0.074 | 0.0 | 0.0 | 0.0 | 0.008 | -0.071 | -0.003 | 0.0 | 0.0 | -0.011 | -0.001 | 0.0 | 0.003 | -0.007 | -0.006 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 17 26 | -0.001 | 0.0 | 0.0 | -0.001 | 0.0 | -0.004 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.019 | 0.009 | 0.0 | -0.006 | -0.126 | 0.027 | 0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.119 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | |
| 18 26 | 0.0 | 0.0 | -0.001 | 0.0 | 0.0 | -0.005 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.008 | -0.024 | 0.0 | 0.003 | 0.028 | -0.121 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.116 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 19 27 | 0.0 | 0.0 | -0.001 | 0.0 | -0.001 | -0.001 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.008 | -0.008 | 0.0 | -0.001 | -0.003 | -0.081 | -0.003 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.001 | 0.079 | 0.009 | 0.019 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | |
|----------|------------|------------|-----|------------|------------|-----|------------|------------|------------|------------|------------|------------|-----|------------|------------|-----------|-----|-----------|------------|------------|------------|------------|------------|------------|------------|-----|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|-----------|
| 20 24 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 3 | 0.0 | 0.0 | -0.01 | 0.0 | 0.0 | 0.0 | -0.00 1 | -0.08 | 0.01 | 0.0 | 0.0 | 0.09 5 | 0.00 2 | 0.0 | -0.00 3 | -0.01 3 | -0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 20 28 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | -0.00 7 | 0.0 | 0.0 | 0.0 | -0.00 3 | -0.07 6 | -0.00 1 | 0.0 | 0.0 | -0.01 4 | 0.0 | 0.0 | 0.00 9 | 0.07 7 | 0.01 8 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 21 24 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | -0.00 1 | -0.00 9 | 0.0 | 0.0 | 0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.01 | -0.07 9 | -0.00 2 | 0.0 | 0.09 4 | -0.01 5 | 0.0 | 0.00 1 | 0.00 2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 21 25 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.0 | -0.00 3 | 0.0 | 0.0 | 0.0 | 0.00 3 | -0.00 9 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 2 | -0.07 9 | 0.01 1 | 0.0 | -0.01 5 | 0.09 4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 2 | 0.0 | 0.0 | 0.0 | 0.0 |
| 22 25 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | 0.0 | 0.0 | 0.0 | -0.01 | 0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.01 | -0.08 | -0.00 1 | 0.00 2 | 0.09 6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 2 | -0.00 4 | -0.01 2 | 0.0 | -0.00 1 | 0.0 |
| 22 35 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | -0.00 7 | -0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | -0.07 5 | -0.00 3 | 0.0 | -0.01 4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 6 | 0.02 1 | 0.07 4 | 0.0 | 0.00 2 | 0.00 1 |
| 23 33 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | -0.00 1 | 0.0 | -0.00 6 | -0.00 6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | -0.07 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | 0.0 | 0.0 | 0.05 5 | 0.01 2 | 0.00 7 | 0.0 | 0.01 2 | 0.00 7 | 0.00 | |
| 27 29 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 2 | 0.00 4 | 0.0 | 0.0 | 0.00 1 | 0.01 4 | -0.00 5 | 0.0 | 0.0 | 0.0 | -0.00 2 | 0.0 | 0.0 | 0.13 8 | -0.03 6 | -0.11 7 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 28 29 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.00 4 | 0.0 | 0.0 | 0.0 | -0.00 6 | 0.01 3 | 0.0 | 0.0 | 0.0 | 0.00 3 | 0.0 | 0.0 | -0.03 6 | 0.14 | -0.11 8 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 30 32 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | 0.00 2 | -0.00 8 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.07 7 | 0.00 6 | 0.07 5 | -0.00 1 | 0.0 | 0.0 | 0.02 1 | -0.00 3 | -0.01 1 | 0.0 | |
| 30 38 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | -0.00 1 | -0.00 8 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.07 7 | -0.00 1 | -0.01 1 | 0.00 6 | 0.00 2 | 0.00 1 | -0.00 3 | 0.02 1 | 0.07 5 | 0.0 | |
| 31 36 | 0.00 2 | 0.00 1 | 0.0 | 0.00 4 | 0.0 | 0.0 | 0.0 | 0.00 9 | 0.02 5 | 0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 5 | 0.09 2 | -0.03 | 0.0 | 0.0 | 0.0 | -0.10 1 | 0.0 | -0.00 1 | 0.0 | |
| 32 36 | -0.00 1 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | -0.00 4 | -0.00 7 | 0.00 4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.01 4 | -0.02 2 | 0.14 4 | 0.00 1 | 0.0 | 0.0 | -0.13 1 | 0.00 3 | 0.00 1 | | |
| 33 34 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 1 | 0.00 3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 5 | 0.01 | 0.0 | -0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 2 | 0.0 | 0.0 | 0.09 4 | -0.10 2 | -0.03 | 0.0 | 0.02 2 | 0.00 7 | 0.0 | |
| 33 37 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 3 | 0.00 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 2 | 0.01 | 0.0 | 0.00 1 | 0.0 | 0.0 | 0.0 | -0.00 5 | 0.0 | -0.00 1 | 0.09 4 | 0.02 2 | 0.00 7 | 0.0 | -0.10 2 | -0.03 | 0.0 | |
| 34 35 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.01 4 | -0.00 4 | 0.0 | 0.00 4 | 0.0 | 0.0 | 0.0 | -0.00 1 | 0.0 | 0.0 | -0.02 3 | -0.13 | 0.14 4 | 0.0 | -0.00 6 | -0.00 2 | 0.0 | |
| 37 38 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.00 4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -0.00 1 | -0.00 4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.01 4 | 0.0 | 0.00 3 | -0.02 3 | -0.00 6 | -0.00 2 | 0.00 1 | -0.13 | 0.14 4 |

