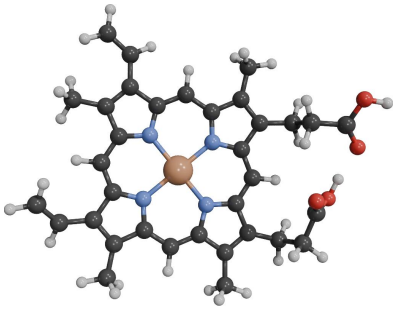
A Report On The Calculation Of The Optimised Structure Of Heme_B At The PBE1PBE/def2SVP Level

osl - 28th May 2025



Abstract

The calculation of optimised structure for the system 'Heme_B' 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 -84218.30 eV after 23 steps. The highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO) were calculated to be -5.50 and -2.30 eV respectively, corresponding to a HOMO-LUMO band gap of 3.20 eV. The permanent dipole moment (PDM) was calculated to be 1.66 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 08:55:31 (1 h, 8 m, 53 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	23
Final energy	-84218.3039 eV
Final energy	-8,125,831 kJ·mol^{-1}

Geometry

Table 3: *Summary of geometry properties.*

Formula	$C_{34}N_4H_{32}FeO_4$
SMILES	[CH2][CH][C]1[C](C)[C]2[CH][C]3[C](C)[C](CC[C]([O])O)[C]4[CH][C]5[C](CC[C]([O])O)[C](C)[C]6[CH][C]7[C]([CH][CH2])[C](C)[C]8[CH][C]1N2[Fe](N87)(N34)N65
Exact mass	616.1773 g·mol^{-1}
Molar mass	616.4873 g·mol^{-1}
Alignment method	Minimal
X extension	15.70 Å
Y extension	12.69 Å
Z extension	3.57 Å
Linearity ratio	0.19
Planarity ratio	0.72

Molecular Orbitals

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

$E_{HOMO,LUMO}$	3.20 eV
E_{HOMO}	-5.50 eV
E_{LUMO}	-2.30 eV

Permanent Dipole Moment

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

Total	1.66 D
X axis angle	52.64 °
XY plane angle	28.48 °

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 **1 h, 8 m, 53 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 23 steps, the results of which are displayed in figure 1. The energy calculated by the final step was -84218.30 eV, corresponding to -8,125,831 KJmol^{-1}. A plot of the total SCF electron density is shown in figure 2.

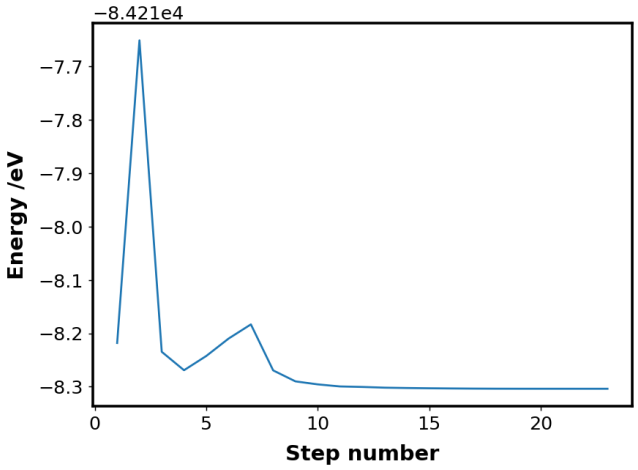


Figure 1: *Graph of calculated energies at the self-consistent field (SCF) level.*

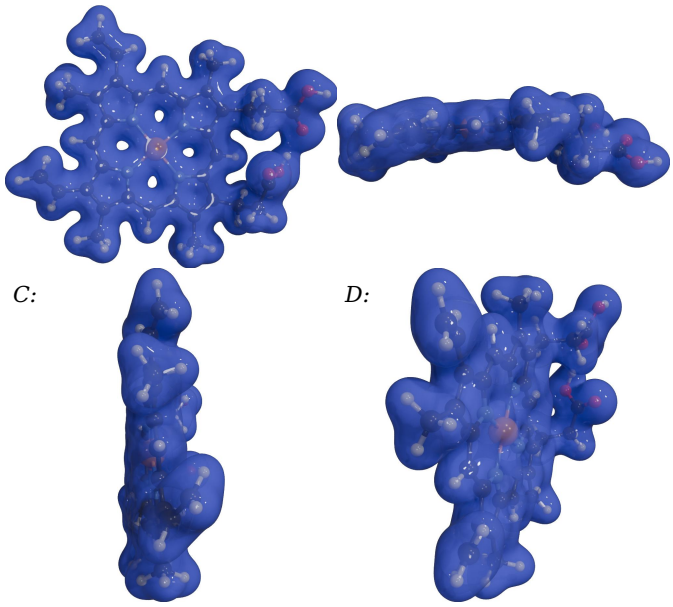


Figure 2: *Plot of the total SCF electron density, plotted with an isovalue of 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Geometry

