

**Supplementary Material**  
**Structural, electronic and vibrational properties of B<sub>24</sub>N<sub>24</sub> nanocapsules: novel anodes  
for magnesium batteries**

Domenico Corona,<sup>1</sup> Francesco Buonocore,<sup>2</sup> Friedhelm Bechstedt,<sup>3</sup> Massimo Celino,<sup>2</sup> and Olivia Pulci<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Rome Tor Vergata,  
and INFN, Via della Ricerca Scientifica 1, 00133 Rome,*

*Italy; domenico.corona@roma2.infn.it (D.C.); olivia.pulci@roma2.infn.it (O.P.)*

<sup>2</sup>*Energy Technologies and Renewable Sources (TERIN) Department, Italian National Agency for New Technologies,  
Energy and Sustainable Economic Development (ENEA), Casaccia Research Centre,  
00123 Rome, Italy; francesco.buonocore@enea.it (F.B.); massimo.celino@enea.it (M.C.)*

<sup>3</sup>*Institut für Festkörpertheorie und -optik, Friedrich Schiller Universität,  
Max Wien Platz 1, 07743 Jena, Germany; friedhelm.bechstedt@uni-jena.de*

(Dated: January 26, 2024)

## I. GEOMETRICAL STRUCTURES

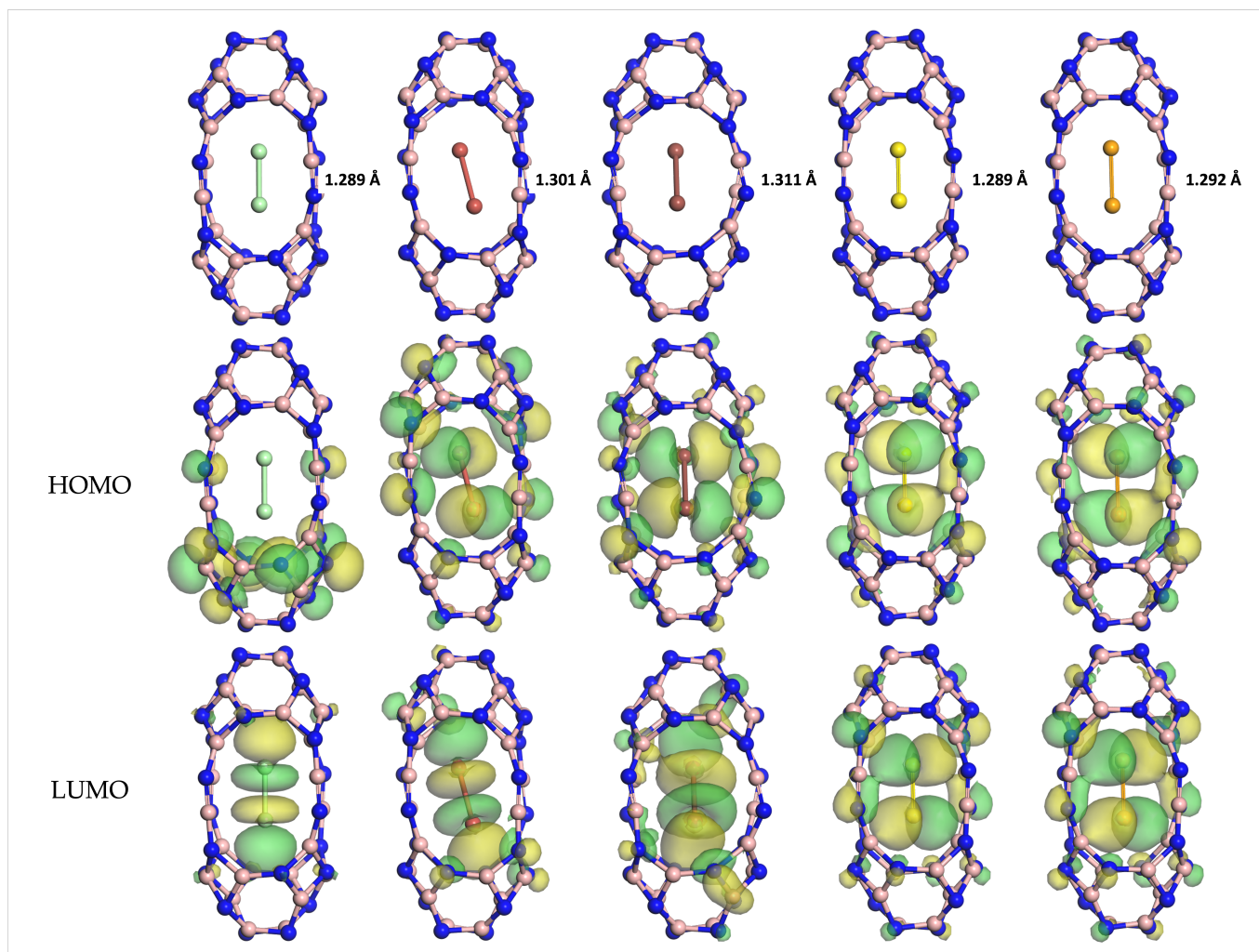


Figure S1. Geometrically optimized structures and molecular orbitals plots for (from left to right): Cl<sub>2</sub>/B<sub>24</sub>N<sub>24</sub>, Br<sub>2</sub>/B<sub>24</sub>N<sub>24</sub>, I<sub>2</sub>/B<sub>24</sub>N<sub>24</sub>, S<sub>2</sub>/B<sub>24</sub>N<sub>24</sub> and Se<sub>2</sub>/B<sub>24</sub>N<sub>24</sub>. Distances are in Å.