7.2. Presentation of molecule:



8. Bond-Bond-Polarizability

8.1. Calculated values:

| | 1 2 | 1 3 | 1 4 | 2 7 | 2 8 | 3 5 | 3 6 | 4 9 | 4 16 | 5 12 | 5 15 | 6 13 | 6 14 | 7 11 | 7 12 | 8 10 | 8 31 | 9 31 | 10 23 | 10 30 | 11 22 | 11 23 | 12 21 | 13 16 | 13 17 | 14 18 | 14 19 | 15 19 | 15 20 | 17 26 | 18 26 | 19 27 | 20 24 | 20 28 | 21 24 | 21 25 | 22 25 | 22 35 | 23 33 | 27 29 | 28 29 | 30 32 | 30 38 | 31 36 | 32 36 | 33 34 | 33 37 | 34 35 | 37 38 | | | | | | |
|------|----------------|----------------|-----------------------|----------------|-----------------------|-----------------------|-----------------------|-----------------------|----------------|----------------|----------------|----------------|-----------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|--|--|--|--|--|
| 1 2 | 0.3 97 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 3 | - 0.0 7 | 0.3 97 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 4 | - 0.0 59 | - 0.0 59 | 0.3 79 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 7 | - 0.0 68 | 0.0 13 | 0.0 06 | 0.3 96 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 8 | - 0.0 68 | 0.0 07 | 0.0 13 | - 0.0 68 | 0.3 97 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 5 | 0.0 13 | - 0.0 68 | 0.0 05 | 0.0 01 | - 0.0 02 | 0.3 96 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 6 | 0.0 07 | - 0.0 68 | 0.0 13 | - 0.0 02 | 0.0 - 0.0 69 | 0.3 98 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 9 | 0.0 16 | 0.0 07 | - 0.0 8 | - 0.0 02 | - 0.0 01 | 0.0 - 0.0 03 | 0.4 45 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 16 | 0.0 07 | 0.0 16 | - 0.0 8 | - 0.0 01 | - 0.0 03 | - 0.0 02 | - 0.0 01 | 0.4 45 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 12 | 0.0 13 | 0.0 02 | - 0.0 02 | 0.0 13 | - 0.0 02 | - 0.0 67 | 0.0 07 | 0.0 01 | 0.3 97 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 15 | - 0.0 02 | 0.0 07 | 0.0 - 0.0 02 | - 0.0 01 | 0.0 - 0.0 67 | 0.0 13 | 0.0 - 0.0 67 | 0.0 01 | - 0.0 67 | 0.3 97 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 13 | - 0.0 02 | 0.0 13 | 0.0 01 | 0.0 01 | 0.0 06 | - 0.0 61 | - 0.0 06 | 0.0 21 | - 0.0 01 | - 0.0 02 | 0.3 77 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 14 | - 0.0 01 | 0.0 07 | - 0.0 02 | 0.0 13 | - 0.0 68 | 0.0 01 | - 0.0 02 | 0.0 01 | - 0.0 02 | 0.0 01 | - 0.0 53 | 0.3 87 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 11 | 0.0 07 | - 0.0 02 | 0.0 - 0.0 67 | - 0.0 13 | - 0.0 02 | 0.0 01 | 0.0 07 | 0.0 - 0.0 01 | 0.0 01 | 0.3 96 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 12 | 0.0 13 | 0.0 02 | - 0.0 67 | - 0.0 13 | 0.0 07 | - 0.0 02 | 0.0 01 | 0.0 07 | - 0.0 68 | 0.0 07 | 0.0 01 | - 0.0 67 | 0.3 97 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

