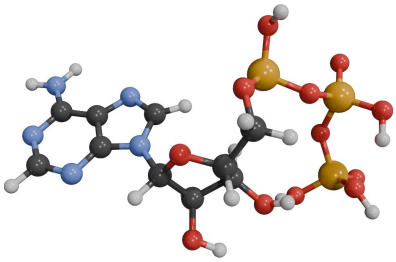
A Report On The Calculation Of The Optimised Structure Of ATP At The PBE1PBE/def2SVP Level

osl - 28th May 2025



Abstract

The calculation of optimised structure for the system 'ATP' 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 -72468.21 eV after 39 steps. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -6.48 and -0.68 eV respectively, corresponding to a HOMO-LUMO band gap of 5.80 eV. The permanent dipole moment (PDM) was calculated to be 12.87 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 08:18:13 (31 m, 35 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	39
Final energy	-72468.2095 eV
Final energy	-6,992,119 kJ·mol^{-1}

Geometry

Table 3: *Summary of geometry properties.*

Formula	$C_{10}H_{16}O_{13}N_5P_3$
SMILES	Nc1ncnc2c1ncn2[C@@H]1O[C@H](CO[P@@](=O)(O)O[P@@](=O)(O)OP(=O)(O)O)[C@@H](O)[C@H]1O
Exact mass	506.9958 g·mol^{-1}
Molar mass	507.1810 g·mol^{-1}
Alignment method	Minimal
X extension	12.44 Å
Y extension	7.54 Å
Z extension	6.02 Å
Linearity ratio	0.39
Planarity ratio	0.20

Molecular Orbitals

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

$E_{HOMO,LUMO}$	5.80 eV
E_{HOMO}	-6.48 eV
E_{LUMO}	-0.68 eV

Permanent Dipole Moment

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

Total	12.87 D
X axis angle	71.50 °
XY plane angle	60.03 °

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 **31 m, 35 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 39 steps, the results of which are displayed in figure 1. The energy calculated by the final step was -72468.21 eV,

corresponding to -6,992,119 KJmol^{-1}. A plot of the total SCF electron density is shown in figure 2.

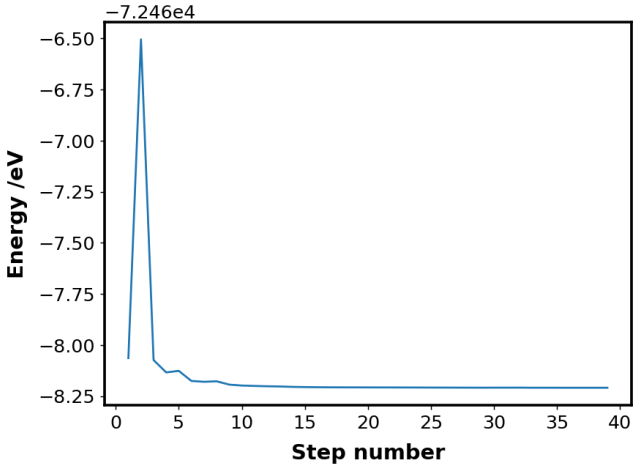


Figure 1: *Graph of calculated energies at the self-consistent field (SCF) level.*

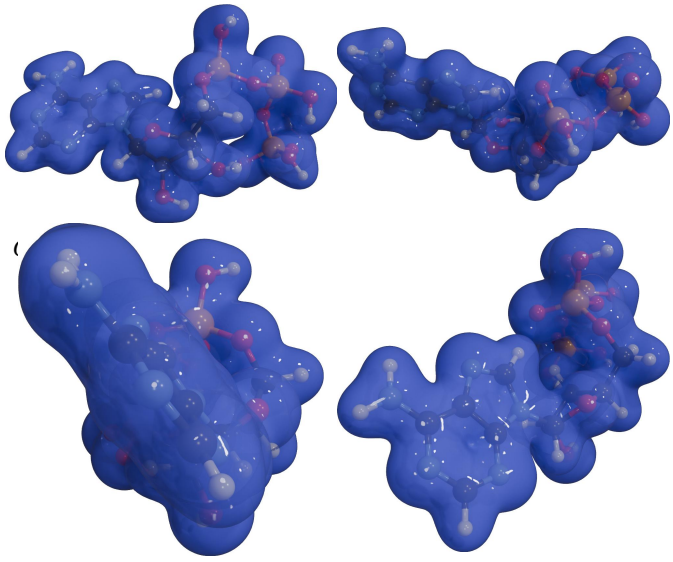


Figure 2: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

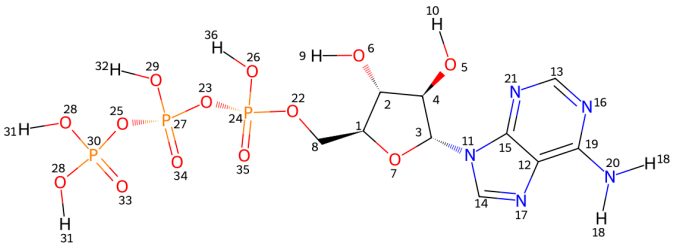


Figure 3: *Labelled structure of ATP.*

The **empirical formula** of the studied system was $C_{10}H_{16}O_{13}N_5P_3$, corresponding to a **molecular mass** of 507.18 gmol^{-1} and an **exact mass**, considering only specific atomic isotopes, of 507.00 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 12.44, 7.54 and 6.02 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 0.39 and 0.20 respectively.

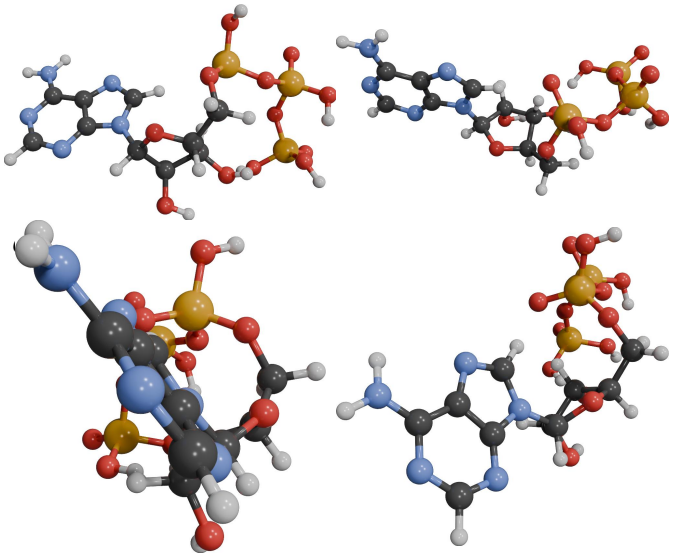


Figure 4: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Permanent Dipole Moment

The calculated **permanent dipole moment** was 12.87 D, with a vector (x,y,z) of 4.09, -4.97, 11.15 D. The angle between the dipole moment vector and the x-axis was 71.50 °, while the angle between the dipole moment and the xy-plane was 60.03 °. A plot of the permanent dipole moment is shown in figure 5.

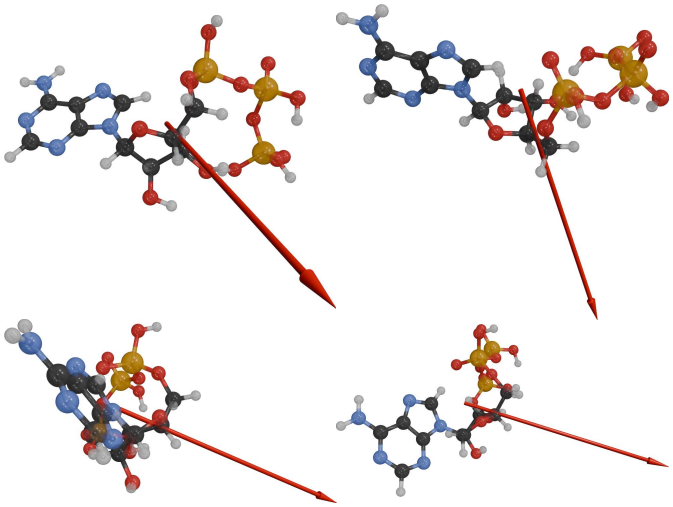


Figure 5: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Molecular Orbitals

In total, 526 doubly occupied molecular orbitals were calculated, divided into 130 occupied orbitals and 396 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -6.48 and -0.68 eV respectively, corresponding to a **HOMO-LUMO band gap** of 5.80 eV (figure 9). Plots of the orbital density for the HOMO and LUMO are shown in figures

6-7 respectively, while the orbital overlap between the HOMO and LUMO is shown in figure 8.

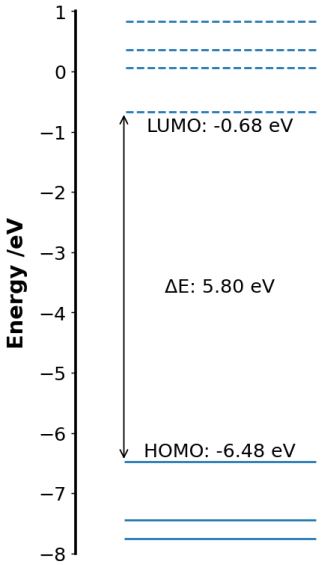


Figure 9: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

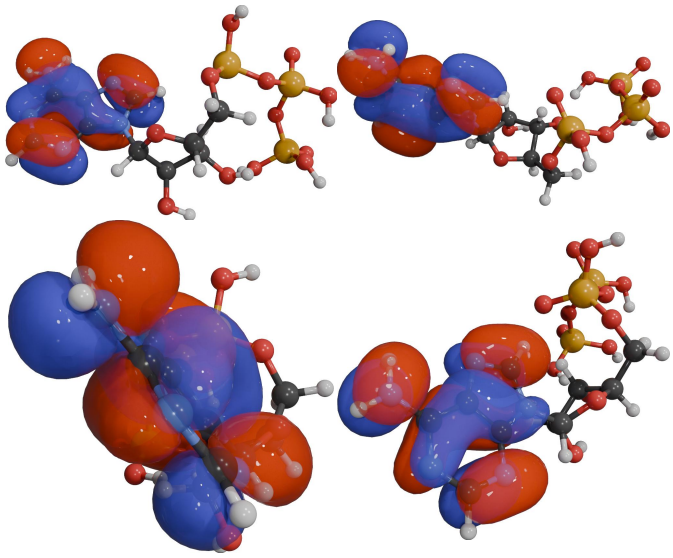


Figure 6: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

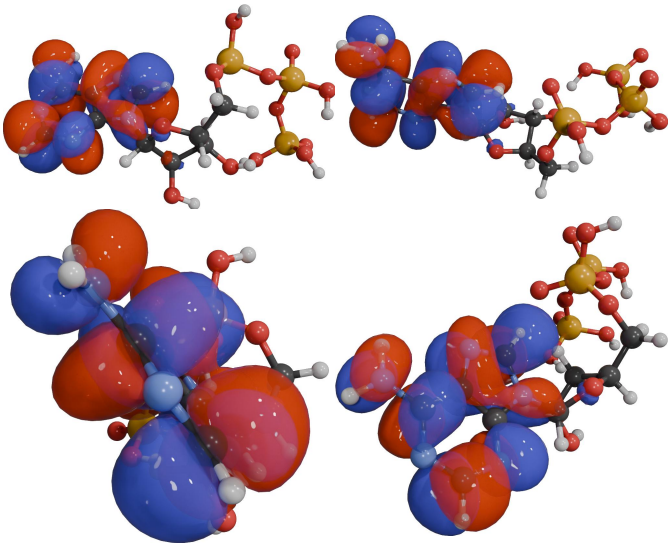


Figure 7: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

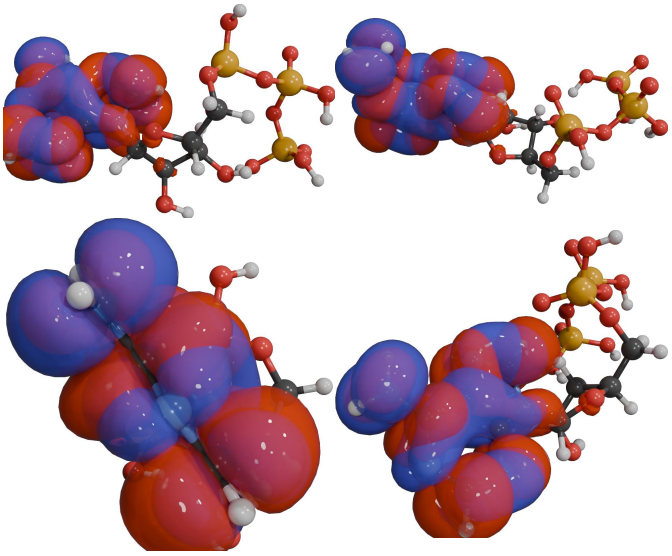


Figure 8: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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}	-0.2396910	-0.9259270	2.0197440
2	C	C_{2}	0.0569740	-1.3767540	0.5890380
3	C	C_{3}	-2.2900600	-1.2693350	0.9839810
4	H	H_{4}	-1.4377280	-2.1316450	-0.8466070
5	O	O_{5}	-1.2392180	-3.3802360	0.8087450
6	C	C_{4}	-1.2414000	-2.1054380	0.2394670
7	H	H_{2}	0.2062800	-0.5132780	-0.0794190
8	O	O_{6}	1.1412530	-2.2763350	0.4713760
9	O	O_{7}	-1.6032820	-0.5671110	1.9934250
10	H	H_{1}	-0.0728110	-1.7935170	2.6888490
11	C	C_{8}	0.5684870	0.2211930	2.5792900
12	H	H_{9}	1.8105540	-2.1266930	1.1547830
13	H	H_{10}	-0.3495750	-3.7413300	0.6793250
14	N	N_{11}	-3.0287600	-0.3454640	0.1643440
15	C	C_{12}	-4.6694680	0.6895450	-0.8705630
16	C	C_{13}	-6.5043280	-1.0006860	0.0576100
17	H	H_{14}	-1.5147280	1.0262810	-0.5586040
18	H	H_{3}	-3.0416700	-1.9504660	1.4124140
19	C	C_{14}	-2.5703260	0.7428050	-0.5481310
20	C	C_{15}	-4.3890820	-0.3908530	-0.0316190
21	N	N_{16}	-6.9225440	-0.0149620	-0.7389610
22	N	N_{17}	-3.5222430	1.3820080	-1.1773610
23	H	H_{18}	-5.7830300	2.5140070	-2.4042970
24	H	H_{18}	-7.4237450	1.9309170	-2.2581960
25	C	C_{19}	-6.0279900	0.8586490	-1.2281070
26	H	H_{13}	-7.2862430	-1.6772930	0.4236770
27	N	N_{20}	-6.4431080	1.8491020	-2.0282090
28	N	N_{21}	-5.2656340	-1.2660400	0.4606770
29	O	O_{22}	0.3483340	1.4468860	1.8871510
30	H	H_{8}	0.2573540	0.4088600	3.6148420
31	H	H_{8}	1.6406010	-0.0287790	2.5847110
32	O	O_{23}	2.5865190	1.3711280	0.8218720
33	P	P_{24}	1.1007940	2.0063380	0.6078010
34	O	O_{25}	3.3865660	0.0739290	-1.1735850
35	O	O_{26}	1.2183470	3.5610900	0.8760710
36	P	P_{27}	3.8186360	1.3217840	-0.2434960
37	O	O_{28}	4.2225000	-1.7621450	0.2119360
38	O	O_{29}	5.0177770	0.8157650	0.6490940
39	P	P_{30}	3.8949140	-1.4666930	-1.3548450
40	H	H_{31}	4.7745140	-2.5486340	0.3515950
41	O	O_{28}	2.5772300	-2.2453100	-1.6973940
42	H	H_{31}	1.9396020	-2.2999750	-0.9253620
43	H	H_{32}	4.9334680	-0.1273960	0.9001110
44	O	O_{33}	5.0040000	-1.6438910	-2.3018550
45	O	O_{34}	4.0332490	2.5770490	-0.9710250
46	O	O_{35}	0.5252820	1.7095120	-0.7206560
47	H	H_{36}	1.5008670	3.8031500	1.7713960

Molecular Orbitals

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

Level	Label	Symmetry	Energy /eV
146	LUMO+15	A	3.0605
145	LUMO+14	A	2.9361
144	LUMO+13	A	2.8123
143	LUMO+12	A	2.7407
142	LUMO+11	A	2.5859
141	LUMO+10	A	2.3296
140	LUMO+9	A	2.2806
139	LUMO+8	A	2.1380
138	LUMO+7	A	1.8743
137	LUMO+6	A	1.8340
136	LUMO+5	A	1.5094
135	LUMO+4	A	1.1080
134	LUMO+3	A	0.8250
133	LUMO+2	A	0.3557
132	LUMO+1	A	0.0569
131	**LUMO**	**A**	**-0.6754**
130	**HOMO**	**A**	**-6.4752**
129	HOMO-1	A	-7.4399
128	HOMO-2	A	-7.7490
127	HOMO-3	A	-8.2056
126	HOMO-4	A	-8.3376
125	HOMO-5	A	-8.3670
124	HOMO-6	A	-8.5759
123	HOMO-7	A	-9.0023
122	HOMO-8	A	-9.0549
121	HOMO-9	A	-9.1621
120	HOMO-10	A	-9.2647
119	HOMO-11	A	-9.3077
118	HOMO-12	A	-9.3645
117	HOMO-13	A	-9.5145
116	HOMO-14	A	-9.6119
115	HOMO-15	A	-9.8307

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