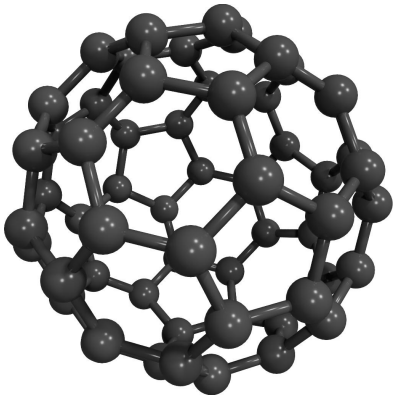
# A Report On The Calculation Of The Optimised Structure Of C60 At The PBE1PBE/def2SVP Level

osl - 28th May 2025




## Abstract

The calculation of optimised structure for the system 'C60' is presented, accompanied by automated analysis and image generation provided by the Digichem software package. The calculation was performed using the Gaussian software package at the PBE1PBE/def2SVP level of theory. The total self-consistent field (SCF) energy of the system was found to be -62103.09 eV after 2 steps. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -6.50 and -3.49 eV respectively, corresponding to a HOMO-LUMO band gap of 3.01 eV. The permanent dipole moment (PDM) was calculated to be 0.00 D.


***Table 1:*** *Summary of overall calculation metadata.*

| Date[a] (Duration[b]) | CPUs (Memory) | Success (Converged) | Computational package | Level of theory | Solvent (model) | Calculations | Wavefunction | Multiplicity | T[c] / K | P[d] / atm |
|---|---|---|---|---|---|---|---|---|---|---|
| 28/05/2025 07:51:23 (4 m, 46 s) | 40 (20 GB) | True (True) | Gaussian (2016+C.01) | PBE1PBE/ def2SVP | Water (IEFPCM) | Optimisation | restricted | 1 (singlet) | N/A | N/A |

*[a]: The date and time at which the calculation was completed. [b]: Total combined duration in real-time (wall-time) for all components of the calculation. [c]: Temperature used for thermochemistry analysis. [d]: Pressure used for thermochemistry analysis.*

## Summary Of Results

### SCF Energy

***Table 2:*** *Summary of SCF energy properties.*

| | |
|---|---|
| **No. of steps** | 2 |
| **Final energy** | -62103.0891 eV |
| **Final energy** | -5,992,037 kJ·mol$^{-1}$ |

### Geometry

***Table 3:*** *Summary of geometry properties.*

| | |
|---|---|
| **Formula** | $C_{60}$ |
| **SMILES** | c12c3c4c5c1c1c6c7c2c2c8c3c3c9c4c4c%10c5c5c1c1c6c6c%11c7c2c2c7c8c3c3c8c9c4c4c9c%10c5c5c1c1c6c6c%11c2c2c7c3c3c8c4c4c9c5c1c1c6c2c3c41 |
| **Exact mass** | 720.0000 g·mol$^{-1}$ |
| **Molar mass** | 720.6420 g·mol$^{-1}$ |
| **Alignment method** | Minimal |
| **X extension** | 6.91 Å |
| **Y extension** | 6.91 Å |
| **Z extension** | 6.91 Å |
| **Linearity ratio** | 0.00 |
| **Planarity ratio** | 0.00 |

### Molecular Orbitals

***Table 4:*** *Summary of HOMO & LUMO properties.*

| | |
|---|---|
| $E_{HOMO,LUMO}$ | 3.01 eV |
| $E_{HOMO}$ | -6.50 eV |
| $E_{LUMO}$ | -3.49 eV |

### Permanent Dipole Moment

***Table 5:*** *Summary of the permanent dipole moment properties.*

| | |
|---|---|
| **Total** | 0.00 D |
| **X axis angle** | 0.00 ° |
| **XY plane angle** | 0.00 ° |

## Methodology

### Metadata

The calculation of the optimised structure was performed using the **Gaussian (2016+C.01)** program, the **DFT** method with the **PBE1PBE** functional and the **def2SVP** basis set. It was completed on the **28th May 2025** after a total duration of **4 m, 46 s** and **finished successfully**. The base multiplicity of the system under study was **1 (singlet)**. Finally, a **restricted wavefunction** was used, resulting in a single set of doubly occupied orbitals. The full calculation metadata is tabulated in table 1.

### Analysis

The report presented here was generated using the Digichem software package. This toolset relies upon a number of third-party applications and libraries which should be cited appropriately in derivative works. In particular, the calculation results described within were parsed by the cclib library.[1] Scientific constants which were used, among other things, for the interconversion of scientific units were provided by SciPy.[2] Three-dimensional plots of atom positions and calculated densities, including molecular orbitals, were rendered using Visual Molecular Dynamics (VMD)[3] and the Tachyon ray-tracer.[4] Finally, two-dimensional graphs were plotted using the

MatPlotlib library,[5] while this report itself was prepared using the Mako template library[6] and the Weasyprint library[7], the latter of which was responsible for generation of the PDF file.

## Discussion

### Total SCF Energy

The total energy of the system was calculated at the **self-consistent field (SCF)** level, corresponding to the energy calculated by the density-functional theory (DFT) method, over a total of two steps, the results of which are displayed in figure 1. The energy calculated by the final step was -62103.09 eV, corresponding to -5,992,037 KJmol$^{-1}$. A plot of the total SCF electron density is shown in figure 2.

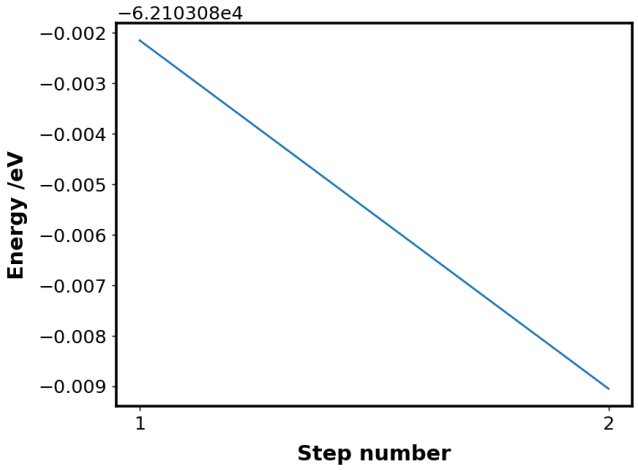



***Figure 1:*** *Graph of calculated energies at the self-consistent field (SCF) level.*

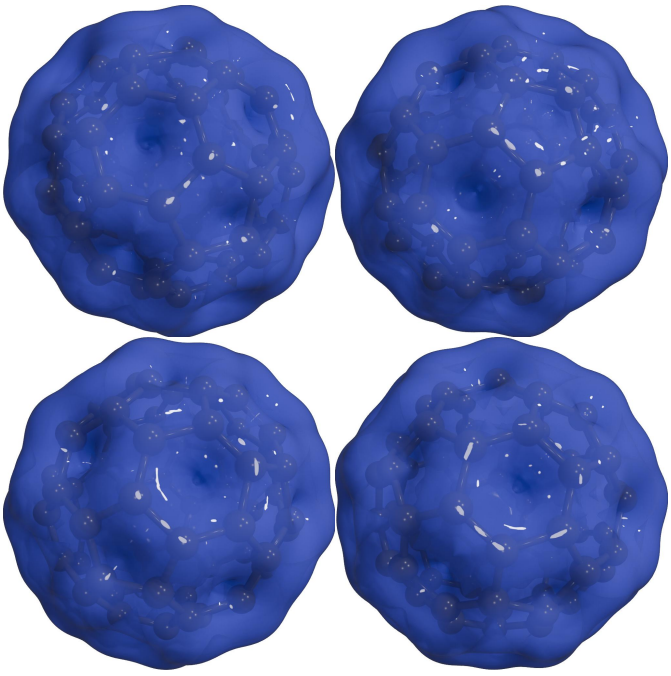


***Figure 2:*** *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

### Geometry

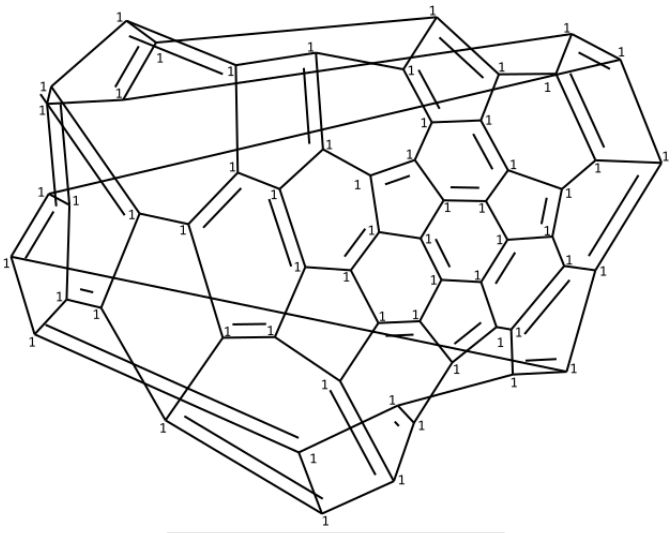


***Figure 3:*** *Labelled structure of C60.*

The **empirical formula** of the studied system was $C_{60}$, corresponding to a **molecular mass** of 720.64 gmol$^{-1}$ and an **exact mass**, considering only specific atomic isotopes, of 720.00 gmol$^{-1}$. The molecular structure, with atom labelling, is shown in figure 3. The molecular geometry was aligned to the cartesian (X, Y and Z) axes by the **Minimal (MIN)** method, and the resulting atomic position are displayed in figure 4. Using this method, the **extent of the molecular system** in the X, Y and Z axes ($L_X$, $L_Y$ and $L_Z$, corresponding to the molecular width, length and height respectively) was determined to be 6.91, 6.91 and 6.91 Å respectively. These extensions give rise to a **molecular linearity ratio** ($1-(L_Y/L_X)$) and **planarity ratio** ($1-(L_X/L_Y)$) of 0.00 and 0.00 respectively.

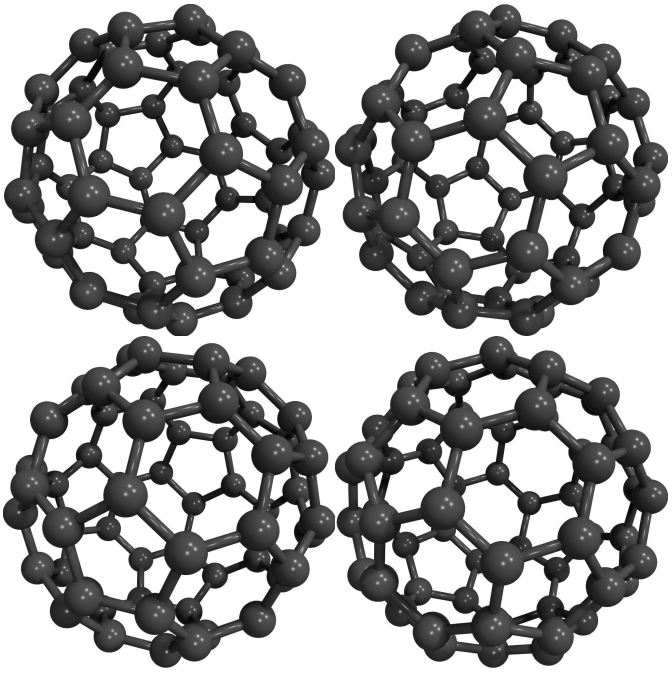


***Figure 4:*** *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

### Permanent Dipole Moment

The calculated **permanent dipole moment** was exactly 0 D.

### Molecular Orbitals

In total, 840 doubly occupied molecular orbitals were calculated, divided into 180 occupied orbitals and 660 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -6.50 and -3.49 eV respectively, corresponding to a **HOMO-LUMO band gap** of 3.01 eV (figure 8). Plots of the orbital density for the HOMO and LUMO are shown in figures 5-6 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 7.

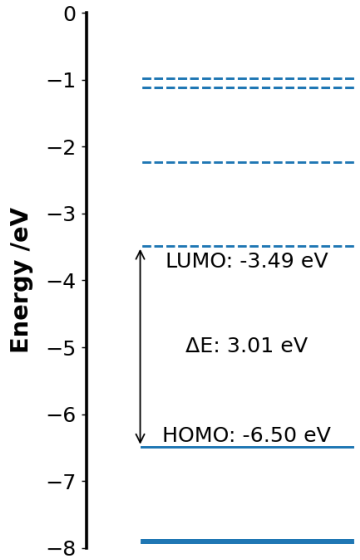



***Figure 8:*** *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

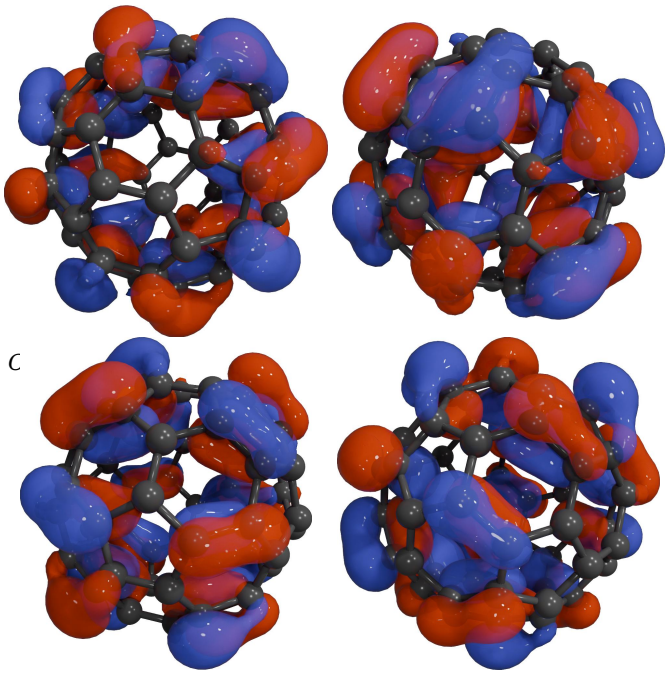



***Figure 5:*** *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

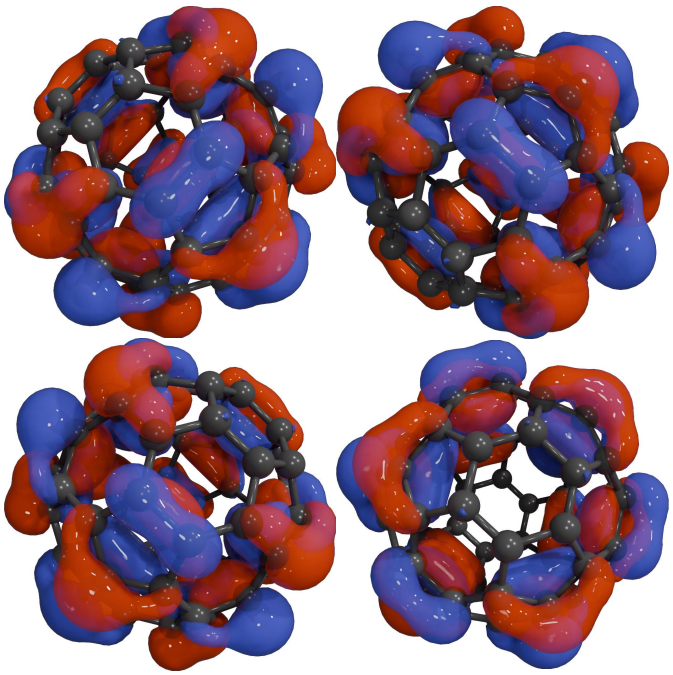


***Figure 6:*** *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

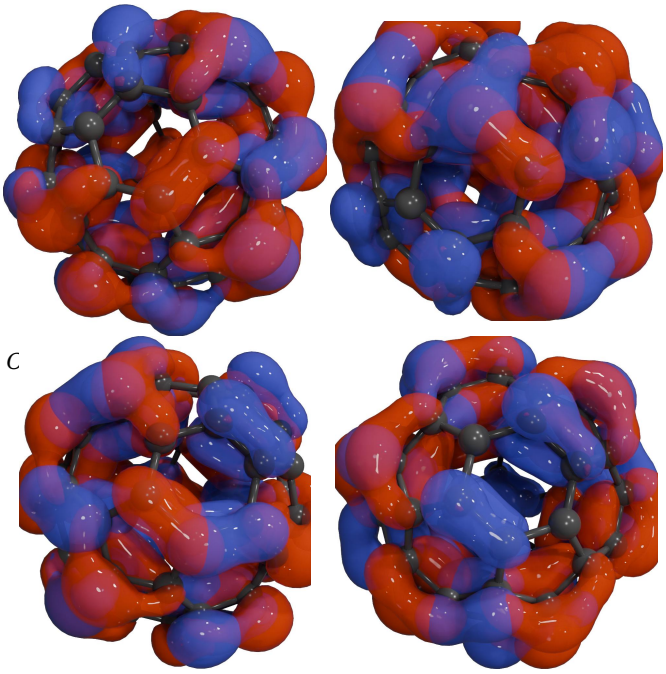



***Figure 7:*** *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

# Tables Of Results

## Atom Coordinates

***Table 6:*** *Coordinates of the atoms of the system under study, as aligned to the cartesian axes by the Minimal method. Atoms that are chemically equivalent have been assigned the same group number.s*

| Index | Element | Group | X Coord /Å | Y Coord /Å | Z Coord /Å |
|---|---|---|---|---|---|
| 1 | C | $C_1$ | -1.4272090 | -0.4657840 | 3.2087360 |
| 2 | C | $C_1$ | -0.0900740 | -0.7701070 | 3.4565470 |
| 3 | C | $C_1$ | -2.2335680 | -1.3532070 | 2.3936320 |
| 4 | C | $C_1$ | -0.2804190 | -2.8269690 | 2.1159540 |
| 5 | C | $C_1$ | -1.6715760 | -2.5104370 | 1.8581250 |
| 6 | C | $C_1$ | -0.4657840 | -3.2087350 | -1.4272090 |
| 7 | C | $C_1$ | -3.2087340 | 1.4272090 | -0.4657820 |
| 8 | C | $C_1$ | -0.7701070 | -3.4565480 | -0.0900750 |
| 9 | C | $C_1$ | -3.4565480 | 0.0900750 | -0.7701070 |
| 10 | C | $C_1$ | -1.8159800 | 0.8976650 | 2.9058940 |
| 11 | C | $C_1$ | 0.8976650 | -2.9058930 | -1.8159810 |
| 12 | C | $C_1$ | -2.9058930 | 1.8159810 | 0.8976680 |
| 13 | C | $C_1$ | 0.4945900 | -1.9741210 | 2.8993440 |
| 14 | C | $C_1$ | -1.9741210 | -2.8993430 | 0.4945920 |
| 15 | C | $C_1$ | -2.8993450 | -0.4945910 | -1.9741200 |
| 16 | C | $C_1$ | -1.3532090 | -2.3936310 | -2.2335690 |
| 17 | C | $C_1$ | -2.3936300 | 2.2335680 | -1.3532060 |
| 18 | C | $C_1$ | 0.9119240 | 0.2766750 | 3.4116530 |
| 19 | C | $C_1$ | 0.2766760 | -3.4116530 | 0.9119230 |
| 20 | C | $C_1$ | -3.4116530 | -0.9119240 | 0.2766760 |
| 21 | C | $C_1$ | -0.8529220 | 1.9038790 | 2.8629010 |
| 22 | C | $C_1$ | 1.9038790 | -2.8629020 | -0.8529260 |
| 23 | C | $C_1$ | -2.8628990 | 0.8529240 | 1.9038810 |
| 24 | C | $C_1$ | -2.8269700 | -2.1159540 | -0.2804190 |
| 25 | C | $C_1$ | -2.1159550 | 0.2804220 | -2.8269680 |
| 26 | C | $C_1$ | -2.5104370 | -1.8581240 | -1.6715750 |
| 27 | C | $C_1$ | -1.8581260 | 1.6715750 | -2.5104360 |
| 28 | C | $C_1$ | 0.5381170 | 1.5872180 | 3.1208250 |
| 29 | C | $C_1$ | 1.5872170 | -3.1208240 | 0.5381150 |
| 30 | C | $C_1$ | -3.1208220 | -0.5381170 | 1.5872180 |
| 31 | C | $C_1$ | 1.4272090 | 0.4657840 | -3.2087360 |
| 32 | C | $C_1$ | 0.4657840 | 3.2087350 | 1.4272090 |
| 33 | C | $C_1$ | 3.2087340 | -1.4272090 | 0.4657820 |
| 34 | C | $C_1$ | 0.0900740 | 0.7701070 | -3.4565470 |
| 35 | C | $C_1$ | 0.7701070 | 3.4565480 | 0.0900750 |
| 36 | C | $C_1$ | 3.4565480 | -0.0900750 | 0.7701070 |
| 37 | C | $C_1$ | 1.8159800 | -0.8976650 | -2.9058940 |
| 38 | C | $C_1$ | -0.8976650 | 2.9058930 | 1.8159810 |
| 39 | C | $C_1$ | 2.9058930 | -1.8159810 | -0.8976680 |
| 40 | C | $C_1$ | -0.4945900 | 1.9741210 | -2.8993440 |
| 41 | C | $C_1$ | 1.9741210 | 2.8993430 | -0.4945920 |
| 42 | C | $C_1$ | 2.8993450 | 0.4945910 | 1.9741200 |
| 43 | C | $C_1$ | 2.2335680 | 1.3532070 | -2.3936320 |
| 44 | C | $C_1$ | 1.3532090 | 2.3936310 | 2.2335690 |
| 45 | C | $C_1$ | 2.3936300 | -2.2335680 | 1.3532060 |
| 46 | C | $C_1$ | -0.9119240 | -0.2766750 | -3.4116530 |
| 47 | C | $C_1$ | -0.2766760 | 3.4116530 | -0.9119230 |
| 48 | C | $C_1$ | 3.4116530 | 0.9119240 | -0.2766760 |
| 49 | C | $C_1$ | 0.8529220 | -1.9038790 | -2.8629010 |
| 50 | C | $C_1$ | -1.9038790 | 2.8629020 | 0.8529260 |
| 51 | C | $C_1$ | 2.8628990 | -0.8529240 | -1.9038810 |
| 52 | C | $C_1$ | 0.2804190 | 2.8269690 | -2.1159540 |
| 53 | C | $C_1$ | 2.8269700 | 2.1159540 | 0.2804190 |
| 54 | C | $C_1$ | 2.1159550 | -0.2804220 | 2.8269680 |
| 55 | C | $C_1$ | 1.6715760 | 2.5104370 | -1.8581250 |
| 56 | C | $C_1$ | 2.5104370 | 1.8581240 | 1.6715750 |
| 57 | C | $C_1$ | 1.8581260 | -1.6715750 | 2.5104360 |
| 58 | C | $C_1$ | -0.5381170 | -1.5872180 | -3.1208250 |
| 59 | C | $C_1$ | -1.5872170 | 3.1208240 | -0.5381150 |
| 60 | C | $C_1$ | 3.1208220 | 0.5381170 | -1.5872180 |

## Molecular Orbitals

***Table 7:*** *Energies of the calculated molecular orbitals.*

| Level | Label | Symmetry | Energy /eV |
|---|---|---|---|
| 196 | LUMO+15 | Au | 0.7489 |
| 195 | LUMO+14 | Au | 0.7489 |
| 194 | LUMO+13 | Ag | -0.9861 |
| 193 | LUMO+12 | Ag | -0.9861 |
| 192 | LUMO+11 | Ag | -0.9867 |
| 191 | LUMO+10 | Ag | -0.9867 |
| 190 | LUMO+9 | Ag | -0.9867 |
| 189 | LUMO+8 | Au | -1.1181 |
| 188 | LUMO+7 | Au | -1.1181 |
| 187 | LUMO+6 | Au | -1.1184 |
| 186 | LUMO+5 | Ag | -2.2392 |
| 185 | LUMO+4 | Ag | -2.2400 |
| 184 | LUMO+3 | Ag | -2.2400 |
| 183 | LUMO+2 | Au | -3.4871 |
| 182 | LUMO+1 | Au | -3.4871 |
| 181 | **LUMO** | **Au** | **-3.4874** |
| 180 | **HOMO** | **Au** | **-6.4951** |
| 179 | HOMO-1 | Au | -6.4951 |
| 178 | HOMO-2 | Au | -6.4954 |
| 177 | HOMO-3 | Au | -6.4954 |
| 176 | HOMO-4 | Au | -6.4956 |
| 175 | HOMO-5 | Ag | -7.8848 |
| 174 | HOMO-6 | Ag | -7.8850 |
| 173 | HOMO-7 | Ag | -7.8850 |
| 172 | HOMO-8 | Ag | -7.8850 |
| 171 | HOMO-9 | Ag | -7.9109 |
| 170 | HOMO-10 | Ag | -7.9109 |
| 169 | HOMO-11 | Ag | -7.9112 |
| 168 | HOMO-12 | Ag | -7.9112 |
| 167 | HOMO-13 | Ag | -7.9112 |
| 166 | HOMO-14 | Au | -9.8206 |
| 165 | HOMO-15 | Au | -9.8209 |

## References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**3.** W. Humphrey, A. Dalke and K. Schulten, *Journal of Molecular Graphics,* 1996, **14,** 33--38

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**7.** K. Community, https://weasyprint.org, (accessed May 2020)