[illegible]

| | 1 2 | 1 3 | 1 4 | 2 7 | 2 8 | 3 5 | 3 6 | 4 9 | 4 16 | 5 12 | 5 15 | 6 13 | 6 14 | 7 11 | 7 12 | 8 10 | 8 31 | 9 31 | 10 23 | 10 30 | 11 22 | 11 23 | 12 21 | 13 16 | 13 17 | 14 18 | 14 19 | 15 19 | 15 20 | 17 26 | 18 26 | 19 27 | 20 24 | 20 28 | 21 24 | 21 25 | 22 25 | 22 35 | 23 33 | 27 29 | 28 29 | 30 32 | 30 38 | 31 36 | 32 36 | 33 34 | 33 37 | 34 35 | 37 38 | | | | | | | | | | | | |
|-------|----------|--------|----------|----------|----------|----------|--------|----------|----------|----------|----------|------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|--------|-------|----------|----------|----------|----------|-------|--------|----------|----------|----------|----------|----------|----------|----------|----------|----------|--------|--------|----------|----------|-------|----------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 20 24 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 15 | 0.0 | 0.0 | 0.0 01 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 15 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 06 | - 0.0 74 | 0.0 | 0.0 | - 0.0 03 | 0.4 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 20 28 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 05 | 0.0 | 0.0 01 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 03 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 16 | - 0.0 64 | 0.0 | 0.0 | 0.0 | - 0.0 84 | 0.4 07 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 21 24 | 0.0 | 0.0 01 | 0.0 | - 0.0 01 | 0.0 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 14 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 07 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 03 | 0.0 01 | - 0.0 72 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 15 | 0.0 | 0.0 | 0.0 01 | - 0.0 82 | 0.0 11 | 0.4 19 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 21 25 | 0.0 01 | 0.0 | 0.0 | - 0.0 02 | 0.0 | - 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 07 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 14 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 15 | - 0.0 02 | - 0.0 71 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | - 0.0 03 | 0.0 | 0.0 | 0.0 | 0.0 12 | - 0.0 02 | - 0.0 88 | 0.4 19 | | | | | | | | | | | | | | | | | | | | | | | | | |
| 22 25 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 01 | 0.0 | 0.0 | 0.0 14 | 0.0 | 0.0 | 0.0 | - 0.0 01 | 0.0 | - 0.0 74 | 0.0 07 | 0.0 15 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 | 0.0 12 | - 0.0 82 | - 0.0 21 | 0.4 | | | | | | | | | | | | | | | | | | | | | | | | |
| 22 35 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 06 | - 0.0 02 | 0.0 01 | 0.0 | 0.0 | - 0.0 02 | 0.0 | - 0.0 64 | 0.0 15 | - 0.0 03 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 11 | - 0.0 83 | 0.4 07 | | | | | | | | | | | | | | | | | | | | | | | |