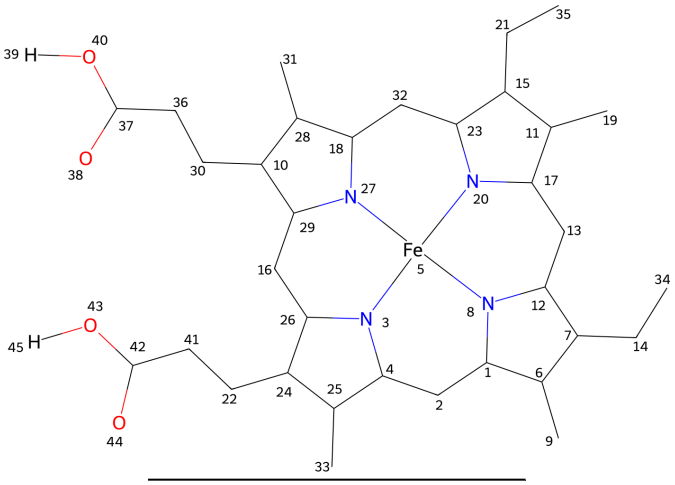


Figure 3: *Labelled structure of Heme_B.*

The **empirical formula** of the studied system was $C_{34}N_4H_{32}FeO_4$, corresponding to a **molecular mass** of 616.49 gmol^{-1} and an **exact mass**, considering only specific atomic isotopes, of 616.18 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 15.70, 12.69 and 3.57 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 0.19 and 0.72 respectively.

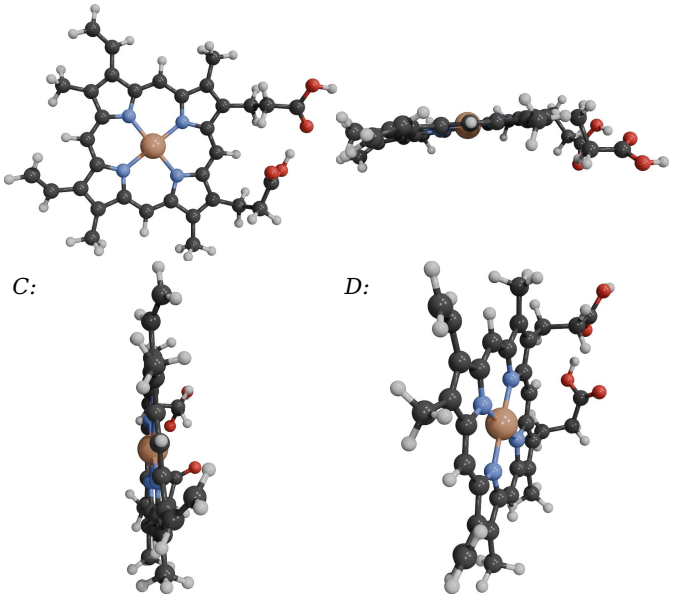


Figure 4: *The molecular structure, aligned using the Minimal (MIN) method. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Permanent Dipole Moment

The calculated **permanent dipole moment** was 1.66 D, with a vector (x,y,z) of 1.01, 1.05, -0.79 D. The angle between the dipole moment vector and the x-axis was 52.64 °, while the angle between the dipole moment and the xy-plane was 28.48 °. A plot of the permanent dipole moment is shown in figure 5.

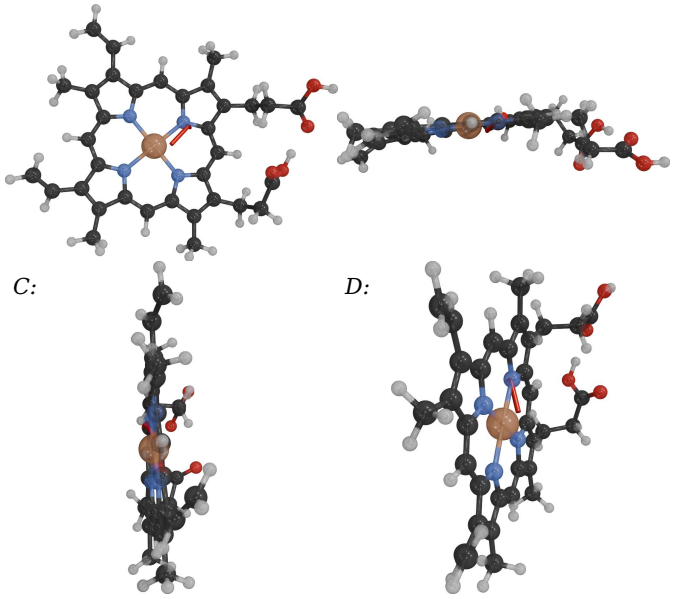


Figure 5: *The permanent dipole moment (red arrow) plotted against the aligned molecular geometry with a scale of 1 Å = 1.0 D. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

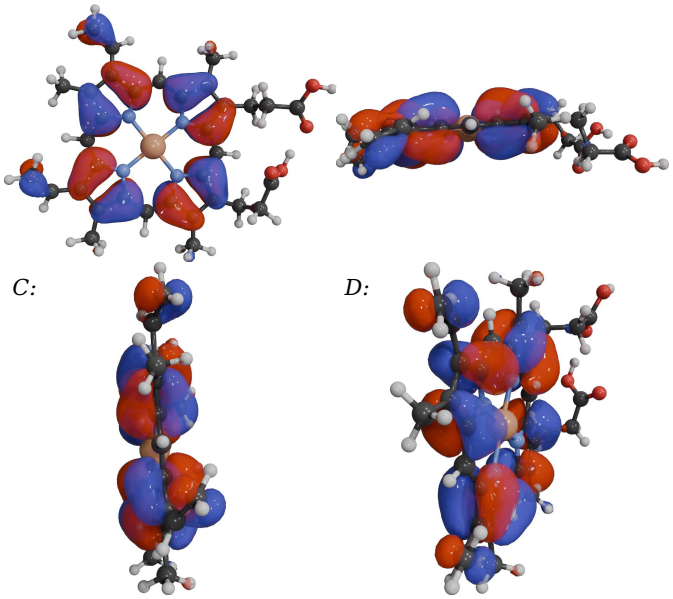


Figure 6: *Orbital density plots of the HOMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

Molecular Orbitals

In total, 779 doubly occupied molecular orbitals were calculated, divided into 161 occupied orbitals and 618 unoccupied (or virtual) orbitals. The calculated energies of the **HOMO and LUMO** were -5.50 and -2.30 eV respectively, corresponding to a **HOMO-LUMO band gap** of 3.20 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.

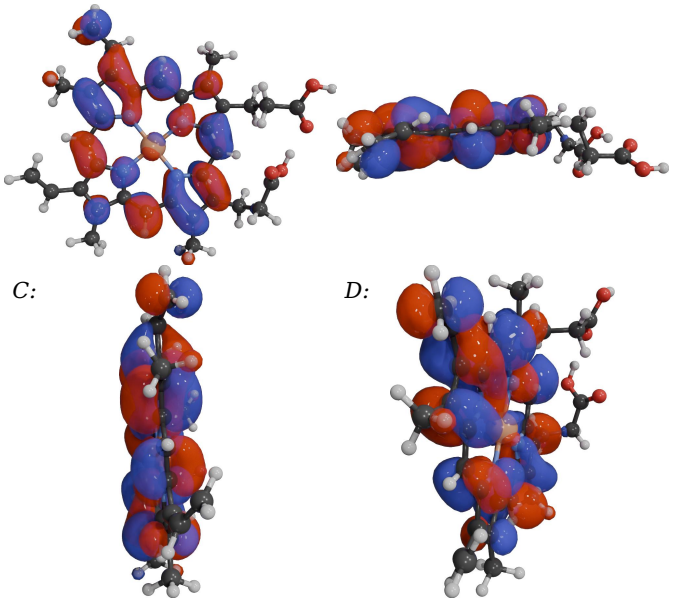


Figure 7: *Orbital density plots of the LUMO, plotted with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

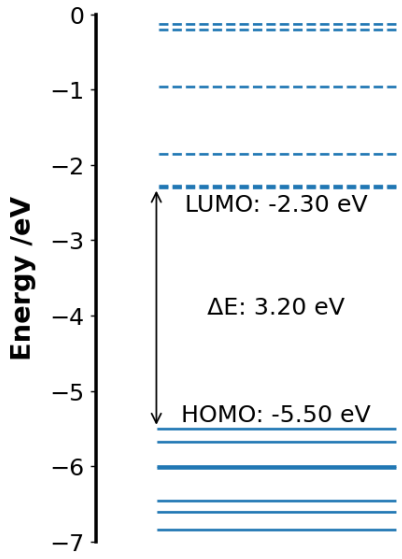


Figure 9: *Graph of the calculated molecular orbital energies in close proximity to the HOMO-LUMO gap. Solid lines: occupied orbitals, dashed lines: virtual orbitals.*

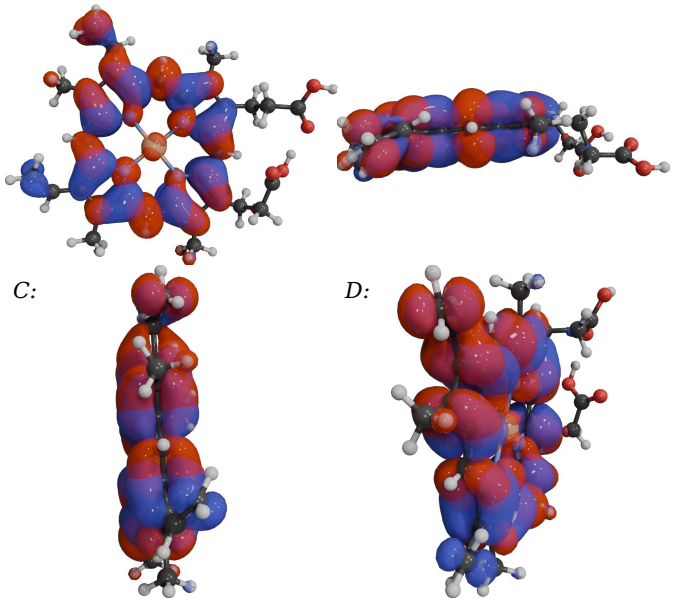


Figure 8: *Orbital density plots of the HOMO (red) and LUMO (blue), plotted simultaneously with isovalue: 0.02. A: In the X/Y plane, B: In the X/Z plane, C: In the Z/Y plane, D: 45° to the axes.*

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}	-2.5484620	-2.7365300	0.0293610
2	C	C_{2}	-1.4021510	-3.4990440	-0.1491290
3	N	N_{3}	0.1920040	-1.6634290	-0.4075550
4	C	C_{4}	-0.1302690	-2.9924370	-0.3541020
5	H	H_{2}	-1.5132650	-4.5836930	-0.1260700
6	Fe	Fe_{5}	-1.0642740	-0.1104150	-0.2531200
7	C	C_{6}	-3.8559900	-3.3072440	0.2525300
8	C	C_{7}	-4.7195100	-2.2449270	0.3971380
9	N	N_{8}	-2.6000200	-1.3691530	0.0139040
10	C	C_{9}	-4.1508130	-4.7639490	0.3440940
11	C	C_{10}	2.6208540	2.0143940	-0.6065290
12	C	C_{11}	-4.2613280	2.7222140	-0.0409210
13	C	C_{12}	-3.9142290	-1.0457230	0.2126590
14	H	H_{13}	-5.5070100	0.3479100	0.2444230
15	C	C_{14}	-6.1467630	-2.3384270	0.6801940
16	C	C_{13}	-4.4279720	0.2396880	0.1523210
17	C	C_{15}	-3.2017490	3.5972330	-0.1589330
18	C	C_{16}	2.2974240	-0.4648250	-0.7026930
19	C	C_{17}	-3.6828710	1.3977280	-0.0191620
20	C	C_{18}	0.4329460	2.5135310	-0.4233130
21	C	C_{19}	-5.7159080	3.0298430	0.0293470
22	N	N_{20}	-2.3196050	1.4469200	-0.1445200
23	C	C_{21}	-3.1990680	5.0503410	-0.2346990
24	C	C_{22}	3.5325420	-3.3237410	-0.9190180
25	C	C_{23}	-2.0064530	2.7726110	-0.2291300
26	C	C_{24}	2.0965290	-2.9634460	-0.7092660
27	C	C_{25}	1.0437380	-3.8230570	-0.5368490
28	C	C_{26}	1.5425740	-1.6244710	-0.6170050
29	N	N_{27}	0.4739260	1.1454040	-0.4546960
30	C	C_{28}	1.7657000	3.0785730	-0.5067940
31	H	H_{16}	3.3680230	-0.5712350	-0.8734630
32	C	C_{29}	1.7955980	0.8224560	-0.5839230
33	C	C_{30}	4.1126980	2.0288020	-0.6035980
34	C	C_{31}	2.0893380	4.5315630	-0.4598690
35	C	C_{32}	-0.7182220	3.2784380	-0.3368630
36	C	C_{33}	1.0430300	-5.3124640	-0.5223390
37	H	H_{32}	-0.5971350	4.3615880	-0.3501410
38	H	H_{19}	-6.3283970	2.1971850	-0.3433800
39	H	H_{19}	-6.0424230	3.2392350	1.0621040
40	H	H_{19}	-5.9545800	3.9214650	-0.5694340
41	H	H_{34}	-6.4824960	-0.5992720	1.8788550
42	H	H_{34}	-7.9647300	-1.6763780	1.5406650
43	C	C_{35}	-4.1444830	5.8871030	0.2234830
44	C	C_{34}	-6.8981260	-1.4872610	1.3957380
45	H	H_{14}	-6.6380970	-3.2346830	0.2822310
46	H	H_{21}	-2.3234680	5.4986520	-0.7178630
47	H	H_{31}	1.5456510	5.0938480	-1.2353880
48	H	H_{31}	1.8141410	4.9754280	0.5104910
49	H	H_{31}	3.1631340	4.7065880	-0.6116690
50	H	H_{30}	4.5124500	1.1860390	-1.1874570
51	H	H_{30}	4.4818100	2.9446640	-1.0902240
52	C	C_{36}	4.6673190	1.9587260	0.8301560
53	H	H_{36}	4.2918010	1.0502500	1.3288860
54	C	C_{37}	6.1599230	1.8550340	0.8383500
55	H	H_{36}	4.3484080	2.8347850	1.4091190
56	O	O_{38}	6.7777680	0.9094080	0.3782460
57	H	H_{39}	7.7354570	2.7339230	1.3313860
58	O	O_{40}	6.7762360	2.8906350	1.3741910
59	H	H_{33}	0.3364800	-5.7248420	-1.2598440
60	H	H_{33}	2.0382720	-5.7171320	-0.7499500
61	H	H_{33}	0.7439460	-5.7053030	0.4628260
62	H	H_{22}	3.9904680	-2.6824280	-1.6882100
63	C	C_{41}	4.4003740	-3.2745870	0.3522030
64	H	H_{22}	3.5758020	-4.3473860	-1.3170220
65	H	H_{41}	3.8535970	-3.6718940	1.2169560
66	H	H_{41}	5.2915220	-3.9031570	0.1927480
67	C	C_{42}	4.9102460	-1.9014070	0.7029700
68	O	O_{43}	5.6452130	-1.3807640	-0.2697860
69	O	O_{44}	4.6892680	-1.3314230	1.7502900
70	H	H_{45}	6.0289270	-0.5009670	0.0087130
71	H	H_{9}	-3.7841430	-5.3060480	-0.5416110
72	H	H_{9}	-3.6645050	-5.2191020	1.2222870
73	H	H_{9}	-5.2289440	-4.9520990	0.4316270
74	H	H_{35}	-5.0333910	5.5384030	0.7533790
75	H	H_{35}	-4.0370010	6.9669590	0.0942500

Molecular Orbitals

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

Level	Label	Symmetry	Energy /eV
177	LUMO+15	A	2.1647
176	LUMO+14	A	2.0194
175	LUMO+13	A	1.9489
174	LUMO+12	A	1.7883
173	LUMO+11	A	1.6773
172	LUMO+10	A	1.3181
171	LUMO+9	A	1.2036
170	LUMO+8	A	0.6999
169	LUMO+7	A	0.4231
168	LUMO+6	A	0.2879
167	LUMO+5	A	-0.1249
166	LUMO+4	A	-0.1984
165	LUMO+3	A	-0.9589
164	LUMO+2	A	-1.8553
163	LUMO+1	A	-2.2781
162	**LUMO**	**A**	**-2.2991**
161	**HOMO**	**A**	**-5.4962**
160	HOMO-1	A	-5.6785
159	HOMO-2	A	-5.9928
158	HOMO-3	A	-6.0181
157	HOMO-4	A	-6.4627

156	HOMO-5	A	-6.6091	150	HOMO-11	A	-7.9582
155	HOMO-6	A	-6.8407	149	HOMO-12	A	-8.5585
154	HOMO-7	A	-7.3454	148	HOMO-13	A	-8.6709
153	HOMO-8	A	-7.3996	147	HOMO-14	A	-8.7150
152	HOMO-9	A	-7.7985	146	HOMO-15	A	-8.8755
151	HOMO-10	A	-7.9411				

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