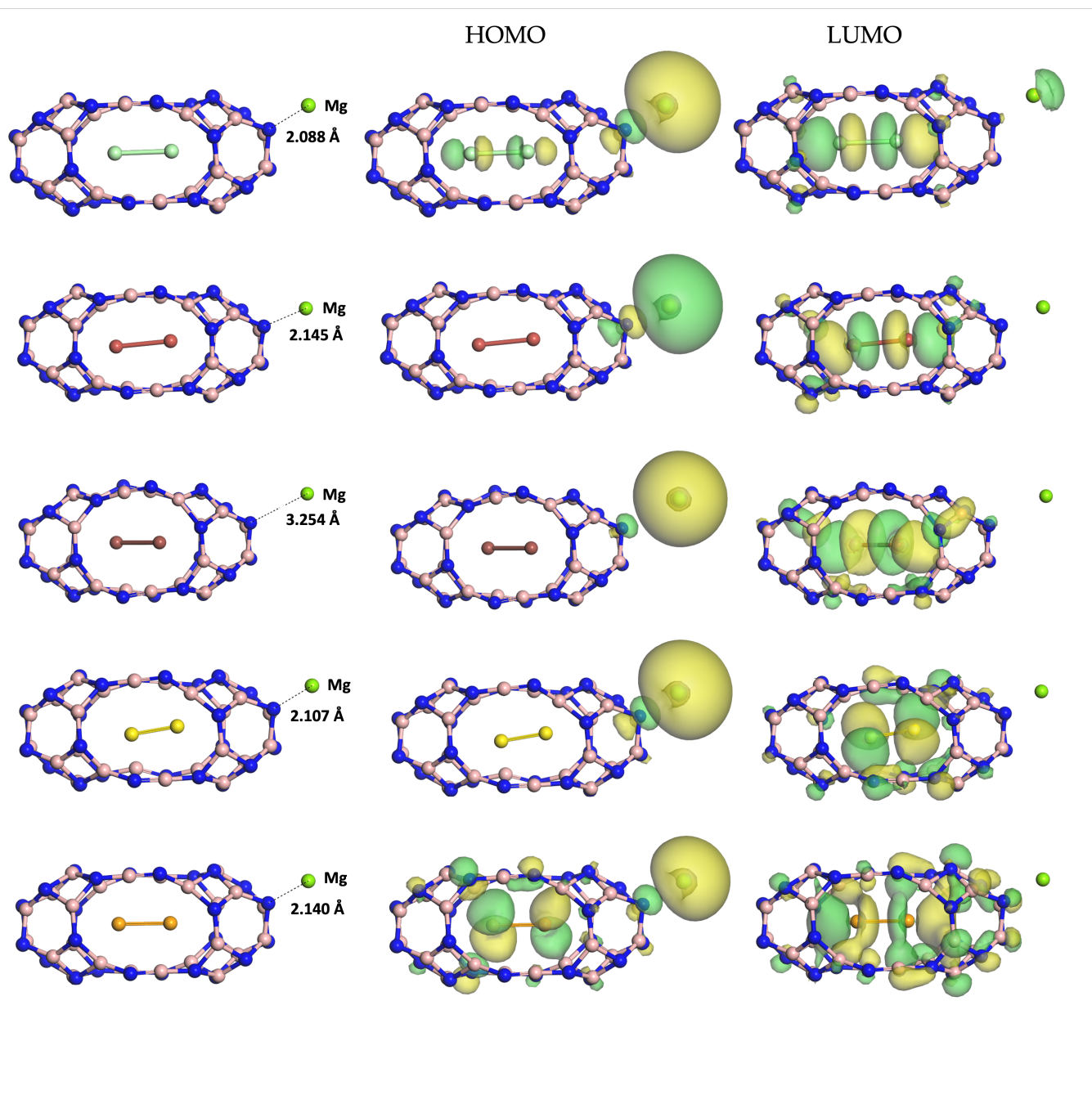


Figure S2. Geometrically optimized structures and molecular orbitals plots for (from top to bottom):  $\text{Cl}_2/\text{B}_{24}\text{N}_{24}@\text{Mg}$ ,  $\text{Br}_2/\text{B}_{24}\text{N}_{24}@\text{Mg}$ ,  $\text{I}_2/\text{B}_{24}\text{N}_{24}@\text{Mg}$ ,  $\text{S}_2/\text{B}_{24}\text{N}_{24}@\text{Mg}$  and  $\text{Se}_2/\text{B}_{24}\text{N}_{24}@\text{Mg}$ . Distances are in Å.

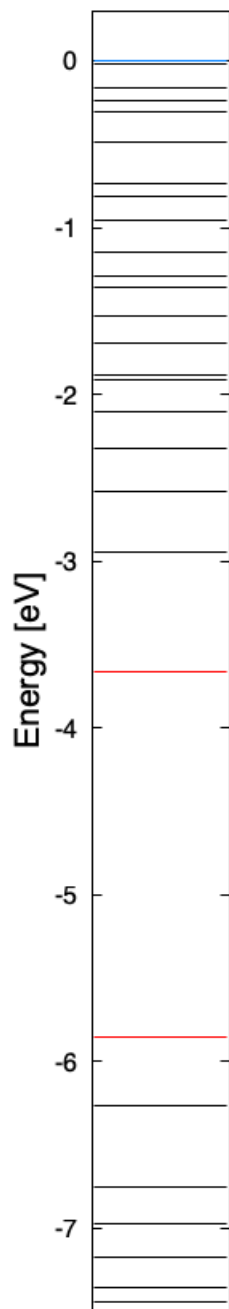


Figure S3. Energy level diagram for  $\text{I}_2/\text{B}_{24}\text{N}_{24}$ . The energy range considered is between -7.5 eV and the vacuum level (blue line), and the frontier orbitals are denoted in red lines.

## II. VIBRATIONAL ANALYSIS

| Frequency (1/cm) | Intensity IR (km/mol) | Intensity Raman (km/mol) |
|------------------|-----------------------|--------------------------|
| 66.19            | 0.01                  | 1.549                    |
| 89.02            | 0.78                  | 20.906                   |
| 95.46            | 0.75                  | 17.194                   |
| 100.65           | 1.16                  | 8.716                    |
| 121.22           | 0.06                  | 5.879                    |



|        |       |        |
|--------|-------|--------|
| 123.63 | 0.31  | 1.747  |
| 127.2  | 0.04  | 1.798  |
| 133.65 | 0.14  | 1.78   |
| 155.24 | 0.07  | 0.138  |
| 162.09 | 0.83  | 0.15   |
| 163.91 | 1.8   | 0.275  |
| 171.23 | 1.53  | 0.008  |
| 214.71 | 0.22  | 3.845  |
| 234.92 | 8.69  | 0.022  |
| 243.31 | 7.31  | 0.088  |
| 277.45 | 0.03  | 0.293  |
| 281.25 | 0.02  | 19.497 |
| 292.09 | 0.03  | 1.716  |
| 318.81 | 2.18  | 0.484  |
| 323.38 | 2.02  | 0.544  |
| 334.26 | 0.26  | 0.052  |
| 337.52 | 0.54  | 0.011  |
| 349.07 | 0.92  | 0.757  |
| 352.7  | 0.15  | 0.117  |
| 356.34 | 0.15  | 0.127  |
| 373.97 | 2.41  | 0.055  |
| 374.95 | 1.81  | 0.079  |
| 384.02 | 0.02  | 0.932  |
| 388.42 | 0.08  | 0.12   |
| 401.97 | 6.2   | 0.23   |
| 404.4  | 0.42  | 0.044  |
| 412.1  | 7.66  | 0.215  |
| 450.21 | 0.07  | 5.425  |
| 461.31 | 26.65 | 0.366  |
| 475.93 | 20.58 | 0.304  |
| 482.4  | 0.41  | 0.05   |
| 484.64 | 1.48  | 0.437  |
| 491.9  | 0.48  | 0.095  |
| 504.42 | 0.41  | 0.294  |
| 505.27 | 0.3   | 0.808  |
| 510.65 | 12.86 | 0.045  |
| 512.92 | 14.17 | 0.017  |
| 514.82 | 6.65  | 0.082  |
| 541.76 | 10.46 | 0.033  |
| 542.18 | 11.02 | 0.085  |
| 546.05 | 11.98 | 0.131  |
| 549.94 | 7.72  | 0.184  |
| 552.83 | 2.4   | 0.174  |
| 565.85 | 9.94  | 0.005  |
| 571.17 | 9.35  | 0.007  |
| 577.98 | 0.14  | 0.018  |
| 582.56 | 0.75  | 0.014  |
| 588.89 | 10.21 | 0.087  |
| 596.54 | 5.23  | 0.14   |
| 602.78 | 2.89  | 0.01   |
| 606.11 | 3.48  | 0.02   |
| 628.67 | 3.82  | 0.048  |
| 634.79 | 3.69  | 0.054  |
| 635.53 | 4.91  | 0.028  |
| 665.3  | 1.33  | 0.193  |
| 668.07 | 6.13  | 0.155  |
| 685.17 | 5.55  | 0.037  |
| 690.55 | 3.91  | 0.403  |
| 691.93 | 98.07 | 1.129  |
| 695.41 | 30.03 | 3.105  |

|          |          |       |
|----------|----------|-------|
| 698.52   | 79.66    | 0.985 |
| 717.72   | 0.05     | 4.11  |
| 724.22   | 28.34    | 0.056 |
| 728.07   | 41.6     | 0.07  |
| 728.79   | 146.78   | 0.016 |
| 729.43   | 59.26    | 0.082 |
| 733.38   | 2.02     | 1.745 |
| 735.72   | 0.72     | 3.649 |
| 740.3    | 140.04   | 0.042 |
| 742.36   | 88.23    | 0.044 |
| 766.07   | 0.41     | 0.01  |
| 772.94   | 2.12     | 0.035 |
| 785.06   | 0.71     | 0.097 |
| 785.8    | 2.62     | 0.145 |
| 792.26   | 350.95   | 0.052 |
| 794.39   | 126.06   | 0.173 |
| 799.33   | 0.75     | 5.977 |
| 835.89   | 16.73    | 0.567 |
| 839.26   | 19.09    | 0.519 |
| 855.62   | 3.86     | 0.047 |
| 861.46   | 1.63     | 0.039 |
| 863.28   | 2.76     | 0.064 |
| 863.59   | 1.84     | 0.089 |
| 866.82   | 1.27     | 0.012 |
| 881.22   | 0.17     | 0.099 |
| 881.91   | 0.71     | 0.258 |
| 882.53   | 0.53     | 0.262 |
| 887.14   | 0.13     | 0.05  |
| 906.19   | 0.36     | 0.052 |
| 912.52   | 1.18     | 0.055 |
| 958.05   | 0.36     | 0.268 |
| 976.55   | 37.15    | 0.013 |
| 978.29   | 35.19    | 0.012 |
| 1.00E+03 | 1.08     | 0.246 |
| 1.01E+03 | 67.49    | 0.07  |
| 1.08E+03 | 7.27     | 0.003 |
| 1.08E+03 | 9.14     | 0.02  |
| 1.11E+03 | 1.28     | 0.186 |
| 1.12E+03 | 8.76     | 0.055 |
| 1.15E+03 | 78.31    | 0.035 |
| 1.16E+03 | 51.27    | 0.047 |
| 1.17E+03 | 1.81     | 0.444 |
| 1.17E+03 | 6.1      | 0.113 |
| 1.19E+03 | 68.16    | 0.062 |
| 1.19E+03 | 150.72   | 0.005 |
| 1.19E+03 | 54.99    | 0.063 |
| 1.21E+03 | 57.63    | 0.023 |
| 1.22E+03 | 49.76    | 0.064 |
| 1.22E+03 | 40.03    | 0.029 |
| 1.23E+03 | 3.01     | 0.065 |
| 1.26E+03 | 48.48    | 0.131 |
| 1.26E+03 | 1.65E+03 | 0.024 |
| 1.27E+03 | 346.67   | 0.11  |
| 1.30E+03 | 985.72   | 0.007 |
| 1.31E+03 | 65.93    | 0.02  |
| 1.31E+03 | 64.04    | 0.017 |
| 1.32E+03 | 7.85     | 0.489 |
| 1.36E+03 | 106.03   | 0.007 |
| 1.37E+03 | 23.43    | 0.004 |
| 1.41E+03 | 1.94E+03 | 0.011 |

|          |          |       |
|----------|----------|-------|
| 1.42E+03 | 1.81E+03 | 0.085 |
| 1.42E+03 | 232.15   | 0.561 |
| 1.44E+03 | 1.35E+03 | 0.123 |
| 1.44E+03 | 548.32   | 0.144 |
| 1.45E+03 | 5.37     | 0.173 |
| 1.49E+03 | 24.24    | 0.012 |
| 1.51E+03 | 27.25    | 0.046 |
| 1.52E+03 | 26.44    | 0.051 |
| 1.56E+03 | 6.13     | 0.113 |
| 1.95E+03 | 0.31     | 7.176 |
| 1.98E+03 | 3.61     | 0.023 |
| 1.98E+03 | 67.74    | 0.451 |
| 2.05E+03 | 5.72E+03 | 0.017 |

Table S1: Vibrational Analysis of the systems  $B_{24}N_{24}$ .

| Frequency (1/cm) | Intensity IR (km/mol) | Intensity Raman (km/mol) |
|------------------|-----------------------|--------------------------|
| 43.64            | 1.54                  | 32.591                   |
| 55.78            | 0.94                  | 31.931                   |
| 87.49            | 0.34                  | 6.495                    |
| 95.91            | 0.14                  | 1.747                    |
| 103.24           | 0.31                  | 0.91                     |
| 116.51           | 6.32                  | 7.21                     |
| 145.77           | 0.72                  | 2.356                    |
| 151.67           | 2.66                  | 1.813                    |
| 152.97           | 3.56                  | 5.533                    |
| 162.52           | 2.42                  | 6.599                    |
| 175.08           | 4.85                  | 3.447                    |
| 186.94           | 6.66                  | 6.005                    |
| 200.78           | 6.4                   | 0.067                    |
| 226.76           | 0.8                   | 0.124                    |
| 236.43           | 0.43                  | 0.305                    |
| 255.6            | 7.22                  | 1.651                    |
| 258.83           | 11.66                 | 1.161                    |
| 272.52           | 24.25                 | 8.532                    |
| 276.69           | 18.6                  | 12.416                   |
| 291.74           | 12.5                  | 1.877                    |
| 299.21           | 12.46                 | 0.961                    |
| 303.85           | 2.61                  | 0.326                    |
| 304.91           | 1.99                  | 2.747                    |
| 310.71           | 19.87                 | 8.88                     |
| 323.58           | 4.11                  | 0.371                    |
| 324.79           | 7.96                  | 0.671                    |
| 332.77           | 1.19                  | 0.214                    |
| 336.78           | 0.54                  | 1.06                     |
| 338.48           | 1.46                  | 0.881                    |
| 345.46           | 22.21                 | 0.621                    |
| 362.22           | 2.57                  | 0.682                    |
| 368.51           | 2.37                  | 0.56                     |
| 378.89           | 2.14                  | 0.785                    |
| 391.47           | 1.56                  | 1.048                    |
| 399.8            | 11.91                 | 1.327                    |
| 402.43           | 47.45                 | 0.853                    |
| 417.35           | 7.69                  | 0.504                    |
| 422.04           | 16.19                 | 0.142                    |
| 423.75           | 49.09                 | 0.936                    |
| 433.63           | 1.27                  | 2.197                    |
| 437.3            | 12.82                 | 0.702                    |
| 455.08           | 8.93                  | 1.024                    |
| 460.06           | 17.88                 | 0.29                     |
| 467.37           | 3.11                  | 0.272                    |
| 475.03           | 52.99                 | 0.276                    |
| 486.35           | 3.41                  | 0.201                    |
| 493.83           | 30.71                 | 0.858                    |
| 497.8            | 14.23                 | 0.176                    |
| 505.37           | 40.83                 | 0.383                    |
| 508.45           | 4.5                   | 0.18                     |
| 510.63           | 4.46                  | 0.279                    |
| 514.3            | 13.24                 | 0.027                    |
| 519.5            | 6.18                  | 0.195                    |
| 523.05           | 22.47                 | 0.236                    |
| 529.18           | 38.69                 | 0.202                    |
| 533.91           | 40.42                 | 0.088                    |
| 545.56           | 50.41                 | 0.304                    |
| 548.32           | 39.27                 | 0.842                    |
| 560.92           | 46.23                 | 0.987                    |

|          |        |       |
|----------|--------|-------|
| 563.06   | 14.26  | 0.172 |
| 571.41   | 22.05  | 0.479 |
| 585.6    | 11.08  | 0.187 |
| 593.67   | 7.81   | 6.218 |
| 609.62   | 22.88  | 0.494 |
| 611.57   | 5.61   | 0.303 |
| 619.11   | 23.91  | 0.157 |
| 627.56   | 0.45   | 0.088 |
| 635.77   | 10.11  | 0.354 |
| 641.25   | 3.15   | 0.38  |
| 656.71   | 17.54  | 0.113 |
| 660.54   | 4.77   | 0.05  |
| 668.12   | 45.97  | 0.347 |
| 673.52   | 5.98   | 0.264 |
| 675.89   | 3.16   | 0.336 |
| 684.5    | 7.68   | 0.389 |
| 689.47   | 5.88   | 2.148 |
| 696.39   | 57.45  | 1.045 |
| 701.33   | 73.57  | 2.96  |
| 704.41   | 33.62  | 2.067 |
| 705.45   | 155.32 | 0.161 |
| 710.7    | 185.98 | 0.153 |
| 710.94   | 98.01  | 0.371 |
| 726.76   | 31.47  | 0.523 |
| 733.99   | 37.04  | 0.183 |
| 738.76   | 5.93   | 1.228 |
| 746.27   | 26.71  | 0.582 |
| 772.58   | 66.2   | 0.903 |
| 773.88   | 43.52  | 0.277 |
| 780.27   | 89.57  | 0.275 |
| 781.63   | 85.55  | 0.649 |
| 784.86   | 114.84 | 0.428 |
| 789.02   | 78.82  | 0.402 |
| 794      | 26.01  | 2.056 |
| 797.04   | 76.51  | 0.732 |
| 823.3    | 28.39  | 0.169 |
| 829.1    | 1.27   | 0.062 |
| 840.23   | 0.11   | 0.722 |
| 882.28   | 4.29   | 0.064 |
| 888.49   | 6.7    | 0.085 |
| 898.14   | 1.54   | 0.219 |
| 922.07   | 1.88   | 0.012 |
| 924.16   | 2.43   | 0.024 |
| 968.67   | 19.31  | 0.033 |
| 975.7    | 17.34  | 0.037 |
| 981.72   | 2.69   | 0.138 |
| 996.48   | 11     | 0.052 |
| 1.00E+03 | 60.56  | 0.122 |
| 1.01E+03 | 35.66  | 0.222 |
| 1.03E+03 | 31.51  | 0.153 |
| 1.04E+03 | 24.08  | 0.198 |
| 1.07E+03 | 13.86  | 0.086 |
| 1.08E+03 | 100.56 | 0.006 |
| 1.10E+03 | 85.04  | 0.043 |
| 1.10E+03 | 39.76  | 0.119 |
| 1.11E+03 | 207.78 | 0.26  |
| 1.13E+03 | 24.64  | 0.174 |
| 1.13E+03 | 21.96  | 0.489 |
| 1.14E+03 | 222.19 | 0.112 |
| 1.15E+03 | 17.95  | 0.046 |

|          |          |       |
|----------|----------|-------|
| 1.16E+03 | 24.61    | 0.066 |
| 1.17E+03 | 13.46    | 0.346 |
| 1.18E+03 | 852.03   | 0.194 |
| 1.22E+03 | 57.82    | 0.016 |
| 1.23E+03 | 386.9    | 0.037 |
| 1.23E+03 | 59.53    | 0.028 |
| 1.24E+03 | 118.48   | 0.027 |
| 1.25E+03 | 212.05   | 0.039 |
| 1.26E+03 | 70.61    | 0.07  |
| 1.28E+03 | 728.1    | 0.007 |
| 1.28E+03 | 343.25   | 0.408 |
| 1.32E+03 | 617.82   | 0.244 |
| 1.33E+03 | 523.84   | 0.106 |
| 1.34E+03 | 655.13   | 0.101 |
| 1.34E+03 | 447.42   | 0.065 |
| 1.37E+03 | 239.9    | 0.126 |
| 1.37E+03 | 14.9     | 0.159 |
| 1.38E+03 | 206.11   | 0.1   |
| 1.38E+03 | 9.52     | 0.146 |
| 1.44E+03 | 1.14E+03 | 0.021 |
| 1.45E+03 | 310.79   | 0.08  |
| 1.76E+03 | 47.88    | 2.048 |
| 1.78E+03 | 110.72   | 0.467 |
| 1.80E+03 | 426.8    | 0.554 |
| 1.83E+03 | 1.97E+03 | 0.229 |

Table S2: Vibrational Analysis of the systems  $I_2/B_{24}N_{24}$ .

| Frequency (1/cm) | Intensity IR (km/mol) | Intensity Raman (km/mol) |
|------------------|-----------------------|--------------------------|
| 40.81            | 0.15                  | 102.148                  |
| 52.66            | 6.56                  | 777.117                  |
| 59.31            | 4.95                  | 321.028                  |
| 63.94            | 5.55                  | 705.092                  |
| 79.69            | 1.02                  | 54.123                   |
| 97.45            | 0.07                  | 19.123                   |
| 106.6            | 0.45                  | 5.46                     |
| 123.78           | 1.14                  | 5.911                    |
| 139.95           | 3.06                  | 6.326                    |
| 145.17           | 0.64                  | 5.969                    |
| 153.65           | 2.25                  | 17.765                   |
| 157.54           | 0.36                  | 25.881                   |
| 169.01           | 0.92                  | 9.41                     |
| 187.82           | 0.29                  | 16.441                   |
| 205.98           | 0.96                  | 8.854                    |
| 220.53           | 1.79                  | 28.951                   |
| 231.33           | 6.83                  | 54.491                   |
| 241.35           | 0.87                  | 1.257                    |
| 251.38           | 9.79                  | 74.171                   |
| 254.14           | 1.32                  | 12.812                   |
| 272.76           | 1.66                  | 9.6                      |
| 284.61           | 4.06                  | 3.776                    |
| 291.65           | 8.14                  | 1.472                    |
| 295.68           | 2.22                  | 6.591                    |
| 300.66           | 9.55                  | 7.018                    |
| 306.11           | 3.06                  | 4.246                    |
| 310.54           | 5.5                   | 4.138                    |
| 319.57           | 5.46                  | 11.647                   |
| 329.4            | 1.62                  | 1.289                    |
| 333.93           | 0.44                  | 3.852                    |
| 339.09           | 4.74                  | 1.389                    |
| 347.87           | 3.17                  | 1.023                    |
| 356.75           | 13.76                 | 4.128                    |
| 364.47           | 5.32                  | 1.416                    |
| 370.8            | 2.82                  | 1.435                    |
| 376.81           | 0.11                  | 8.805                    |
| 386.17           | 6.19                  | 10.516                   |
| 399.68           | 0.43                  | 0.512                    |
| 410.22           | 3.59                  | 3.208                    |
| 418.35           | 9.66                  | 10.856                   |
| 426.88           | 8.26                  | 2.759                    |
| 431.4            | 63.48                 | 23.551                   |
| 437.78           | 18.96                 | 3.556                    |
| 445.69           | 21.25                 | 1.609                    |
| 455.9            | 45.01                 | 7.708                    |
| 460.95           | 24.04                 | 3.19                     |
| 466.97           | 22.53                 | 3.132                    |
| 481.58           | 3.8                   | 0.578                    |
| 483.78           | 15.34                 | 2.468                    |
| 495.39           | 21.49                 | 13.84                    |
| 497.48           | 21.01                 | 9.468                    |
| 505.23           | 9.06                  | 0.786                    |
| 509.91           | 24.95                 | 1.893                    |
| 512.37           | 6.18                  | 1.791                    |
| 516.76           | 5.5                   | 0.538                    |
| 518.69           | 11.91                 | 1.214                    |
| 521.46           | 22.79                 | 2.892                    |
| 529.85           | 33.64                 | 8.788                    |
| 531.27           | 8.51                  | 12.982                   |

|          |        |        |
|----------|--------|--------|
| 545.06   | 118.63 | 41.645 |
| 548.62   | 35.38  | 5.192  |
| 555.75   | 12.46  | 1.586  |
| 557.43   | 25.02  | 2.139  |
| 567.76   | 30.81  | 5.589  |
| 576.49   | 49.77  | 26.682 |
| 584.41   | 2.44   | 5.439  |
| 597.03   | 0.49   | 3.773  |
| 605.86   | 17.81  | 1.036  |
| 609.79   | 21.77  | 2.495  |
| 626.79   | 5.88   | 0.119  |
| 638.76   | 4.86   | 2.435  |
| 646.9    | 35.27  | 2.134  |
| 651.74   | 2.9    | 0.479  |
| 657.88   | 4.89   | 1.428  |
| 665.59   | 18.26  | 6.052  |
| 673.4    | 5.06   | 2.487  |
| 676.15   | 57.31  | 0.554  |
| 680.3    | 24.85  | 1.841  |
| 688.52   | 2.9    | 2.638  |
| 693.76   | 43.49  | 7.725  |
| 695.77   | 107.41 | 3.64   |
| 697.95   | 69.48  | 0.561  |
| 700.09   | 10.38  | 0.761  |
| 704.46   | 131.2  | 7.601  |
| 711.72   | 122.69 | 1.555  |
| 722.76   | 79.4   | 4.708  |
| 726.09   | 61.01  | 2.17   |
| 730.31   | 47.84  | 0.234  |
| 740.32   | 1.61   | 0.126  |
| 750.96   | 22.93  | 1.955  |
| 772.76   | 4.37   | 0.845  |
| 781.08   | 91.74  | 11.637 |
| 783.4    | 7.14   | 0.375  |
| 788.67   | 217.02 | 17.083 |
| 790.93   | 2.4    | 3.78   |
| 795.62   | 127.35 | 10.465 |
| 802.17   | 6.35   | 1.67   |
| 817.65   | 17.31  | 1.721  |
| 833.33   | 2.91   | 0.844  |
| 847.46   | 0.79   | 2.4    |
| 889.09   | 6.76   | 0.664  |
| 898      | 12.15  | 3.186  |
| 904.13   | 9.82   | 9.087  |
| 911.49   | 4.73   | 3.032  |
| 937.4    | 6.83   | 0.485  |
| 941.26   | 2.39   | 0.645  |
| 979.79   | 17.34  | 0.44   |
| 990.07   | 6.58   | 4.348  |
| 993.47   | 14.08  | 1.103  |
| 1.01E+03 | 35.7   | 6.052  |
| 1.02E+03 | 20.45  | 0.687  |
| 1.04E+03 | 52.79  | 3.504  |
| 1.05E+03 | 24.05  | 10.378 |
| 1.07E+03 | 3.91   | 6.669  |
| 1.09E+03 | 34.5   | 11.565 |
| 1.10E+03 | 36.76  | 3.018  |
| 1.11E+03 | 48.47  | 9.507  |
| 1.12E+03 | 35.08  | 0.656  |
| 1.14E+03 | 110.75 | 13.704 |



|          |        |        |
|----------|--------|--------|
| 1.14E+03 | 102.38 | 4.244  |
| 1.15E+03 | 114.41 | 8.184  |
| 1.16E+03 | 170.48 | 9.044  |
| 1.17E+03 | 55.99  | 0.734  |
| 1.19E+03 | 7.38   | 1.188  |
| 1.20E+03 | 244.09 | 57.727 |
| 1.21E+03 | 225.81 | 4.098  |
| 1.22E+03 | 115.57 | 0.559  |
| 1.24E+03 | 324.48 | 5.574  |
| 1.25E+03 | 78.15  | 6.596  |
| 1.26E+03 | 95.82  | 18.456 |
| 1.26E+03 | 324.01 | 5.976  |
| 1.28E+03 | 15.74  | 4.718  |
| 1.29E+03 | 466.82 | 52.478 |
| 1.30E+03 | 358.72 | 17.495 |
| 1.33E+03 | 286.51 | 5.121  |
| 1.35E+03 | 314.74 | 13.703 |
| 1.36E+03 | 71.53  | 20.418 |
| 1.37E+03 | 295.11 | 26.973 |
| 1.39E+03 | 217.18 | 5.549  |
| 1.41E+03 | 91.43  | 23.857 |
| 1.42E+03 | 359.8  | 21.148 |
| 1.44E+03 | 703.18 | 27.066 |
| 1.48E+03 | 97.84  | 1.63   |
| 1.78E+03 | 165.17 | 19.242 |
| 1.81E+03 | 24.31  | 3.789  |
| 1.82E+03 | 30.77  | 9.256  |
| 1.84E+03 | 781.78 | 68.734 |

Table S3: Vibrational Analysis of the systems  $I_2/B_{24}N_{24}@Mg^{2+}$ .

| From   | To      | TD-ex[eV] | KS-ex[eV] | TD-ex[nm] | KS-ex[nm] | [Ha]     | f.osc    |
|--------|---------|-----------|-----------|-----------|-----------|----------|----------|
| HOMO   | LUMO-   | 4.25      | 4.27      | 292       | 291       | 0.156207 | 0.000000 |
| HOMO-1 | LUMO+   | 4.25      | 4.27      | 292       | 291       | 0.156257 | 0.000000 |
| HOMO   | LUMO+   | 4.29      | 4.27      | 289       | 290       | 0.157714 | 0.003411 |
| HOMO-1 | LUMO-   | 4.29      | 4.27      | 289       | 290       | 0.157765 | 0.003463 |
| HOMO   | LUMO+1- | 4.50      | 4.50      | 276       | 275       | 0.165278 | 0.003308 |
| HOMO-1 | LUMO+1- | 4.50      | 4.51      | 276       | 275       | 0.165323 | 0.003289 |
| HOMO   | 148-    | 4.59      | 4.51      | 270       | 275       | 0.168822 | 0.005800 |
| 140    | LUMO-   | 4.72      | 4.67      | 263       | 266       | 0.173379 | 0.007334 |
| 139    | LUMO+   | 4.72      | 4.67      | 263       | 266       | 0.173428 | 0.007323 |
| 141    | LUMO-   | 4.75      | 4.78      | 261       | 259       | 0.174663 | 0.050667 |
| 139    | LUMO+2+ | 4.95      | 4.91      | 251       | 253       | 0.181776 | 0.012384 |
| 135    | LUMO+   | 5.04      | 5.02      | 246       | 247       | 0.185345 | 0.002741 |
| 136    | LUMO+   | 5.04      | 5.02      | 246       | 247       | 0.185350 | 0.003125 |
| 138    | LUMO+2+ | 5.06      | 5.02      | 245       | 247       | 0.185824 | 0.010157 |
| 138    | 148+    | 5.06      | 5.02      | 245       | 247       | 0.185889 | 0.009080 |
| 138    | LUMO+1- | 5.14      | 5.14      | 241       | 241       | 0.188818 | 0.139794 |
| HOMO   | 151-    | 5.19      | 5.16      | 239       | 240       | 0.190633 | 0.004675 |
| HOMO-1 | 151-    | 5.19      | 5.17      | 239       | 240       | 0.190677 | 0.004214 |
| 132    | LUMO-   | 5.28      | 5.26      | 235       | 236       | 0.193995 | 0.002773 |

Table S4: Optical Absorption Analysis of the system  $B_{24}N_{24}$ . The HOMO corresponds to Kohn-Sham state 144 while the LUMO corresponds to state 145.

| From   | To      | TD-ex[eV] | KS-ex[eV] | TD-ex[nm] | KS-ex[nm] | [Ha]     | f <sub>osc</sub> |
|--------|---------|-----------|-----------|-----------|-----------|----------|------------------|
| HOMO   | LUMO+   | 2.11      | 2.18      | 588       | 568       | 0.077457 | 0.000000         |
| HOMO   | LUMO-   | 2.35      | 2.18      | 527       | 568       | 0.086397 | 0.000131         |
| HOMO-1 | LUMO-   | 2.52      | 2.59      | 492       | 478       | 0.092635 | 0.000000         |
| HOMO-1 | LUMO+   | 2.74      | 2.59      | 452       | 478       | 0.100876 | 0.005351         |
| HOMO   | LUMO+1+ | 2.89      | 2.91      | 429       | 426       | 0.106086 | 0.000000         |
| HOMO   | LUMO+1- | 2.96      | 2.91      | 419       | 426       | 0.108734 | 0.007053         |
| 194    | LUMO-   | 3.12      | 3.08      | 397       | 403       | 0.114752 | 0.001736         |
| HOMO-2 | LUMO-   | 3.14      | 3.08      | 395       | 403       | 0.115421 | 0.007628         |
| HOMO-1 | LUMO+1- | 3.36      | 3.32      | 369       | 373       | 0.123489 | 0.001091         |
| 193    | LUMO+   | 3.44      | 3.42      | 360       | 363       | 0.126508 | 0.003252         |
| HOMO   | 201-    | 3.55      | 3.54      | 349       | 350       | 0.130637 | 0.001283         |
| HOMO   | 202-    | 3.57      | 3.54      | 347       | 350       | 0.131151 | 0.002797         |
| 191    | LUMO-   | 3.58      | 3.57      | 347       | 348       | 0.131495 | 0.014285         |
| HOMO-1 | LUMO+2+ | 3.73      | 3.71      | 332       | 334       | 0.137091 | 0.002083         |
| 187    | LUMO+   | 3.78      | 3.76      | 328       | 330       | 0.138747 | 0.020050         |
| 185    | LUMO+   | 3.79      | 3.80      | 327       | 326       | 0.139139 | 0.007428         |
| HOMO   | 203-    | 3.83      | 3.80      | 324       | 326       | 0.140745 | 0.020258         |
| 194    | LUMO+1+ | 3.85      | 3.80      | 322       | 326       | 0.141385 | 0.003758         |
| HOMO-2 | LUMO+1+ | 3.86      | 3.80      | 322       | 326       | 0.141703 | 0.010796         |
| HOMO-1 | 201-    | 3.96      | 3.95      | 313       | 314       | 0.145686 | 0.007286         |
| HOMO   | 204-    | 3.97      | 3.95      | 312       | 314       | 0.146048 | 0.001403         |
| 184    | LUMO-   | 3.98      | 3.96      | 312       | 313       | 0.146151 | 0.001075         |
| HOMO-1 | 202+    | 3.99      | 3.98      | 311       | 311       | 0.146571 | 0.004207         |
| HOMO   | 205-    | 4.03      | 4.01      | 308       | 309       | 0.147940 | 0.002025         |
| 182    | LUMO-   | 4.10      | 4.07      | 303       | 304       | 0.150533 | 0.023020         |
| 181    | LUMO-   | 4.13      | 4.12      | 300       | 301       | 0.151633 | 0.002792         |
| HOMO-1 | 203+    | 4.20      | 4.17      | 295       | 297       | 0.154487 | 0.001216         |
| 191    | LUMO+1- | 4.21      | 4.18      | 295       | 297       | 0.154604 | 0.021723         |
| HOMO-2 | LUMO+2- | 4.23      | 4.20      | 293       | 295       | 0.155420 | 0.001850         |
| 194    | LUMO+2- | 4.23      | 4.20      | 293       | 295       | 0.155466 | 0.001439         |
| 190    | LUMO+1- | 4.26      | 4.23      | 291       | 293       | 0.156383 | 0.002032         |
| 180    | LUMO+   | 4.28      | 4.30      | 290       | 289       | 0.157240 | 0.005432         |
| 189    | LUMO+1- | 4.33      | 4.30      | 287       | 289       | 0.158996 | 0.000462         |
| HOMO   | 208-    | 4.41      | 4.40      | 281       | 282       | 0.161950 | 0.003536         |
| 188    | LUMO+1+ | 4.45      | 4.44      | 279       | 279       | 0.163401 | 0.014101         |
| HOMO-2 | 201+    | 4.45      | 4.44      | 278       | 279       | 0.163673 | 0.003904         |
| 194    | 202+    | 4.46      | 4.44      | 278       | 279       | 0.163915 | 0.001292         |
| 186    | LUMO+1+ | 4.47      | 4.44      | 277       | 279       | 0.164367 | 0.001231         |
| HOMO-2 | 202-    | 4.50      | 4.49      | 276       | 276       | 0.165232 | 0.012259         |
| 194    | 201+    | 4.50      | 4.49      | 276       | 276       | 0.165310 | 0.009893         |
| HOMO   | 210+    | 4.51      | 4.51      | 275       | 275       | 0.165602 | 0.000000         |
| 185    | LUMO+1+ | 4.51      | 4.51      | 275       | 275       | 0.165886 | 0.002675         |
| HOMO   | 209+    | 4.53      | 4.52      | 274       | 275       | 0.166304 | 0.005343         |
| HOMO   | 209+    | 4.53      | 4.52      | 274       | 275       | 0.166357 | 0.004306         |
| HOMO   | 210+    | 4.57      | 4.58      | 271       | 271       | 0.168084 | 0.003717         |
| HOMO   | 211-    | 4.60      | 4.59      | 269       | 270       | 0.169088 | 0.002742         |
| 190    | LUMO+2- | 4.62      | 4.60      | 268       | 270       | 0.169719 | 0.001051         |
| HOMO-1 | 206-    | 4.64      | 4.65      | 267       | 267       | 0.170446 | 0.006771         |
| HOMO-2 | 203-    | 4.68      | 4.67      | 265       | 266       | 0.171937 | 0.001548         |
| 184    | LUMO+1+ | 4.69      | 4.67      | 265       | 266       | 0.172201 | 0.002729         |
| 193    | 202-    | 4.69      | 4.67      | 264       | 266       | 0.172437 | 0.002457         |
| 189    | LUMO+2- | 4.70      | 4.67      | 264       | 266       | 0.172633 | 0.006328         |
| 183    | LUMO+1- | 4.71      | 4.71      | 263       | 263       | 0.172988 | 0.006702         |
| HOMO   | 213-    | 4.77      | 4.76      | 260       | 260       | 0.175437 | 0.001207         |
| HOMO-1 | 207+    | 4.79      | 4.78      | 259       | 259       | 0.175933 | 0.003281         |
| 187    | LUMO+2- | 4.80      | 4.78      | 258       | 259       | 0.176283 | 0.002755         |
| HOMO-1 | 208-    | 4.81      | 4.78      | 258       | 259       | 0.176651 | 0.007351         |
| HOMO-1 | 208+    | 4.81      | 4.78      | 258       | 259       | 0.176704 | 0.008183         |
| 191    | 202-    | 4.83      | 4.81      | 257       | 258       | 0.177347 | 0.004978         |

|        |         |      |      |     |     |          |          |
|--------|---------|------|------|-----|-----|----------|----------|
| 178    | LUMO+   | 4.84 | 4.85 | 256 | 256 | 0.177977 | 0.001109 |
| 190    | 201-    | 4.86 | 4.86 | 255 | 255 | 0.178590 | 0.001413 |
| HOMO-2 | 204-    | 4.87 | 4.86 | 255 | 255 | 0.178788 | 0.001296 |
| 190    | 202-    | 4.87 | 4.86 | 255 | 255 | 0.178947 | 0.001519 |
| 194    | 204+    | 4.87 | 4.87 | 255 | 254 | 0.178999 | 0.001102 |
| 185    | LUMO+2- | 4.89 | 4.87 | 254 | 254 | 0.179599 | 0.001008 |
| 194    | 205-    | 4.91 | 4.91 | 252 | 252 | 0.180571 | 0.001810 |
| 190    | 202+    | 4.91 | 4.92 | 252 | 252 | 0.180612 | 0.015348 |
| HOMO-2 | 205-    | 4.93 | 4.92 | 252 | 252 | 0.181040 | 0.005843 |
| 189    | 201-    | 4.93 | 4.92 | 252 | 252 | 0.181146 | 0.001410 |
| HOMO   | 214+    | 4.94 | 4.93 | 251 | 252 | 0.181674 | 0.006570 |
| HOMO   | 214-    | 4.95 | 4.93 | 251 | 251 | 0.181748 | 0.008750 |
| HOMO-1 | 209+    | 4.96 | 4.93 | 250 | 251 | 0.182431 | 0.006916 |
| 180    | LUMO+1- | 4.97 | 4.97 | 249 | 250 | 0.182657 | 0.002505 |
| 189    | 202-    | 4.98 | 4.98 | 249 | 249 | 0.182933 | 0.015722 |
| HOMO-1 | 210-    | 4.99 | 4.99 | 249 | 248 | 0.183202 | 0.002432 |
| 192    | 203-    | 5.01 | 5.01 | 248 | 247 | 0.184039 | 0.013617 |
| 191    | 203+    | 5.02 | 5.01 | 247 | 247 | 0.184385 | 0.001724 |
| 196    | 211+    | 5.02 | 5.02 | 247 | 247 | 0.184607 | 0.001863 |
| 196    | 211-    | 5.03 | 5.02 | 247 | 247 | 0.184676 | 0.002251 |
| 184    | 200-    | 5.05 | 5.04 | 246 | 246 | 0.185454 | 0.003399 |
| 177    | LUMO+   | 5.06 | 5.06 | 245 | 245 | 0.185871 | 0.015113 |
| 187    | 202+    | 5.06 | 5.06 | 245 | 245 | 0.186073 | 0.002004 |
| 187    | 202-    | 5.07 | 5.07 | 244 | 244 | 0.186417 | 0.001093 |
| 183    | 200+    | 5.08 | 5.07 | 244 | 244 | 0.186794 | 0.001695 |
| 195    | 206-    | 5.10 | 5.08 | 243 | 244 | 0.187271 | 0.004179 |
| 194    | 206+    | 5.10 | 5.08 | 243 | 244 | 0.187334 | 0.002049 |
| HOMO   | 216+    | 5.11 | 5.10 | 243 | 243 | 0.187710 | 0.006542 |
| 190    | 203+    | 5.11 | 5.11 | 243 | 243 | 0.187789 | 0.001338 |
| 186    | 201-    | 5.12 | 5.11 | 242 | 243 | 0.187984 | 0.001086 |
| 186    | 202-    | 5.12 | 5.12 | 242 | 242 | 0.188108 | 0.008424 |
| 182    | 200+    | 5.14 | 5.14 | 241 | 241 | 0.188876 | 0.005290 |
| 185    | 201-    | 5.14 | 5.14 | 241 | 241 | 0.188982 | 0.029862 |
| 196    | 212-    | 5.16 | 5.15 | 240 | 241 | 0.189638 | 0.002540 |
| 189    | 203+    | 5.17 | 5.17 | 240 | 240 | 0.189972 | 0.003113 |
| 174    | LUMO+   | 5.17 | 5.17 | 240 | 240 | 0.190058 | 0.005158 |
| HOMO   | 217+    | 5.18 | 5.17 | 239 | 240 | 0.190249 | 0.001012 |
| 192    | 205-    | 5.20 | 5.19 | 238 | 239 | 0.191272 | 0.001719 |
| 196    | 213+    | 5.21 | 5.22 | 238 | 238 | 0.191457 | 0.002868 |
| 191    | 204-    | 5.22 | 5.24 | 238 | 237 | 0.191697 | 0.004051 |
| 181    | 200+    | 5.22 | 5.24 | 237 | 236 | 0.191992 | 0.018638 |
| 190    | 204-    | 5.29 | 5.29 | 234 | 234 | 0.194542 | 0.001190 |
| 184    | 201+    | 5.30 | 5.29 | 234 | 234 | 0.194706 | 0.002393 |

Table S5: Optical Absorption Analysis of the system  $I_2/B_{24}N_{24}$ . The HOMO corresponds to Kohn-Sham state 197 while the LUMO corresponds to state 198.