| 23 33 | 0.0 01 | 0.0 | 0.0 | - 0.0 02 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 06 | 0.0 | 0.0 06 | 0.0 | 0.0 | - 0.0 59 | 0.0 14 | 0.0 14 | - 0.0 6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | - 0.0 03 | 0.0 01 | 0.0 01 | 0.3 8 | | | | | | | | | | | | | | | | | | | | | |
| 27 29 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 01 | 0.0 | 0.0 | 0.0 | - 0.0 03 | 0.0 | - 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 03 | 0.0 13 | 0.0 21 | - 0.0 02 | 0.0 | 0.0 01 | - 0.1 1 | - 0.0 06 | 0.0 33 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.4 58 | | | | | | | | | | | | | | | | | | | |
| 28 29 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | - 0.0 03 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 01 | - 0.0 05 | - 0.0 02 | 0.0 2 | 0.0 | 0.0 34 | 0.0 16 | - 0.1 07 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.1 65 | 0.4 58 | | | | | | | | | | | | | | | | | | | | |
| 30 32 | 0.0 | 0.0 | 0.0 | 0.0 01 | - 0.0 02 | 0.0 | 0.0 | 0.0 02 | - 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 16 | 0.0 01 | - 0.0 08 | 0.0 06 | - 0.0 67 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 | 0.0 | 0.4 08 | | | | | | | | | | | | | | | | | | |
| 30 38 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 06 | - 0.0 02 | 0.0 02 | 0.0 16 | - 0.0 67 | 0.0 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 01 | 0.0 01 | 0.0 | 0.0 | - 0.0 77 | 0.4 08 | | | | | | | | | | | | | | | | | |
| 31 36 | - 0.0 03 | 0.0 01 | - 0.0 05 | 0.0 07 | 0.0 | 0.0 | 0.0 | 0.0 24 | - 0.0 05 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 16 | - 0.0 76 | - 0.1 26 | - 0.0 02 | - 0.0 01 | 0.0 | 0.0 01 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | | | | | | |
| 32 36 | 0.0 01 | 0.0 | 0.0 02 | 0.0 | - 0.0 03 | 0.0 | 0.0 | - 0.0 06 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 23 | 0.0 29 | - 0.0 02 | 0.0 2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | | | | | | |
| 33 34 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 06 | - 0.0 03 | - 0.0 01 | 0.0 17 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | - 0.0 06 | 0.0 29 | - 0.0 78 | 0.0 | 0.0 | 0.0 02 | - 0.0 08 | 0.0 | - 0.0 01 | 0.4 4 | | | | | | | | | | | | | | |
| 33 37 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 | 0.0 | 0.0 | 0.0 17 | - 0.0 01 | - 0.0 03 | 0.0 07 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | | | | |
| 34 35 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 03 | 0.0 01 | 0.0 | 0.0 | 0.0 | - 0.0 03 | 0.0 01 | 0.0 2 | - 0.0 02 | 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 17 | - 0.1 11 | 0.0 24 | 0.0 | 0.0 | - 0.0 01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | | | | | |
| 37 38 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | - 0.0 02 | 0.0 01 | - 0.0 01 | - 0.0 02 | 0.0 2 | 0.0 01 | - 0.0 03 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

8.2. Presentation of molecule:

