

Supplementary Material

for

"The First Coordination Sphere of Lanthanide (III) Motexafins (Ln-Motex²⁺, Ln=La, Gd, Lu) and its Effects on Structure, Reduction Potentials and UV-Vis Absorption Spectra. Theoretical Studies"

Authors: X. Cao, N. Heinz, J. Zhang, M. Dolg

Journal: PCCP

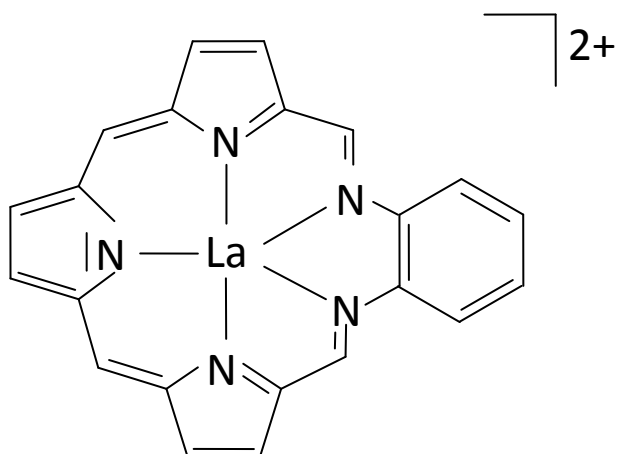
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I. [La-Tex]²⁺ and [Mg-Por]⁰ Model Systems

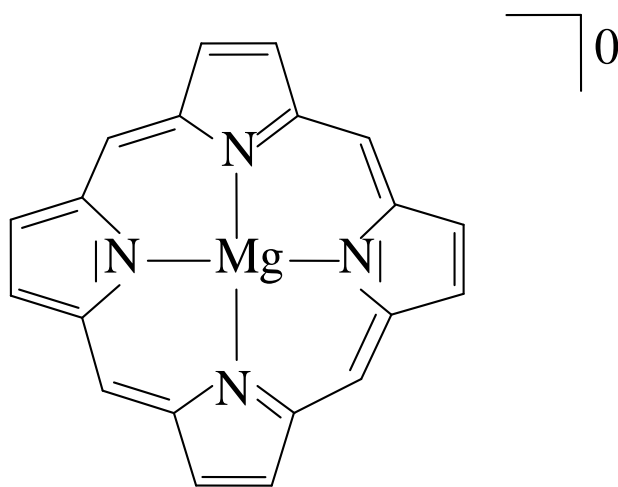
I.a Structures

In the following orbital plots and UV-Vis spectra Tex stands for the inner macrocyclic ringsystem without side chains, which is common to both texaphyrin and motexafin. Model calculations were performed for [La-Tex]²⁺ (C_s symmetry) and [Mg-Tex]⁰ (C_{2v} symmetry).



Scheme 1: [La-Tex]²⁺ model system.

The UV-Vis spectra of the above model systems are compared to those obtained for a porphyrin ligand (Por), i.e., [La-Por]⁺ (C_{4v} symmetry) and [Mg-Por] (D_{4h} symmetry).



Scheme 2: [Mg-Por]⁰ model system.

The calculations were performed with DFT/BP86 as well as DFT/B3LYP, def2-TZVP basis sets and a large-core pseudopotential for La (ECP46MWB). The TURBOMOLE quantum chemistry code and the TmoleX visualization tool was applied to plot the orbitals. UV-Vis spectra were obtained from the calculated TD-DFT wavelengths and oscillator strengths using a superposition of Gaussian functions with exponents 0.0015 for broadening. The plots were generated with the program xmgrace.

I.b Cartesian Coordinates of Optimized Structures of [M-Por]ⁿ⁺ (M=Mg, n=0; M=La, n=1) and [M-TeX]ⁿ⁺ (M=Mg, n=1; M=La, n=2) Model Complexes

Program used: TURBOMOLE V 6.3 and V6.6

All energies are given in units of Hartree

All cartesian atomic coordinates are given in units of Bohr

The input coordinates given below are for the optimized structures for basis sets B (cf. text). A scalar-relativistic large-core pseudopotential was used for La (ECP46MWB).

Mg-Por{0}:

input coordinates and input keywords

Energy: -1189.026432347

\$symmetry d4h

\$dft

functional b-p

gridsize 5

\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	mg
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-3.90226867673658	0.0000000000000000	0.0000000000000000	n
0.0000000000000000	-3.90226867673658	0.0000000000000000	n
3.90226867673658	0.0000000000000000	0.0000000000000000	n
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5.44926689609175	2.09070768773674	0.0000000000000000	c
-2.09070768773674	5.44926689609175	0.0000000000000000	c
-5.44926689609175	-2.09070768773674	0.0000000000000000	c
2.09070768773674	5.44926689609175	0.0000000000000000	c
5.44926689609175	-2.09070768773674	0.0000000000000000	c
-2.09070768773674	-5.44926689609175	0.0000000000000000	c
-5.44926689609175	2.09070768773674	0.0000000000000000	c
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-8.06479622908092	1.29350846917633	0.0000000000000000	c
-1.29350846917633	-8.06479622908092	0.0000000000000000	c
8.06479622908092	-1.29350846917633	0.0000000000000000	c
1.29350846917633	-8.06479622908092	0.0000000000000000	c
-8.06479622908092	-1.29350846917633	0.0000000000000000	c
-1.29350846917633	8.06479622908092	0.0000000000000000	c
8.06479622908092	1.29350846917633	0.0000000000000000	c
4.60188816079825	4.60188816079825	0.0000000000000000	c
-4.60188816079825	4.60188816079825	0.0000000000000000	c
-4.60188816079825	-4.60188816079825	0.0000000000000000	c
4.60188816079825	-4.60188816079825	0.0000000000000000	c
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-6.06023556199707	6.06023556199707	0.0000000000000000	h
-6.06023556199707	-6.06023556199707	0.0000000000000000	h
6.06023556199707	-6.06023556199707	0.0000000000000000	h
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-2.55462778373038	9.68662668102763	0.0000000000000000	h

```

-9.68662668102763      -2.55462778373038      0.0000000000000000    h
 2.55462778373038      -9.68662668102763      0.0000000000000000    h
 9.68662668102763      -2.55462778373038      0.0000000000000000    h
-2.55462778373038      -9.68662668102763      0.0000000000000000    h
-9.68662668102763      2.55462778373038      0.0000000000000000    h
 2.55462778373038      9.68662668102763      0.0000000000000000    h
$user-defined bonds
$end

La-Por{1+}:
input coordinates and input keywords
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$dft
  functional b-p
  gridsize 5
$COORD
  0.0000000000000000      0.0000000000000000      2.76873930988451      la
  0.0000000000000000      3.96983403347725      0.55944302284604      n
-3.96983403347725      0.0000000000000000      0.55944302284604      n
  0.0000000000000000      -3.96983403347725      0.55944302284604      n
  3.96983403347725      0.0000000000000000      0.55944302284604      n
  2.10805931075750      -5.48405924211208      0.23490999582939      c
  5.48405924211208      2.10805931075750      0.23490999582939      c
-2.10805931075750      5.48405924211208      0.23490999582939      c
-5.48405924211208      -2.10805931075750      0.23490999582939      c
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  5.48405924211208      -2.10805931075750      0.23490999582939      c
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-8.05061288492005      1.29446600956499      -0.21035541740218      c
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  1.29446600956499      -8.05061288492005      -0.21035541740218      c
-8.05061288492005      -1.29446600956499      -0.21035541740218      c
-1.29446600956499      8.05061288492005      -0.21035541740218      c
  8.05061288492005      1.29446600956499      -0.21035541740218      c
  4.61377843298900      4.61377843298900      0.17153669157488      c
-4.61377843298900      4.61377843298900      0.17153669157488      c
-4.61377843298900      -4.61377843298900      0.17153669157488      c
  4.61377843298900      -4.61377843298900      0.17153669157488      c
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-6.05730368777488      -6.05730368777488      -0.11627695603158      h
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-2.54528589814625      9.64303022460962      -0.55299837134757      h
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-9.64303022460962      2.54528589814625      -0.55299837134757      h
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Mg-TeX{1+}:

```

input coordinates and input keywords

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\$symmetry c2v

\$dft

functional b-p

gridsize 5

\$coord

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-2.45096546856552	0.000000000000000	4.32398390193171	n
2.45096546856552	0.000000000000000	4.32398390193171	n
-4.06573302934695	0.000000000000000	-0.52092504721885	n
4.06573302934695	0.000000000000000	-0.52092504721885	n
-2.66038619468382	0.000000000000000	9.01339722653809	c
2.66038619468382	0.000000000000000	9.01339722653809	c
-1.35555465979436	0.000000000000000	6.67622512967927	c
1.35555465979436	0.000000000000000	6.67622512967927	c
1.33619009465224	0.000000000000000	11.26186314834687	c
-1.33619009465224	0.000000000000000	11.26186314834687	c
-4.89031894208279	0.000000000000000	3.96499421906642	c
4.89031894208279	0.000000000000000	3.96499421906642	c
-5.75116792975639	0.000000000000000	1.42678808641339	c
5.75116792975639	0.000000000000000	1.42678808641339	c
-5.53388563008337	0.000000000000000	-2.67681644674320	c
5.53388563008337	0.000000000000000	-2.67681644674320	c
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8.31876238414557	0.000000000000000	0.55486425532940	c
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4.59684315828511	0.000000000000000	-5.12893842397108	c
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2.05770965360799	0.000000000000000	-5.86597125173972	c
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-1.28790509413637	0.000000000000000	-8.48613793880356	c
8.18665219506485	0.000000000000000	-2.03047080605879	c
-8.18665219506485	0.000000000000000	-2.03047080605879	c
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2.56593009829349	0.000000000000000	-10.09317675576040	h
-9.99270600139220	0.000000000000000	1.74310105557470	h
9.99270600139220	0.000000000000000	1.74310105557470	h
9.73413306026754	0.000000000000000	-3.38044031221072	h
-9.73413306026754	0.000000000000000	-3.38044031221072	h
2.35522723468817	0.000000000000000	13.05253785928624	h
-2.35522723468817	0.000000000000000	13.05253785928624	h
-4.71879709420213	0.000000000000000	9.05567730810048	h
4.71879709420213	0.000000000000000	9.05567730810048	h
6.29325492590607	0.000000000000000	5.49231617818378	h
-6.29325492590607	0.000000000000000	5.49231617818378	h
5.98895408000285	0.000000000000000	-6.65020704145737	h
-5.98895408000285	0.000000000000000	-6.65020704145737	h

\$end

La-Tex{2+}:

input coordinates and input keywords

Energy: -1152.282555433

\$symmetry cs

\$dft

functional b-p

```

gridsize 5
$coord
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 3.44582215179102      2.49367946182532      2.52833989883181     n
-1.29180980510179      1.38939481303799      4.23047753280381     n
-1.29180980510179      1.38939481303799     -4.23047753280381     n
 7.97247986886390      3.68993661302022     -2.66216907700546     c
 7.97247986886390      3.68993661302022      2.66216907700546     c
 5.72260550369673      3.07655090741766     -1.36271890345225     c
 5.72260550369673      3.07655090741766      1.36271890345225     c
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10.14572462627036      4.27872256395233     -1.33512426279900     c
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 2.95702821517125      2.89529972931024      4.94062240644242     c
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 0.50537610835823      2.28576401501107     -5.86713547569544     c
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-3.44200949800528      0.98937868376536      5.64422182663612     c
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 4.33696002368173      3.73694041922826      6.23259790371924     h
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 0.51984003259913      3.13801221479941     -10.03877625843513     h
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11.88200146543749      4.71367550543324     -2.35501647218371     h
 8.02785153816106      3.64958531720271     -4.71990267419009     h
 8.02785153816106      3.64958531720271      4.71990267419009     h
-7.27893281092065     -0.09635599382893     -5.97947581220406     h
-7.27893281092065     -0.09635599382893      5.97947581220406     h

```

\$end

La-Tex{2+}:

input coordinates and input keywords

Energy: -1151.451132042

\$symmetry cs

\$dft

functional b3-lyp

gridsize 5

\$coord

```

 0.00786351726535      -0.04106290429020      0.0000000000000000    la
-4.80257595945856     -0.00786607645340      0.0000000000000000    n
 3.45733228862855      2.45621668104915     -2.53215659671373     n

```


3.45733228862855	2.45621668104915	2.53215659671373	n
-1.27491600223196	1.33867330580490	4.22865549490517	n
-1.27491600223196	1.33867330580490	-4.22865549490517	n
7.95879898563286	3.68261381613768	-2.64524959929876	c
7.95879898563286	3.68261381613768	2.64524959929876	c
5.72336788448860	3.05629107146076	-1.35234424957033	c
5.72336788448860	3.05629107146076	1.35234424957033	c
10.11802895769101	4.28920643014498	1.32795141595875	c
10.11802895769101	4.28920643014498	-1.32795141595875	c
2.95119489707461	2.88150144618995	-4.90964393226199	c
2.95119489707461	2.88150144618995	4.90964393226199	c
0.49821959923551	2.26004420025620	5.83957301865703	c
0.49821959923551	2.26004420025620	-5.83957301865703	c
-3.42933746175497	0.96483491372929	-5.62505974551631	c
-3.42933746175497	0.96483491372929	5.62505974551631	c
-2.94849279413384	1.65360890328704	-8.21017515933510	c
-2.94849279413384	1.65360890328704	8.21017515933510	c
-5.71570418660658	0.16034561243938	-4.61635276685774	c
-5.71570418660658	0.16034561243938	4.61635276685774	c
-6.36031889295750	-0.24437423408186	-2.07249016964043	c
-6.36031889295750	-0.24437423408186	2.07249016964043	c
-8.90577518042120	-0.75941048796275	1.28564938705172	c
-8.90577518042120	-0.75941048796275	-1.28564938705172	c
-0.50091947801868	2.48648880300020	8.33371397912678	c
-0.50091947801868	2.48648880300020	-8.33371397912678	c
-4.30430495660595	1.55716394882571	9.73041506417987	h
-4.30430495660595	1.55716394882571	-9.73041506417987	h
4.29749391909618	3.75472462418912	-6.19110351406139	h
4.29749391909618	3.75472462418912	6.19110351406139	h
0.49450605289822	3.18057695234169	9.97154731735152	h
0.49450605289822	3.18057695234169	-9.97154731735152	h
-10.49221642015325	-1.02446025165658	-2.53870537469529	h
-10.49221642015325	-1.02446025165658	2.53870537469529	h
11.83583250151632	4.73732421791364	2.34251368428897	h
11.83583250151632	4.73732421791364	-2.34251368428897	h
8.01424111497546	3.64210140269542	-4.68738376990824	h
8.01424111497546	3.64210140269542	4.68738376990824	h
-7.25104541971506	-0.07667229755576	-5.95021755735321	h
-7.25104541971506	-0.07667229755576	5.95021755735321	h

\$end

I.c Orbital Isosurfaces of $[\text{La-Tex}]^{2+}$

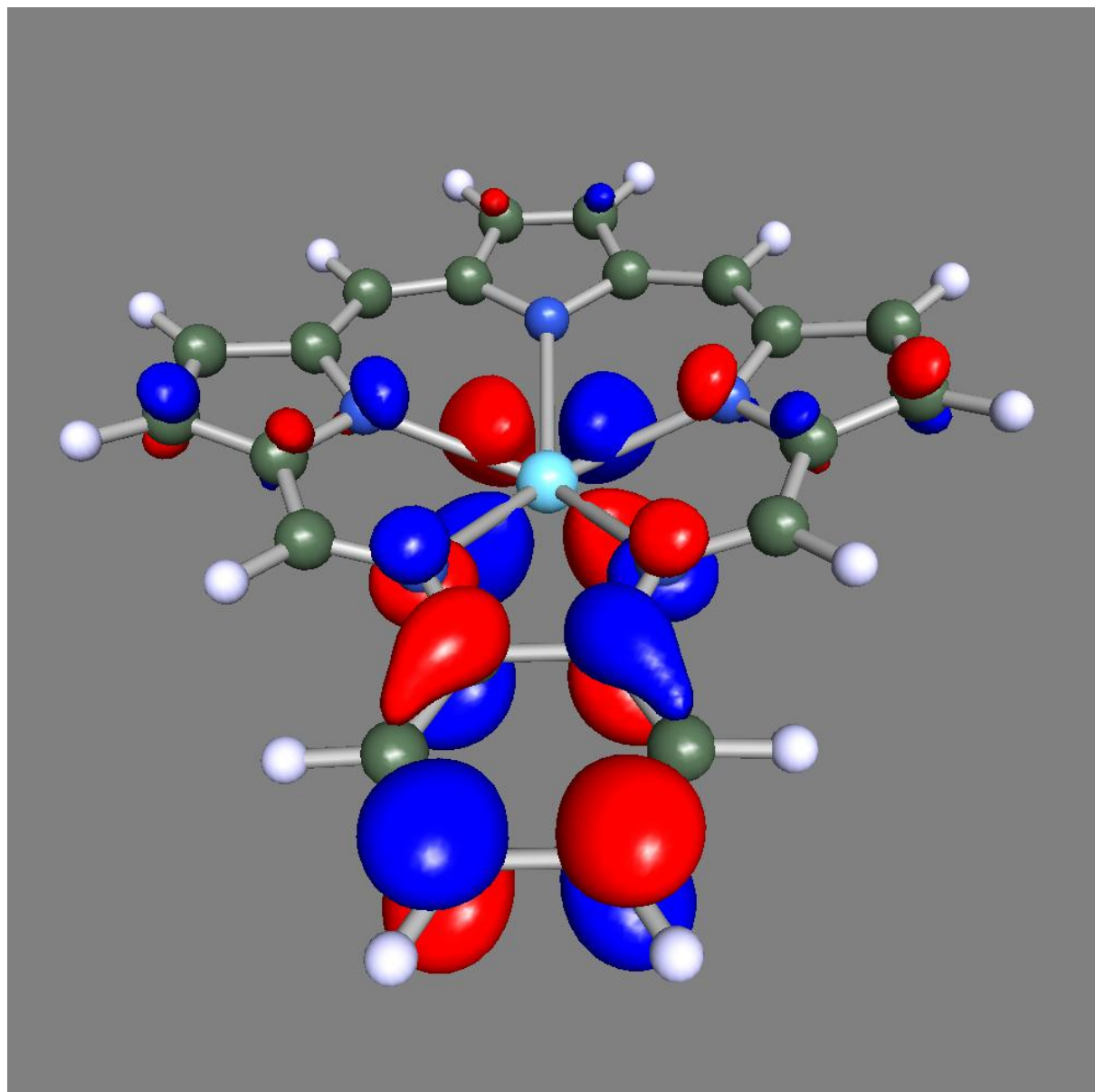


Fig. S1a:

LUMO+9 of $[\text{La-Tex}]^{2+}$

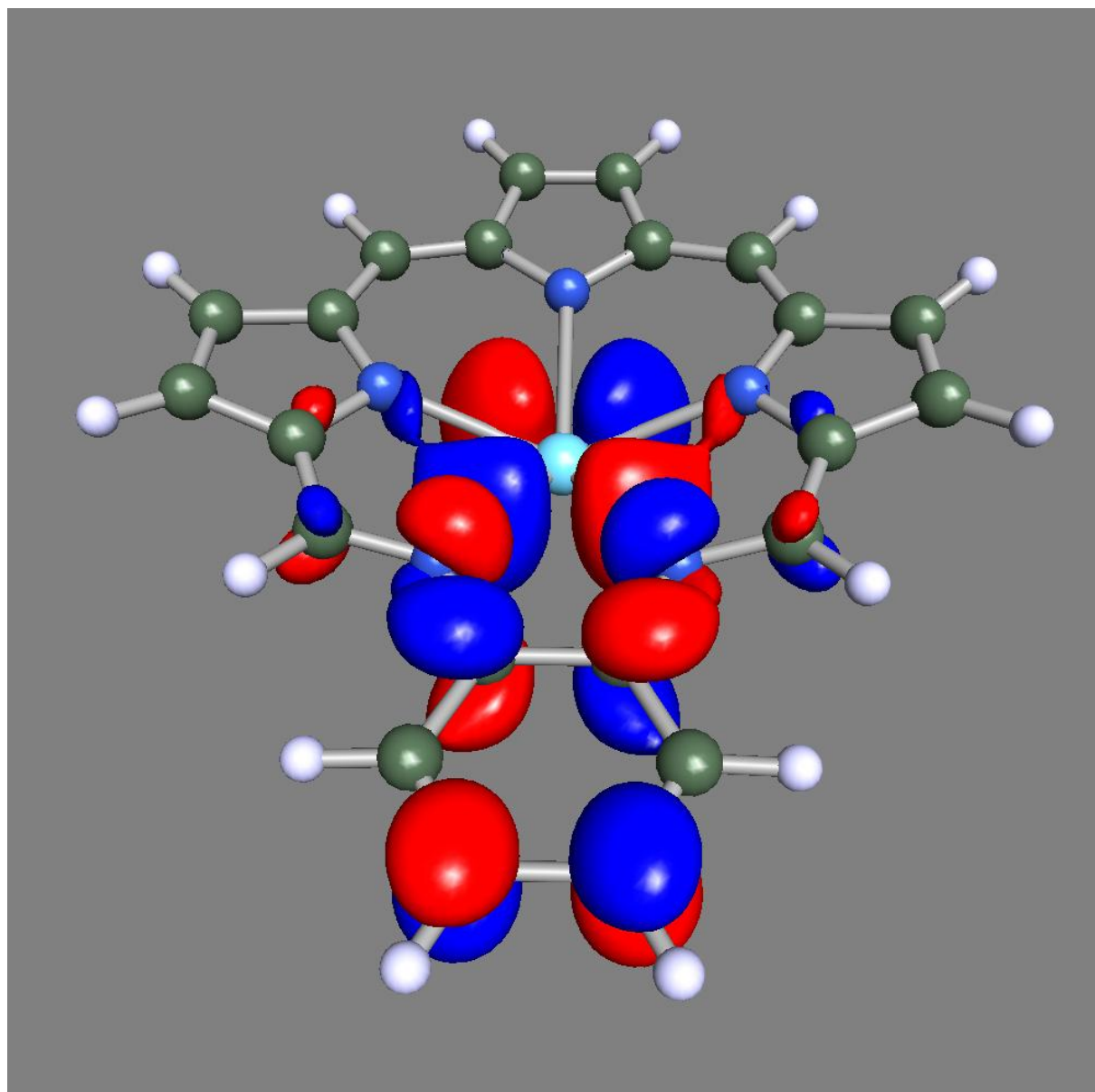


Fig. S1b:

LUMO+8 of [La-Tex]²⁺

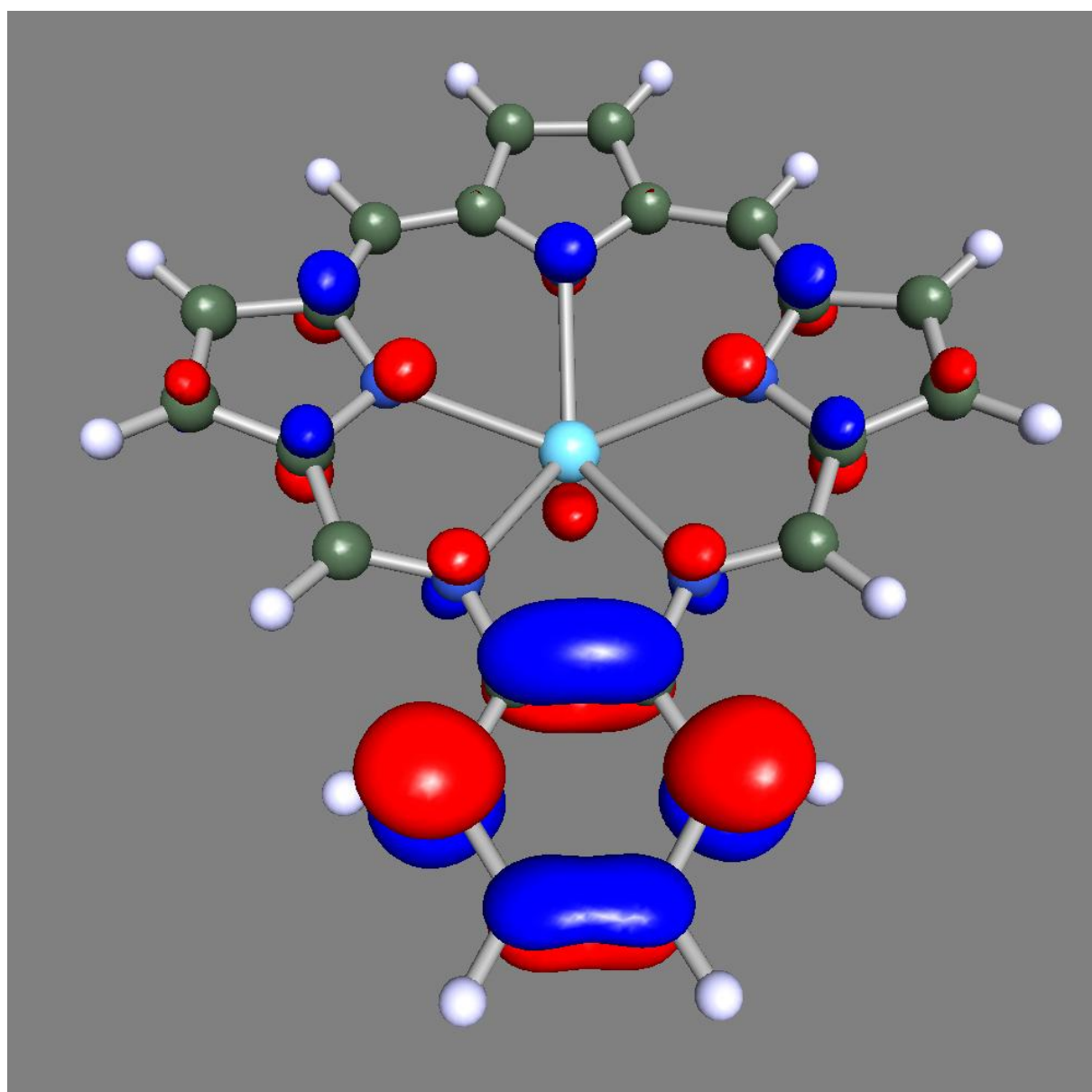


Fig. S1c:

LUMO+7 of [La-Tex]²⁺

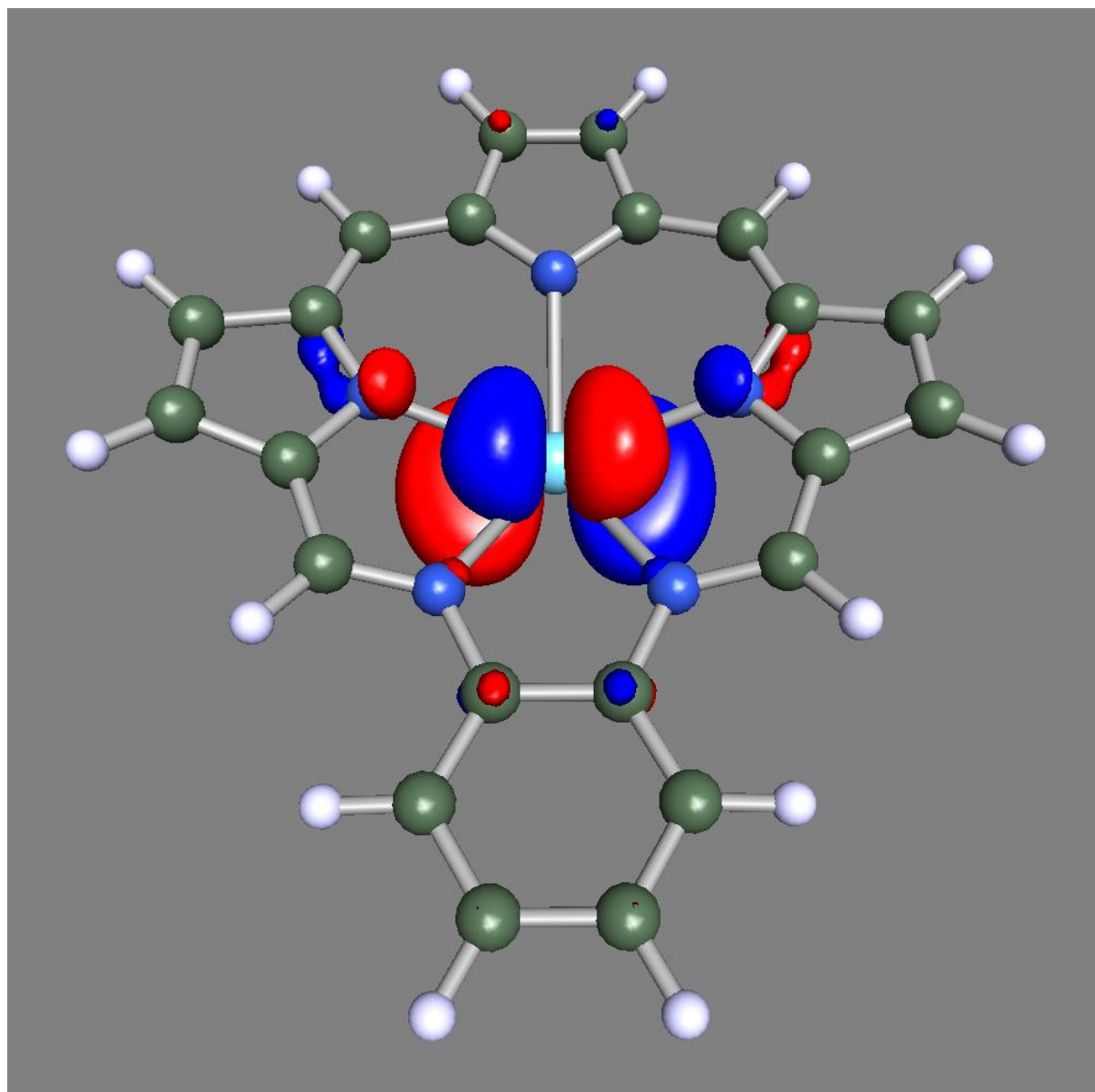


Fig. S1d:

LUMO+6 of [La-Tex]²⁺

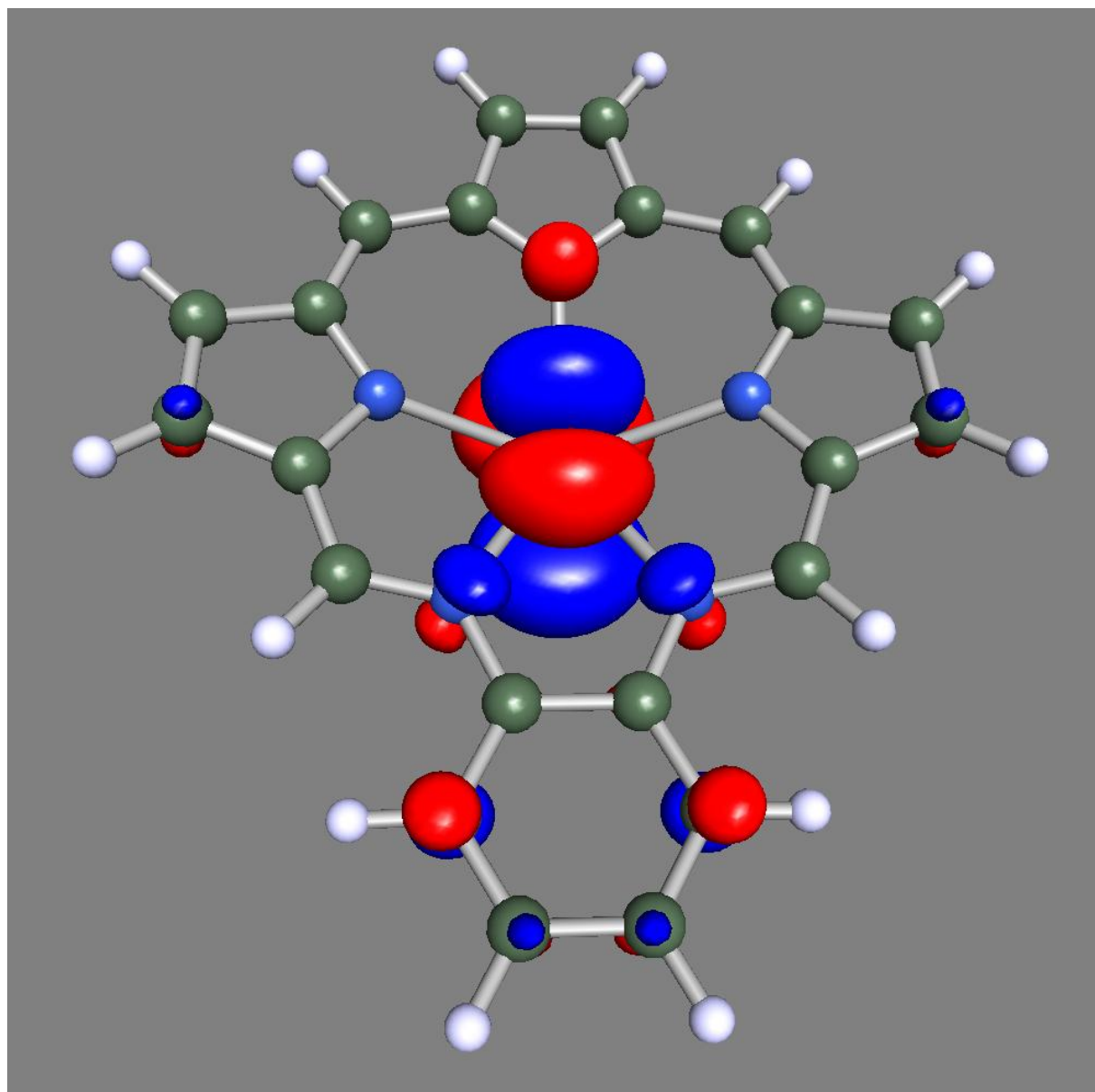


Fig. S1e:

LUMO+5 of [La-Tex]²⁺

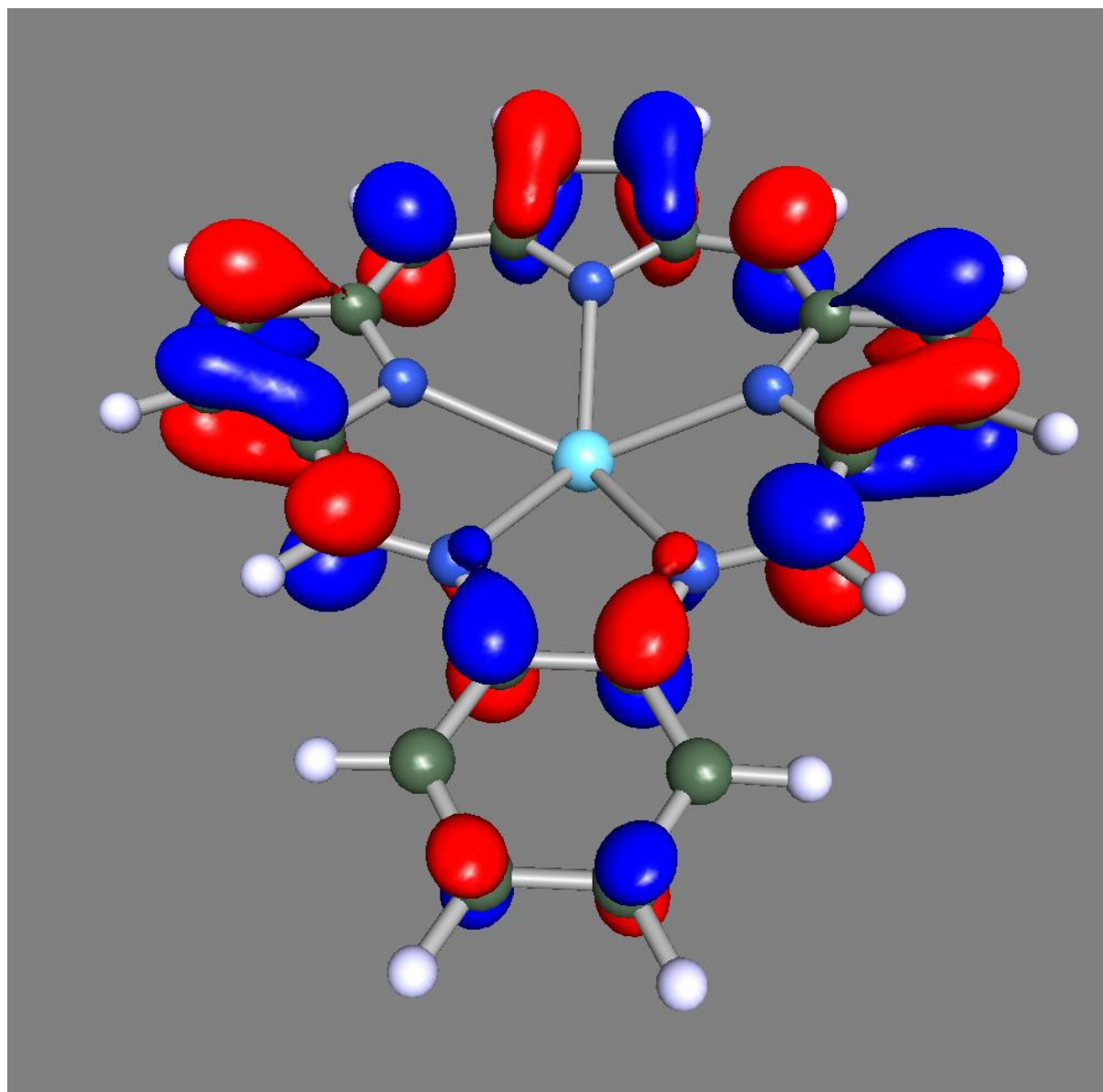


Fig. S1f:
LUMO+4 of [La-Tex]²⁺

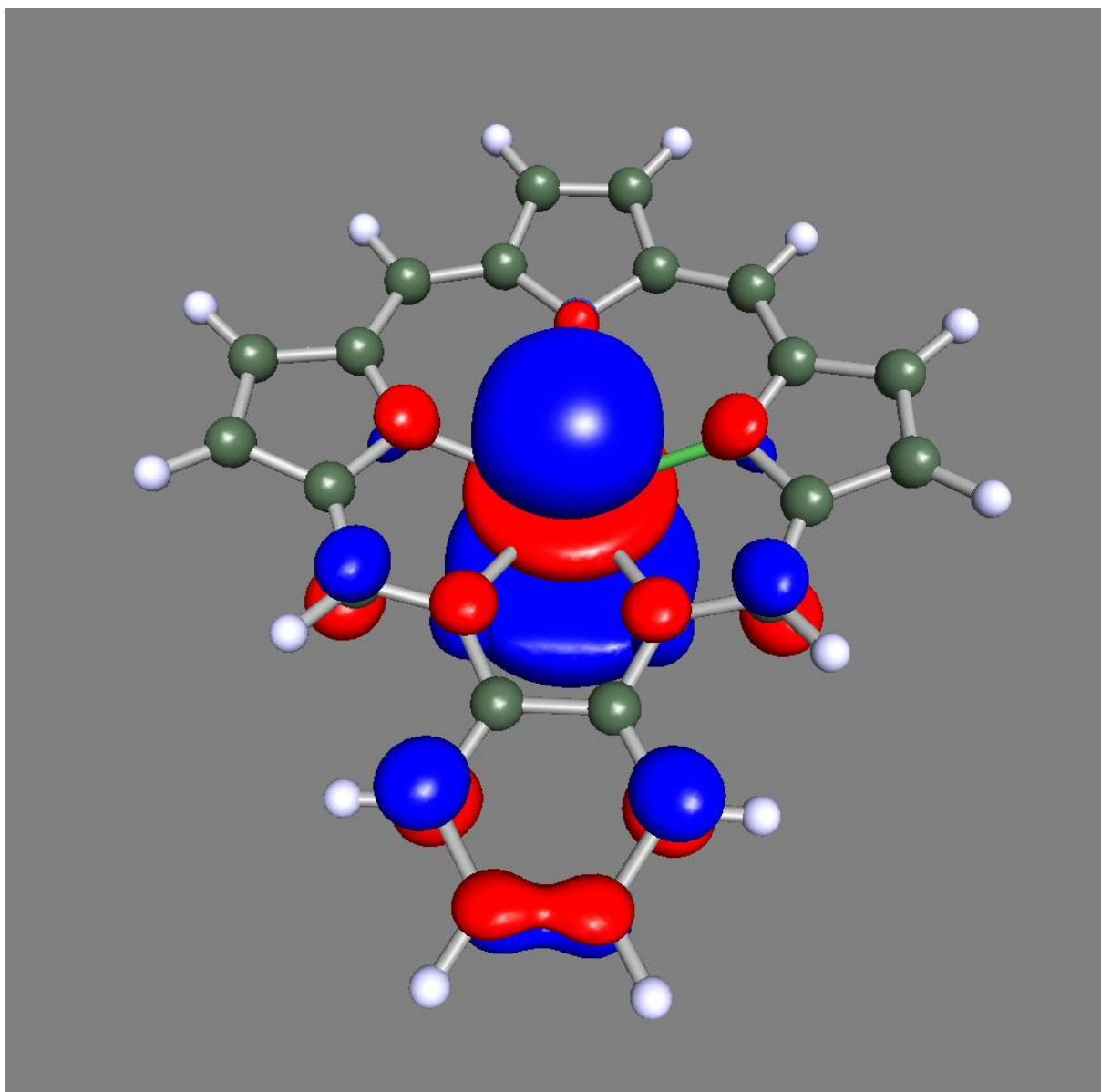


Fig. S1g:
LUMO+3 of [La-Tex]²⁺

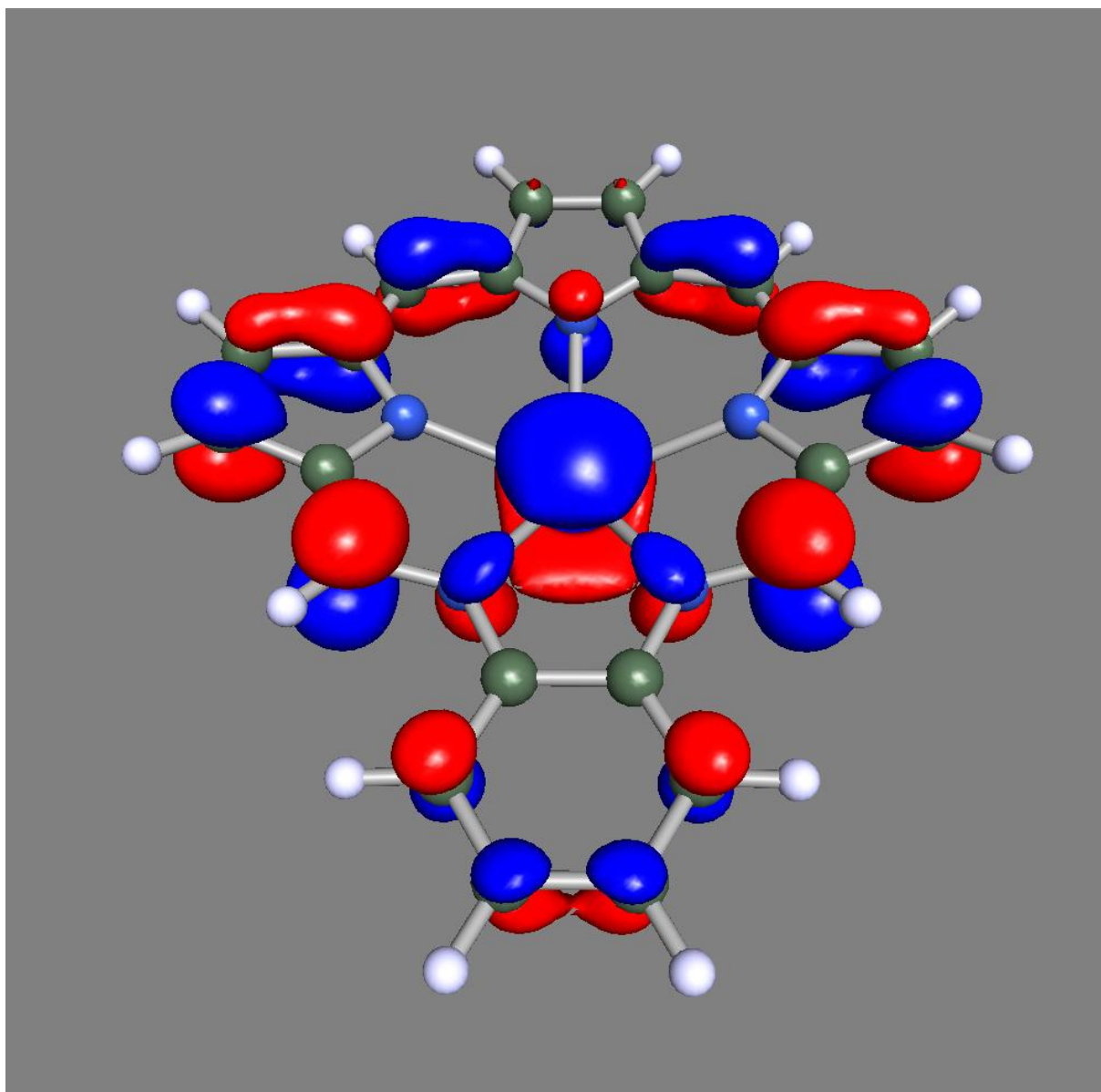


Fig. S1h:

LUMO+2 of [La-Tex]²⁺

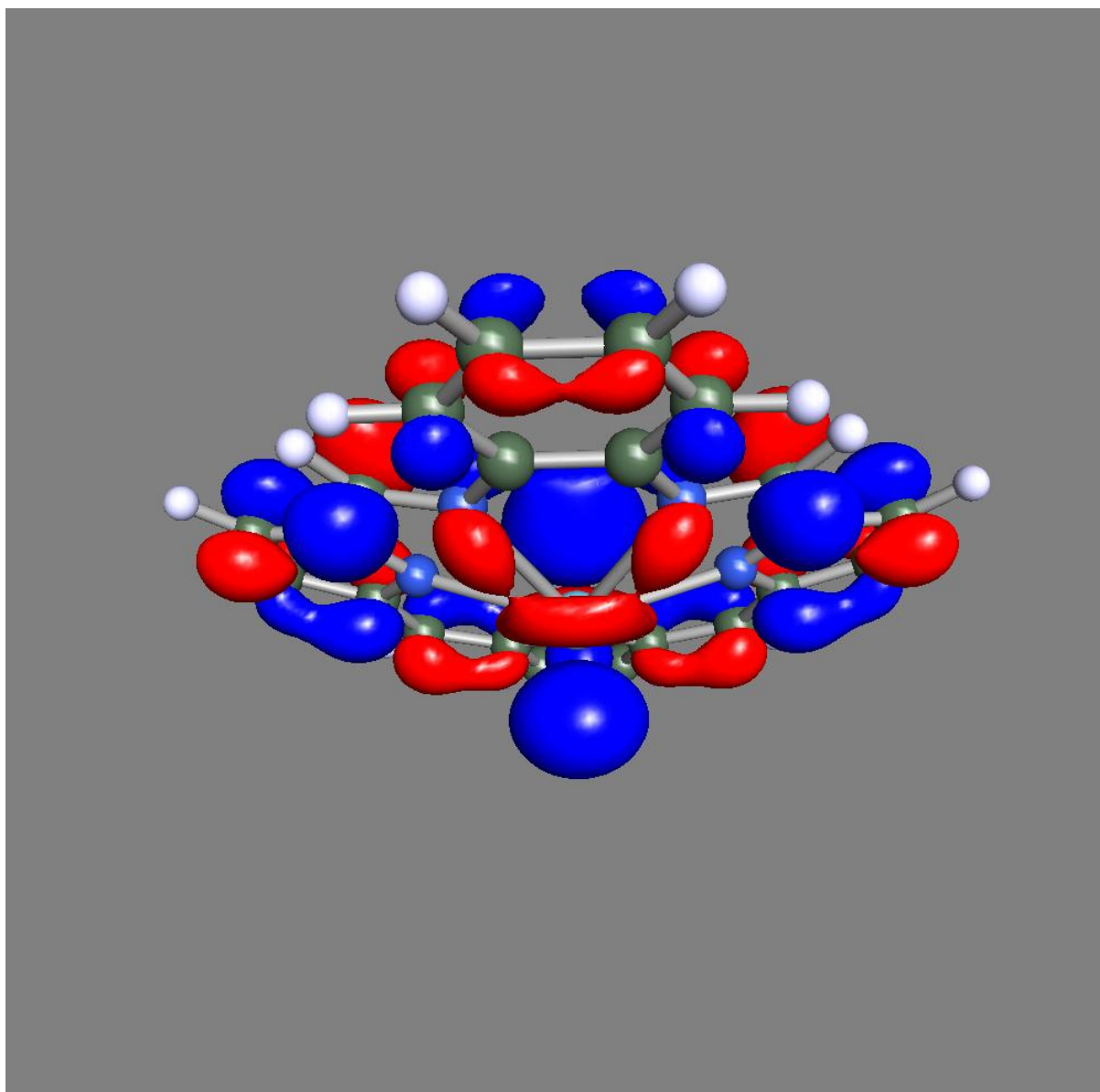


Fig. S1i:

LUMO+2 of [La-Tex]²⁺

Alternative view emphasizing the d_z^2 character of the La atomic orbital contributing to the π -type molecular orbital.

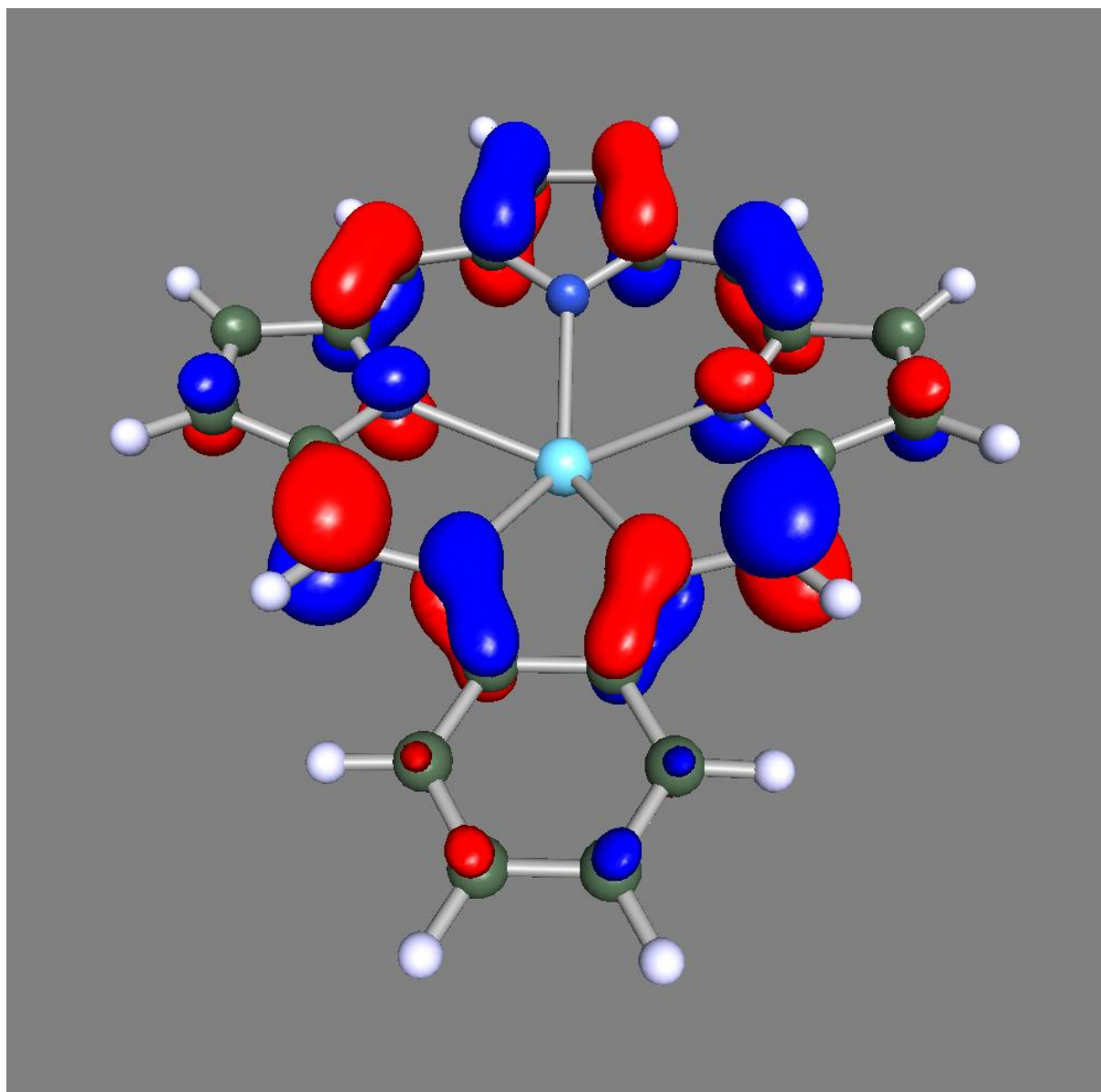


Fig. S1j:
LUMO+1 of [La-Tex]²⁺

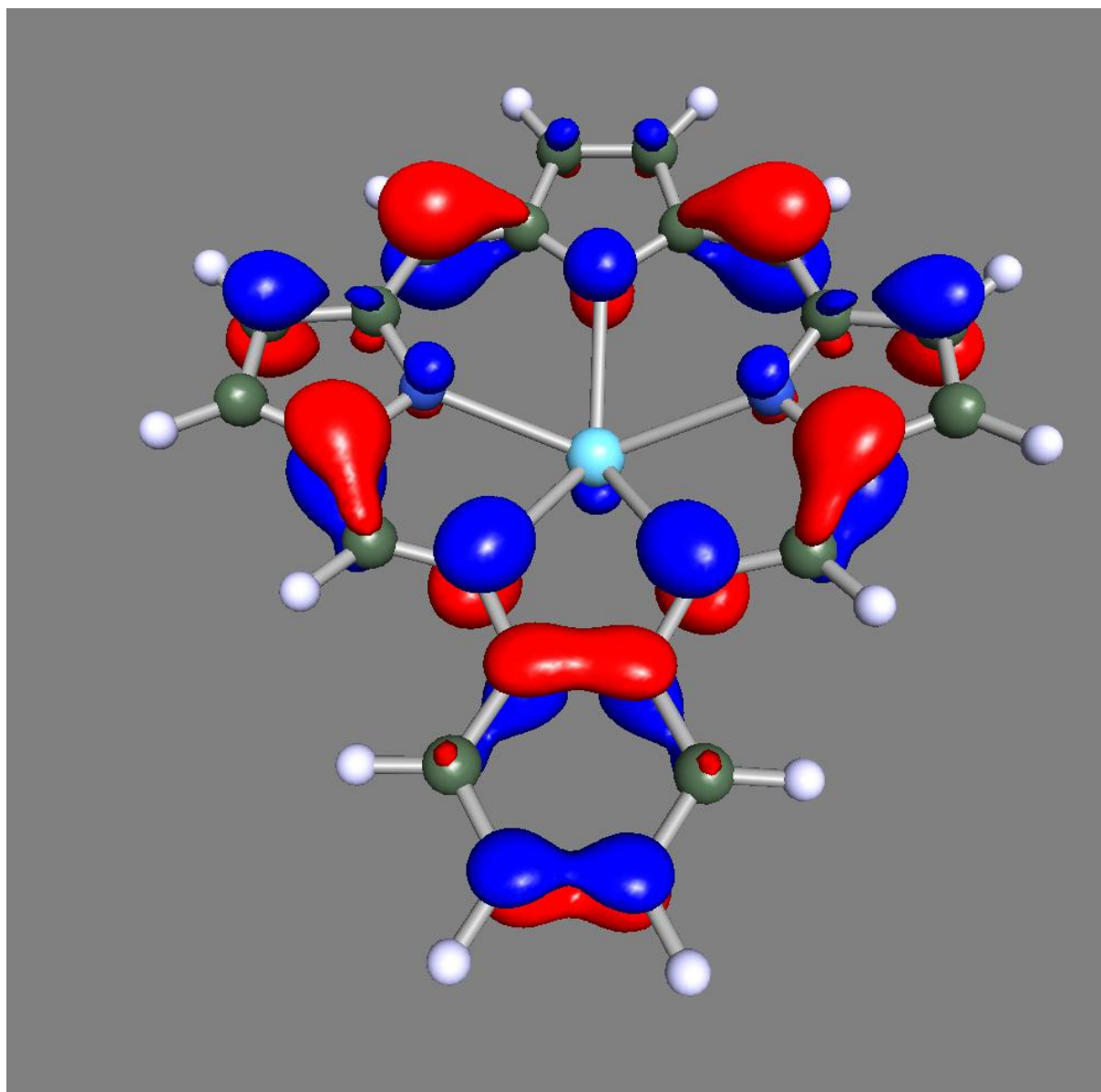


Fig. S1k:

LUMO of [La-Tex]²⁺

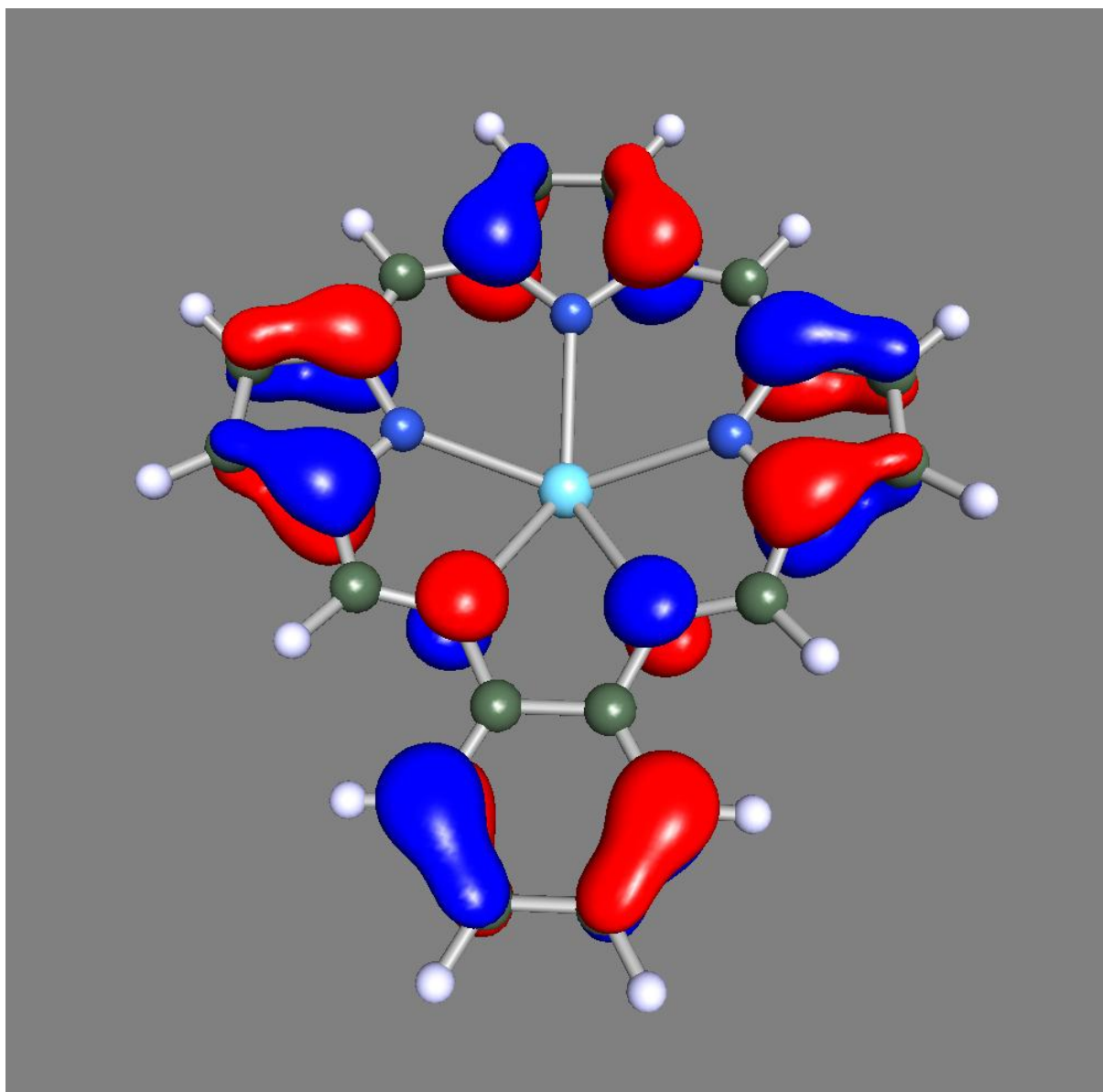


Fig. S1l:

HOMO of [La-Tex]²⁺

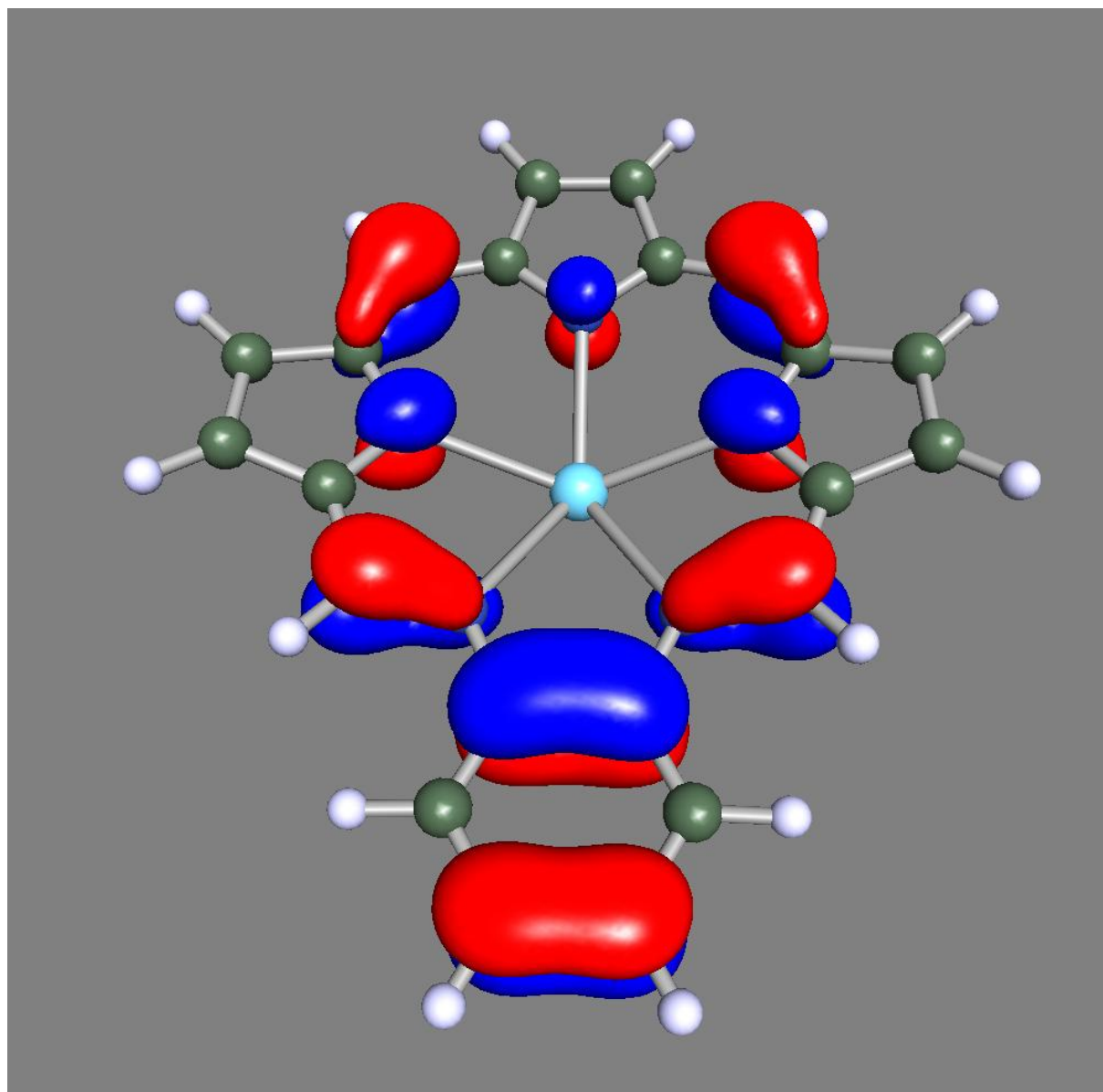


Fig. S1m:

HOMO-1 of [La-Tex]²⁺

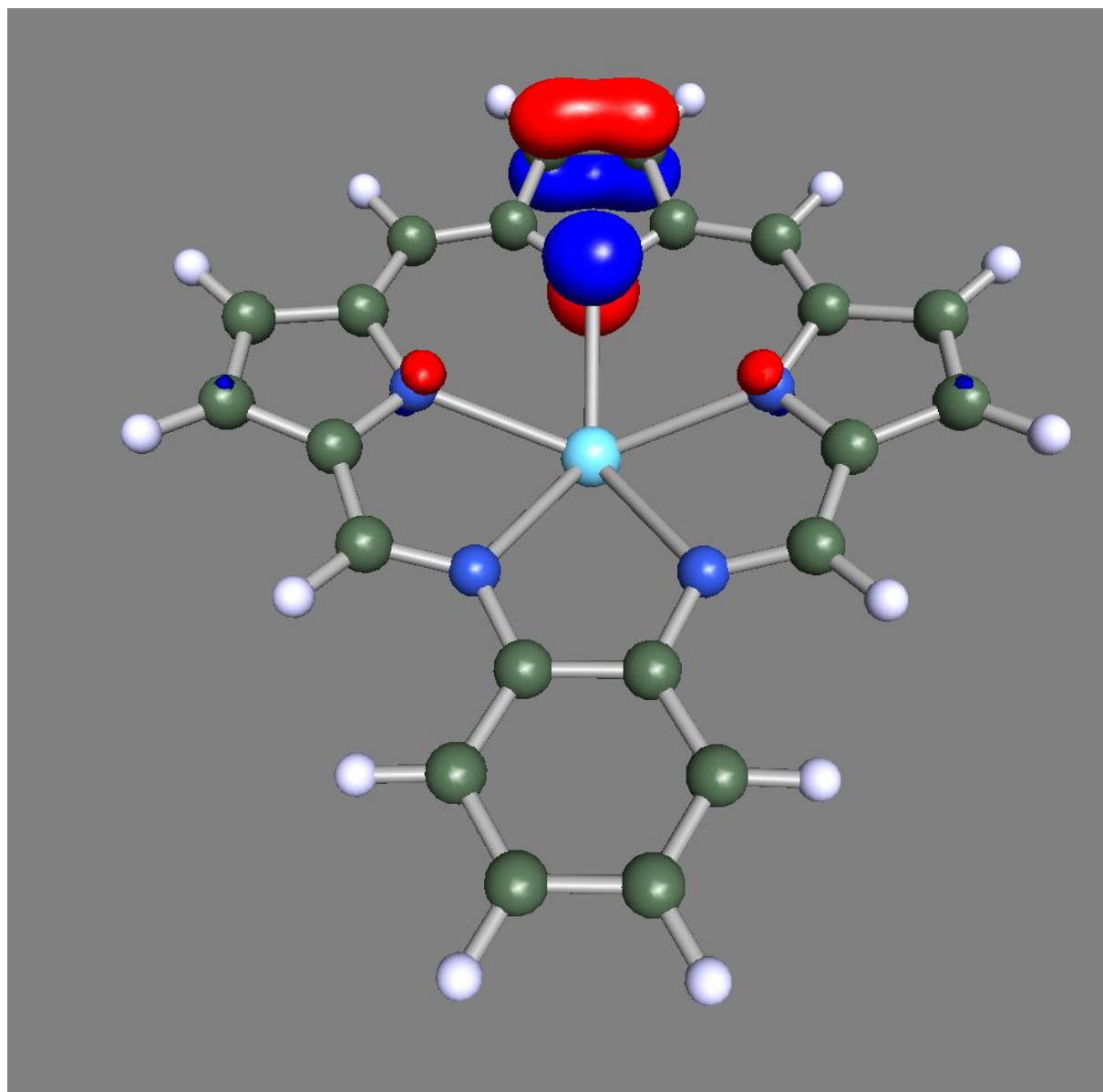


Fig. S1n:

HOMO-2 of [La-Tex]²⁺

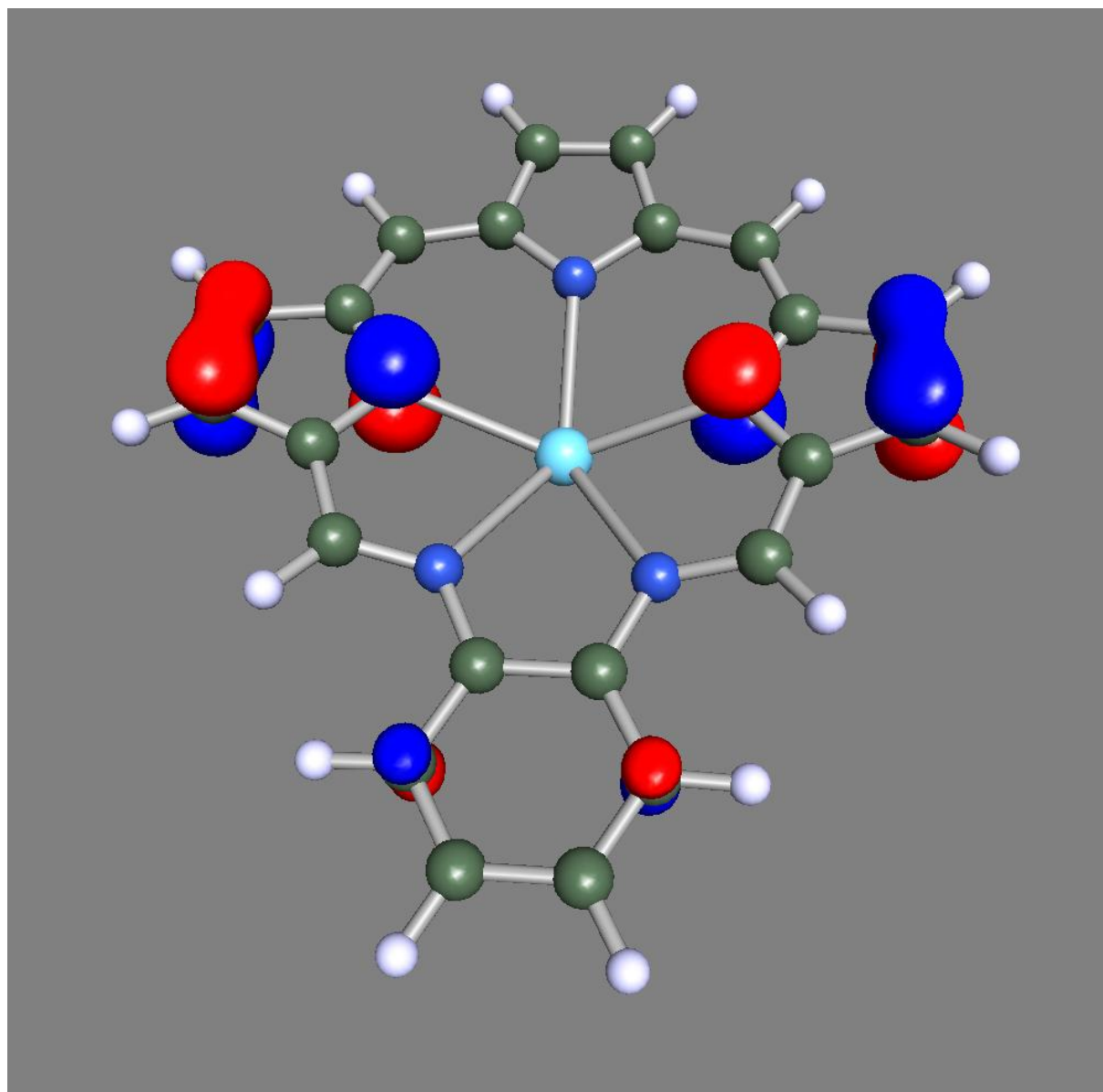


Fig. S1o:

HOMO-3 of [La-Tex]²⁺

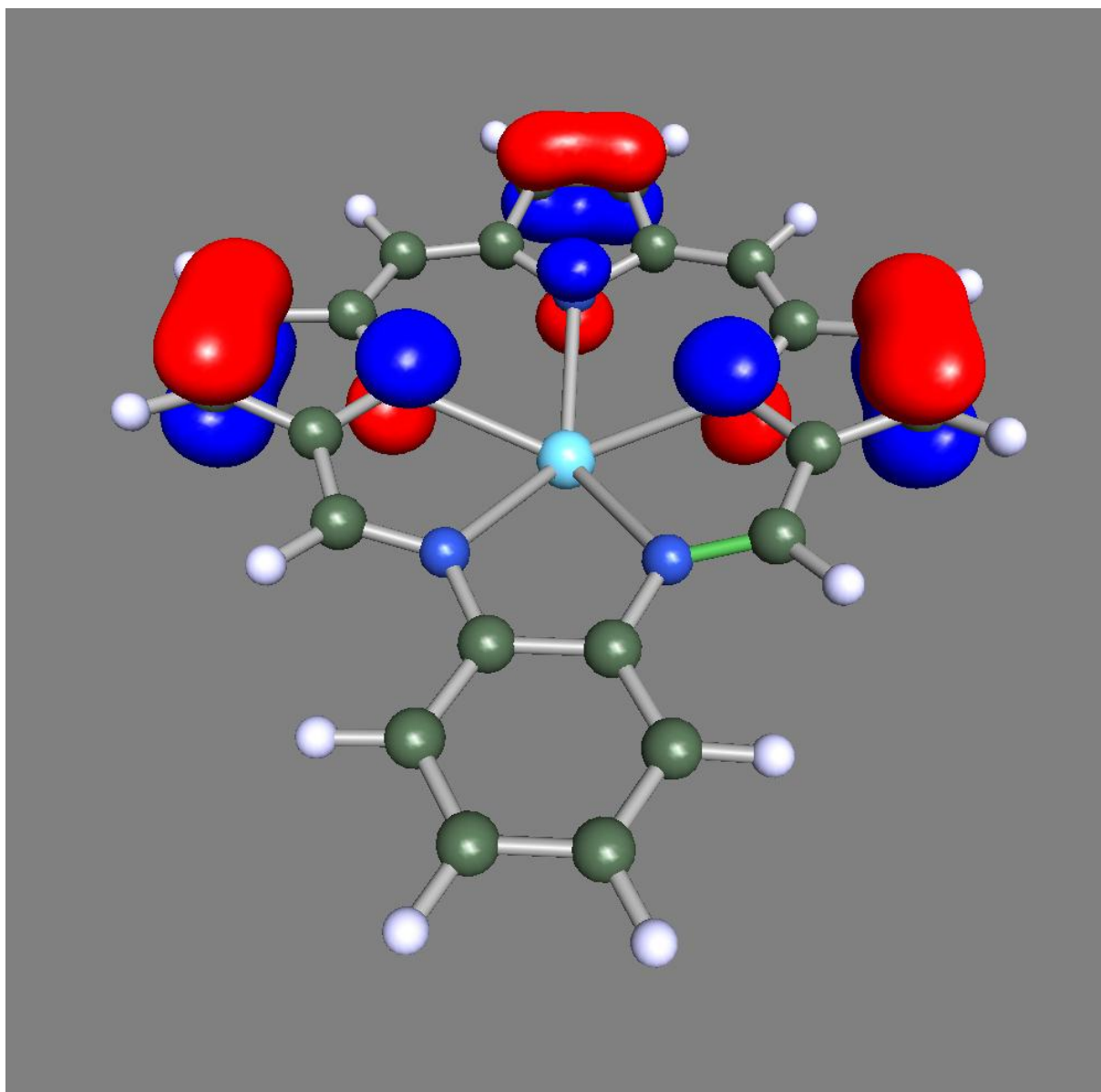


Fig. S1p:

HOMO-4 of [La-Tex]²⁺

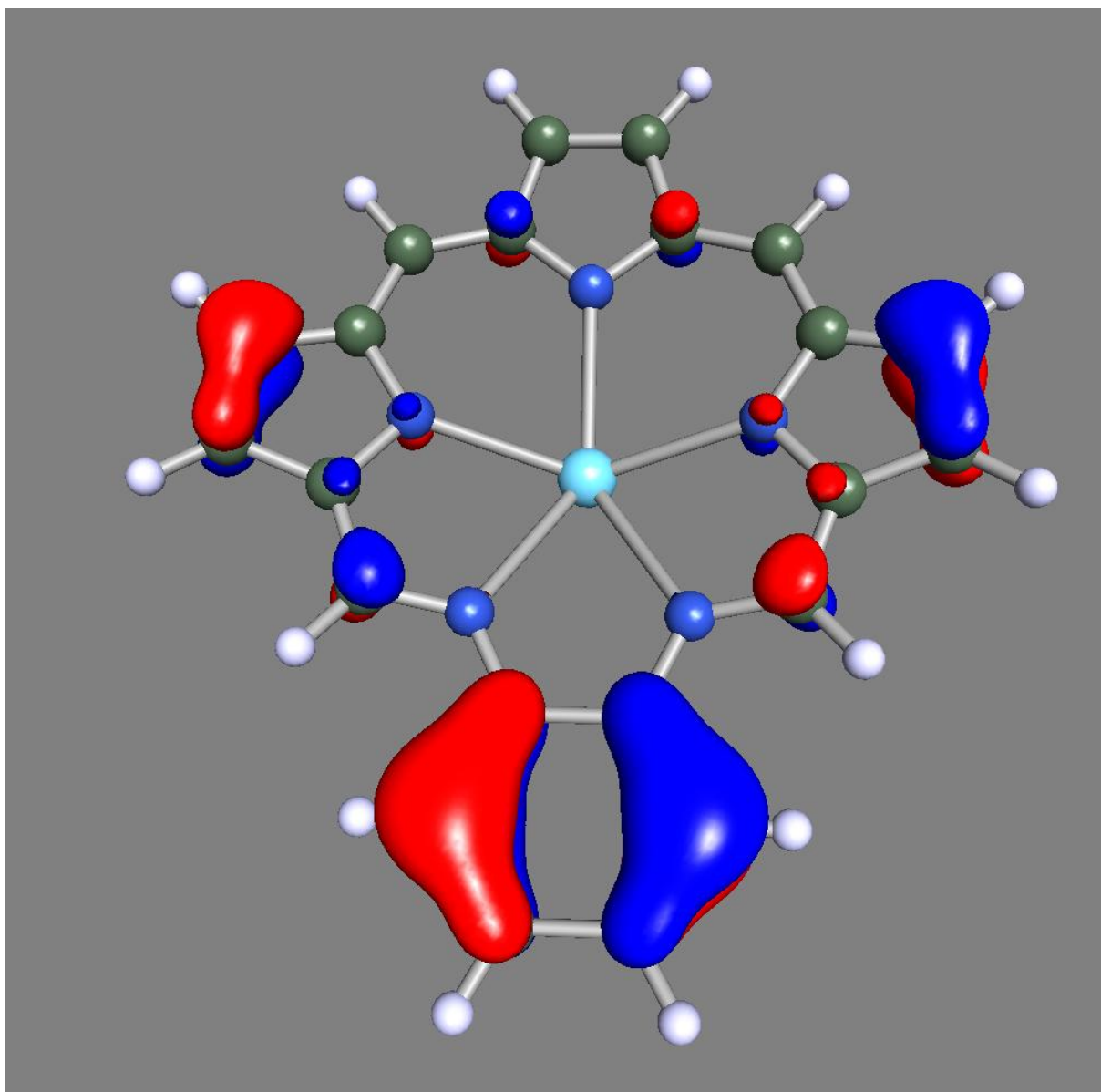


Fig. S1q:

HOMO-5 of [La-Tex]²⁺

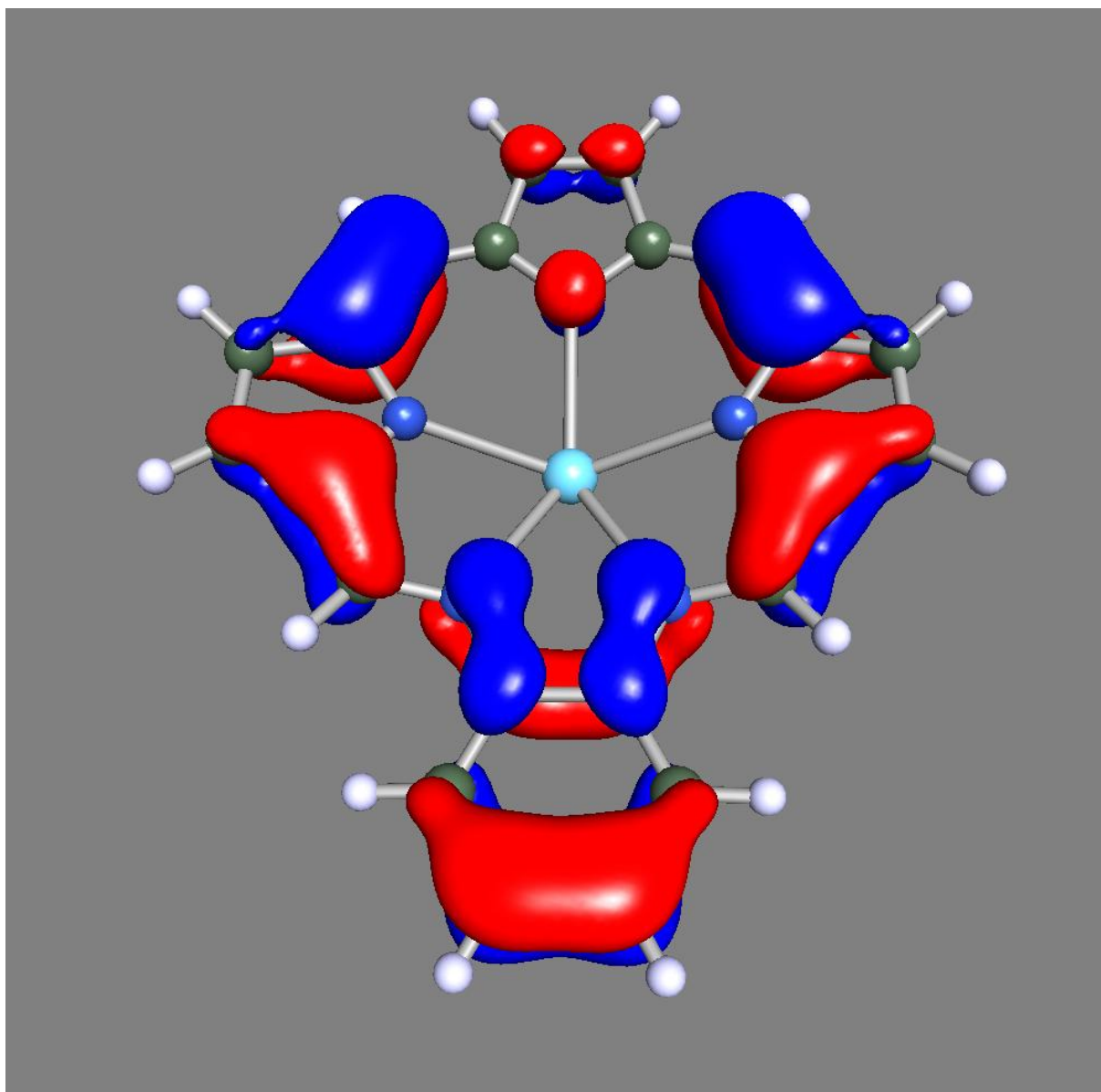


Fig. S1r:
HOMO-6 of [La-Tex]⁶⁺

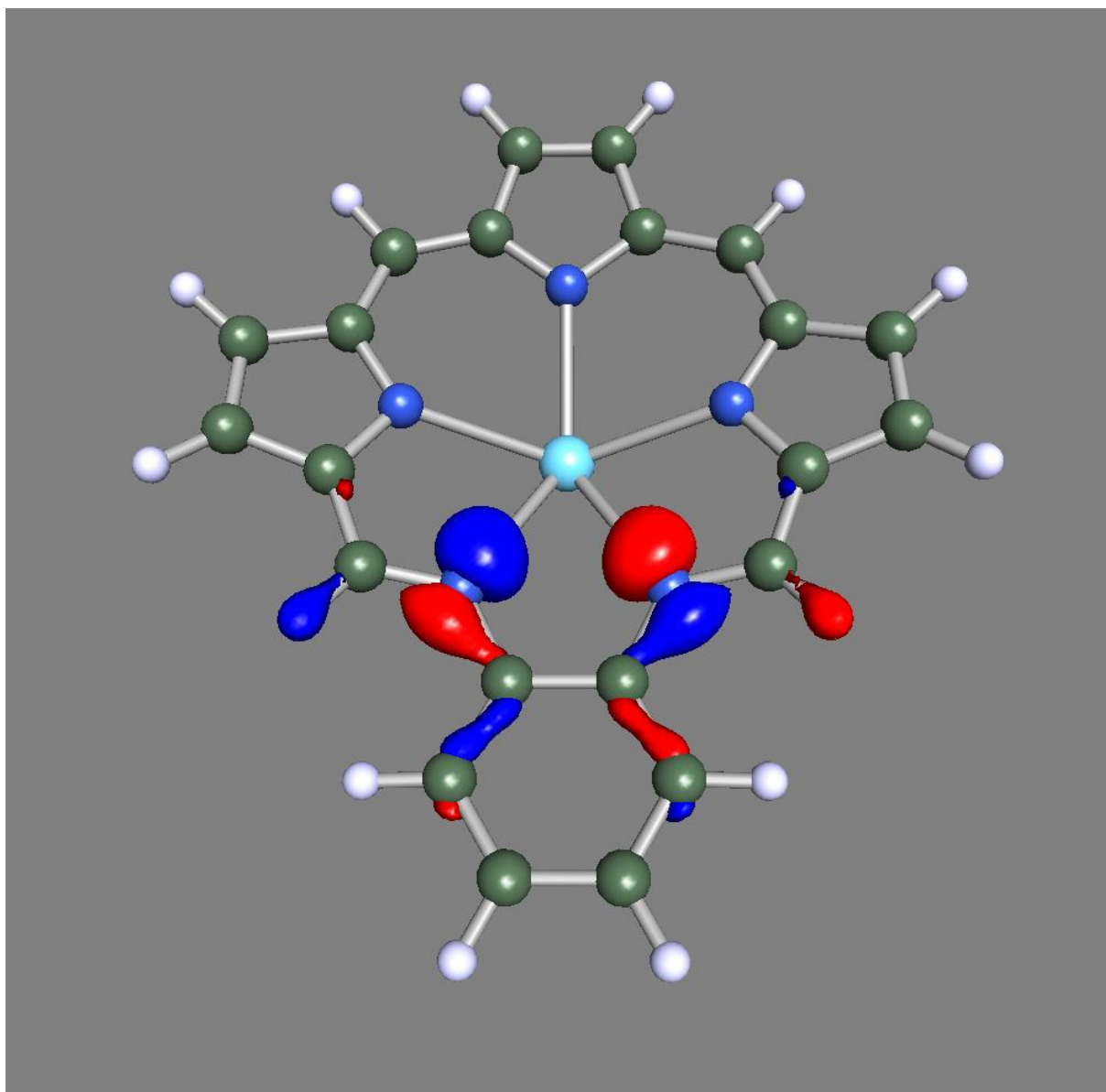


Fig. S1s:
HOMO-7 of [La-Tex]²⁺

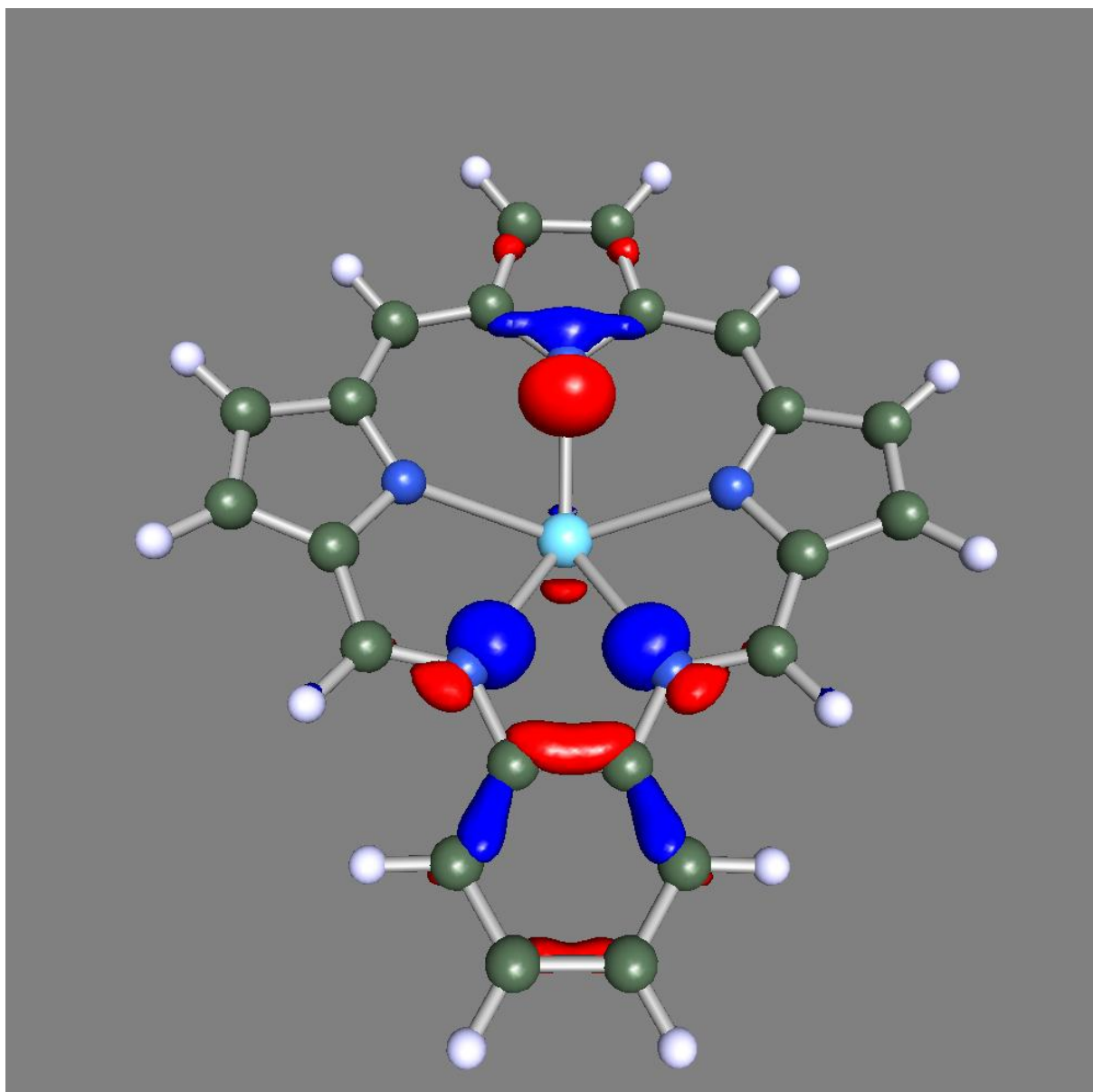


Fig. S1t:
HOMO-8 of [La-Tex]²⁺

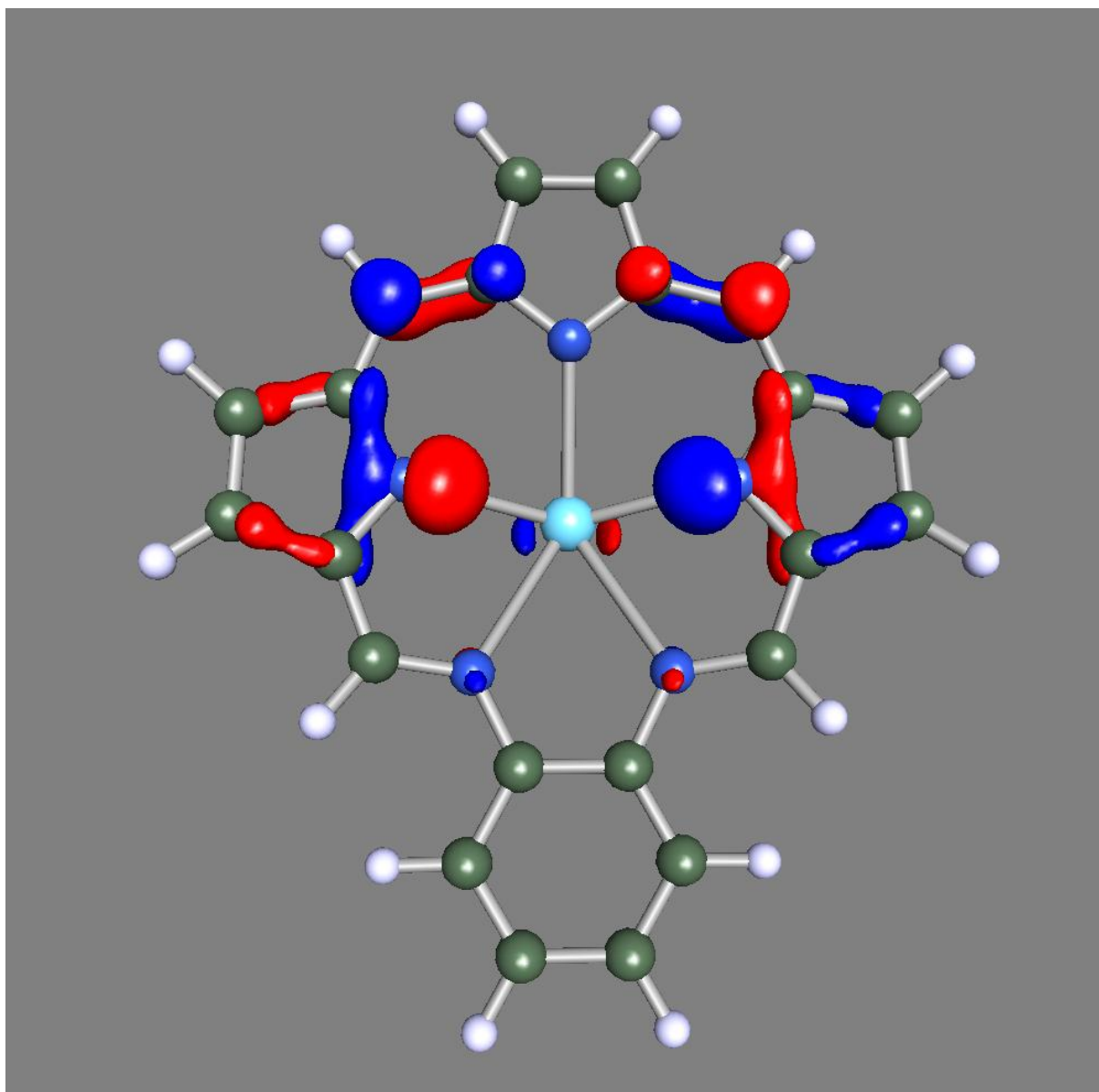


Fig. S1u:
HOMO-9 of [La-Tex]²⁺

I.d UV-Vis Absorption Spectra of $[\text{La-Tex}]^{2+}$

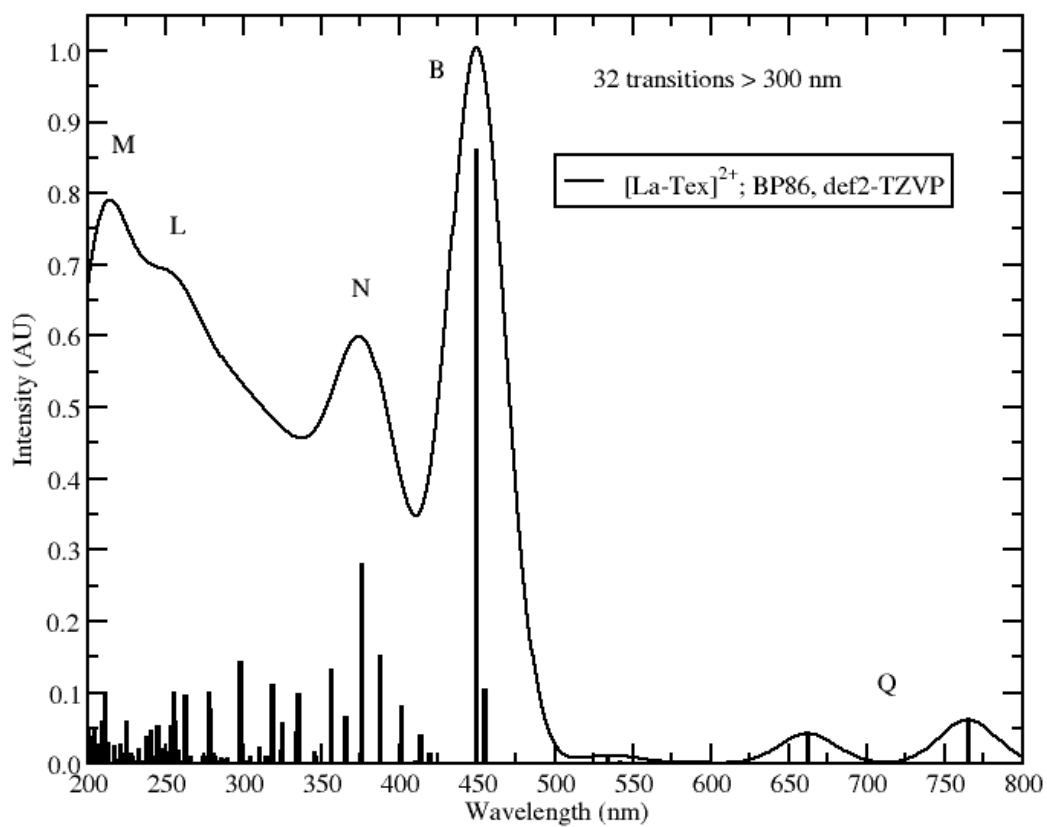


Fig. S2a:

UV-Vis absorption spectrum of $[\text{La-Tex}]^{2+}$ in gas phase calculated by TD-DFT (BP86, def2-TZVP).

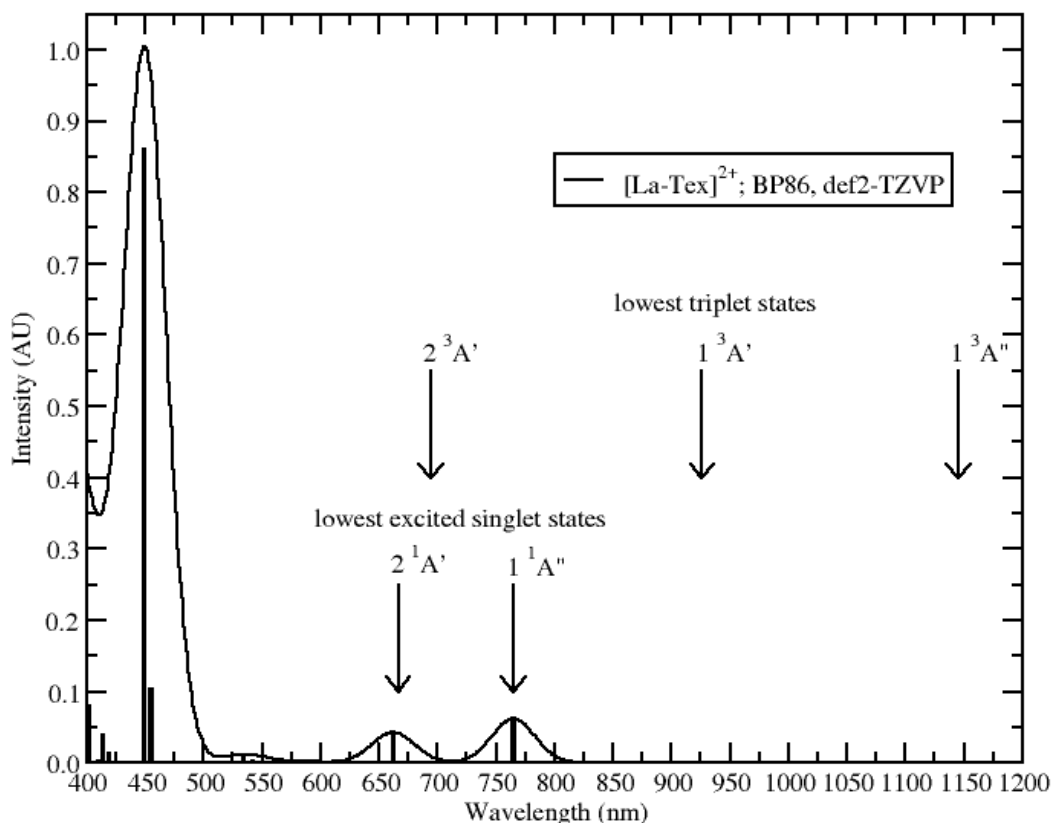


Fig. S2b:

Lowest excited singlet and triplet states of [La-Tex]²⁺ from TD-DFT gas phase calculations using the BP86 functional and def2-TZVP basis sets.

Triplet states located below the lowest excited singlet state $1\ ^1A''$ at a term energy of 1.620 eV (765 nm) are found at 1.082 eV (1146 nm, $1\ ^3A''$) and 1.338 eV (927 nm, $1\ ^3A'$) above the $1\ ^1A'$ ground state (all term symbols for C_{2v} symmetry), i.e., below the high wavelength limit of the “therapeutic window” (near-infrared window) in biological tissue set by the excitation of O_2 from the $^3\Sigma_g^+$ ground state to the $^1\Delta_g$ excited state at 0.977 eV (1269 nm). The low wavelength limit is given by the onset of significant absorption by hemoglobin (HbO_2 , Hb) at around 650 nm and below.

Table S1:

**Summary of the 15 lowest singlet-singlet transitions for [La-Tex]²⁺
from TD-DFT (BP86, def2-TZVP) calculations.**

no.	excitation energy (nm)		oscillator strength		excited state
	occ. MO	Energy (eV)	virt. MO	Energy (eV)	100*coeff.^2
1	765.21		0.44720377015216E-01		1 ¹ A''
	HOMO	-11.77	LUMO	-10.50	90.1
2	662.51		0.30994047368661E-01		1 ¹ A'
	HOMO-1	-12.05	LUMO	-10.50	68.6
	HOMO	-11.77	LUMO+1	-9.76	27.5
3	606.95		0.26484985771929E-04		2 ¹ A'
	HOMO-2	-12.40	LUMO	-10.50	96.3
4	584.31		0.13464541898481E-02		2 ¹ A''
	HOMO-3	-12.52	LUMO	-10.50	96.5
5	541.95		0.17340800088197E-02		3 ¹ A'
	HOMO-4	-11.68	LUMO	-10.50	88.3
	HOMO	-11.77	LUMO+1	-9.76	7.7
6	534.25		0.70291845293752E-02		3 ¹ A''
	HOMO-5	-12.69	LUMO	-10.50	81.6
	HOMO-1	-12.05	LUMO+1	-9.76	13.8
7	455.31		0.79612345453637E-01		4 ¹ A''
	HOMO-1	-12.05	LUMO+1	-9.76	40.8
	HOMO	-11.77	LUMO+2	-8.92	26.0
	HOMO-2	-12.40	LUMO+1	-9.76	22.1
	HOMO-5	-12.69	LUMO	-10.50	4.6
8	449.86		0.61991505830949E+00		4 ¹ A'

	HOMO	-11.77	LUMO+1	-9.76	48.5
	HOMO-1	-12.05	LUMO	-10.50	21.7
	HOMO-6	-13.32	LUMO	-10.50	8.3
	HOMO-4	-12.68	LUMO	-10.50	7.0
	HOMO-3	-12.52	LUMO+1	-9.76	5.3
9	449.29		0.18435112046824E-01		5 ¹ A''
	HOMO-2	-12.40	LUMO+1	-9.76	75.3
	HOMO-1	-12.05	LUMO+1	-9.76	17.0
10	419.52		0.70381602626991E-02		5 ¹ A'
	HOMO-3	-12.52	LUMO+1	-9.76	80.0
	HOMO-6	-13.32	LUMO	-10.50	14.4
11	414.04		0.31463767405582E-01		6 ¹ A'
	HOMO-5	-12.69	LUMO+1	-9.76	46.3
	HOMO-6	-13.32	LUMO	-10.50	37.3
	HOMO-3	-12.52	LUMO+1	-9.76	6.6
12	410.29		0.29482580877750E-02		6 ¹ A''
	HOMO-4	-12.68	LUMO+1	-9.76	75.3
	HOMO	-11.77	LUMO+2	-8.92	18.7
13	401.69		0.58522332684448E-01		7 ¹ A'
	HOMO-1	-12.05	LUMO+2	-8.92	47.5
	HOMO-5	-12.69	LUMO+1	-9.76	35.4
	HOMO-6	-13.32	LUMO	-10.50	8.8
14	388.51		0.10958399733025E+00		7 ¹ A''
	HOMO-7	-13.68	LUMO	-10.50	55.8
	HOMO	-11.77	LUMO+2	-8.92	19.1
	HOMO-4	-12.68	LUMO+1	-9.76	10.8
	HOMO-1	-12.05	LUMO+1	-9.76	4.9
15	376.34		0.19762505142552E+00		8 ¹ A''
	HOMO-7	-13.68	LUMO	-10.50	40.4
	HOMO	-11.77	LUMO+2	-8.92	17.5
	HOMO-4	-12.68	LUMO+1	-9.76	8.2
	HOMO-1	-12.05	LUMO+1	-9.76	7.6
	HOMO	-11.77	LUMO+4	-8.41	7.4
	HOMO-6	-13.32	LUMO+1	-9.76	4.5
	HOMO-5	-12.69	LUMO	-10.50	3.6
	HOMO-9	-14.02	LUMO	-10.50	2.6

Table S2:

**Summary of the 2 lowest (spin-forbidden) singlet-triplet transitions
for [La-Tex]²⁺ from TD-DFT (BP86, def2-TZVP) calculations.**

no.	excitation energy (nm)		excited state		
	occ. MO	Energy (eV)	virt. MO	Energy (eV)	100*coeff.^2
1	1146.09		1 ³ A''		
	HOMO	-11.77	LUMO	-10.50	99.1
2	926.94		1 ³ A'		
	HOMO-1	-12.05	LUMO	-10.50	98.8

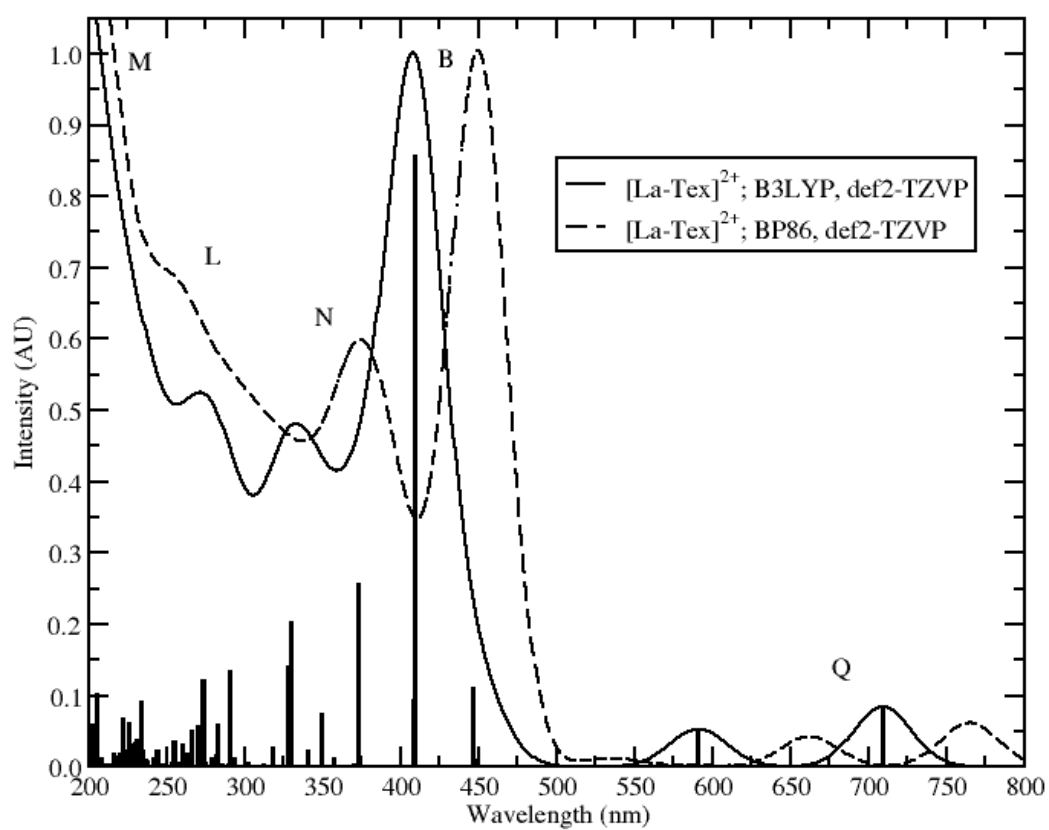


Fig. S3a:
UV-Vis absorption spectrum of [La-Tex]²⁺ calculated by TD-DFT (B3LYP and BP86, def2-TZVP).

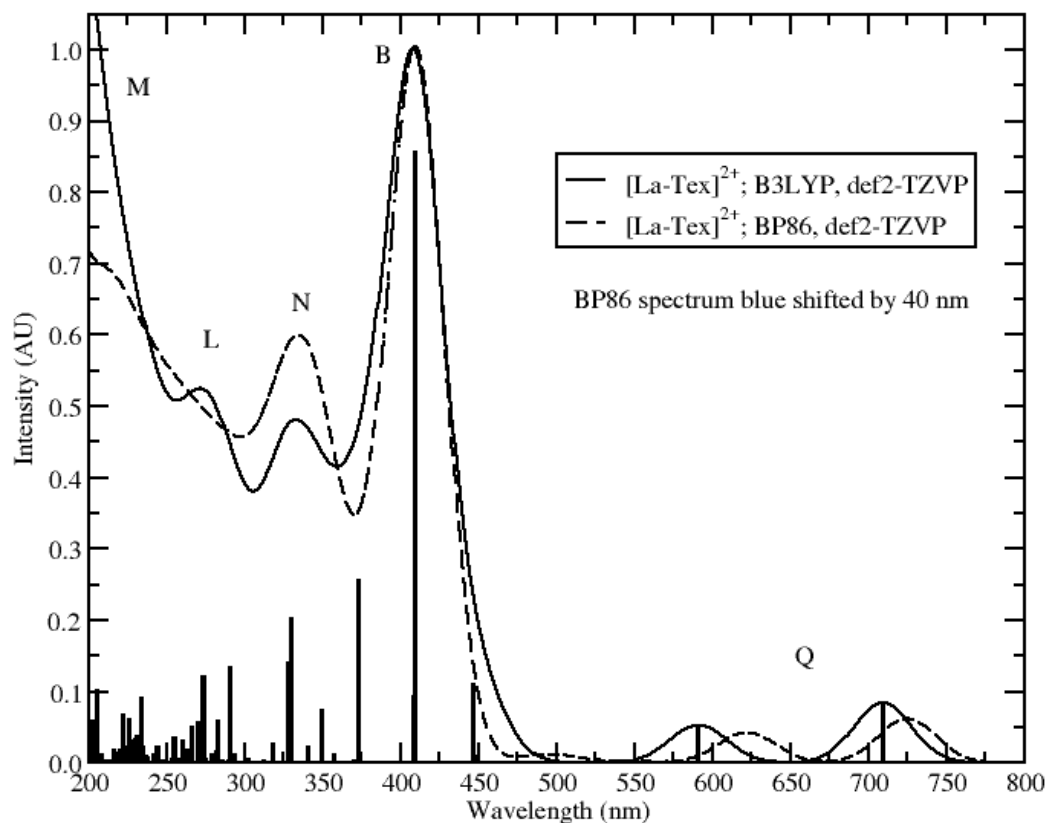


Fig. S3b:
UV-Vis absorption spectrum of $[\text{La-Tex}]^{2+}$ calculated by TD-DFT (B3LYP and BP86, def2-TZVP).

The BP86 spectrum was shifted to shorter wavelengths by 40 nm in order to have the B-bands at nearly the same position.

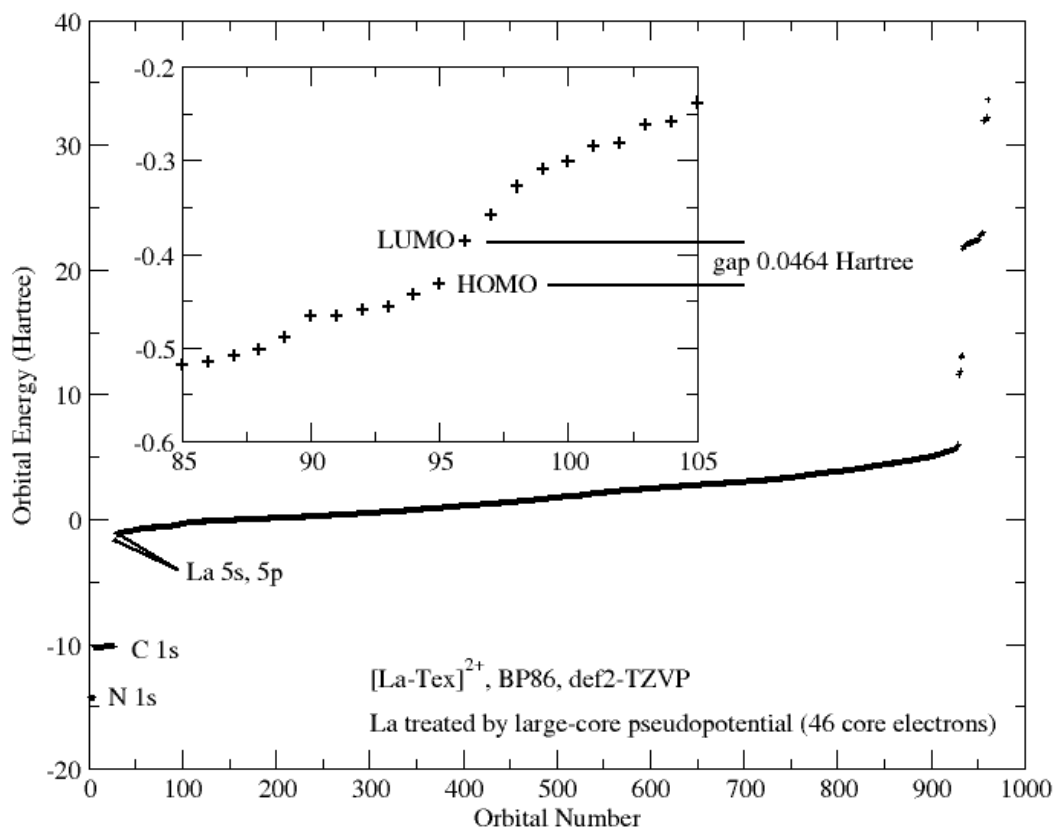


Fig. S4a:
Orbital energies from BP86 calculations of $[\text{La-Tex}]^{2+}$.

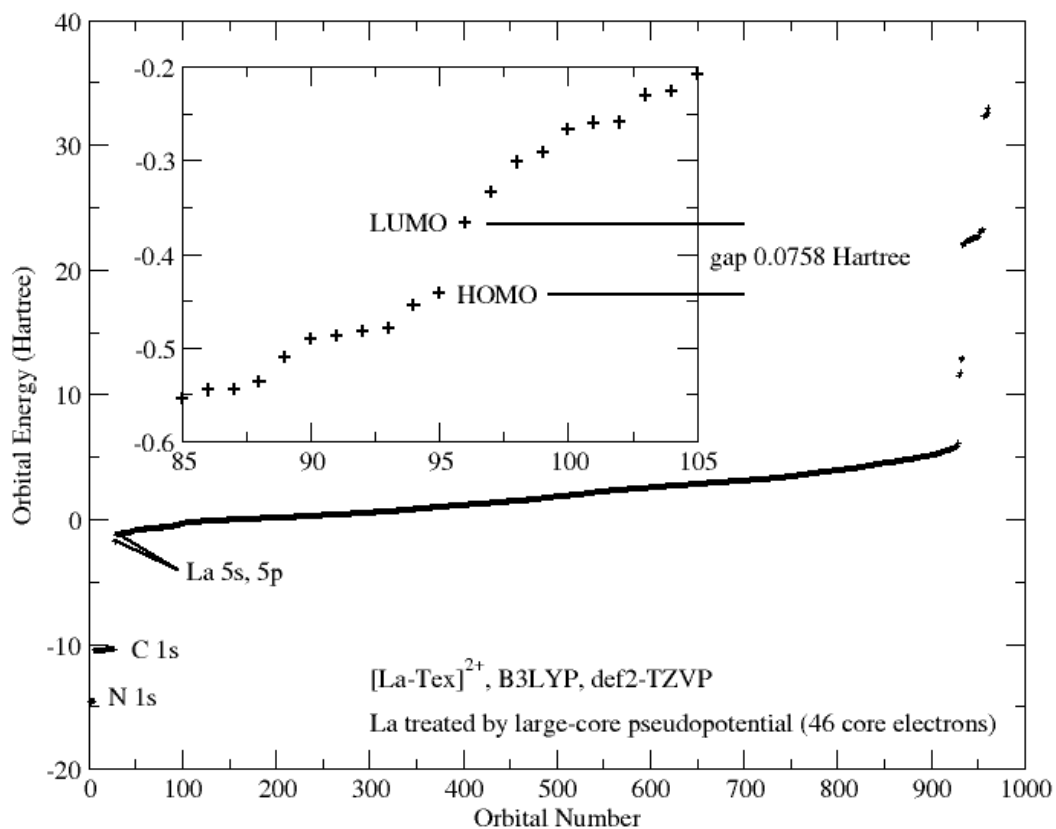


Fig. S4b:

Orbital energies from B3LYP calculations of $[\text{La-Tex}]^{2+}$.

The HOMO-LUMO gap as well as the spread of the orbital energies (e.g. between no. 85 und 105) is significantly larger for B3LYP than for BP86, (cf. Figure S4a) leading to a blue shift of the B3LYP spectrum with respect to the BP86 one (cf. Figure S3b).

I.e UV-Vis Absorption Spectra of $[M\text{-Por}]^{n+}$ ($M=\text{Mg},n=0$;
 $M=\text{La},n=1$) and $[M\text{-Tex}]^{n+}$ ($M=\text{Mg},n=1$; $M=\text{La},n=2$)

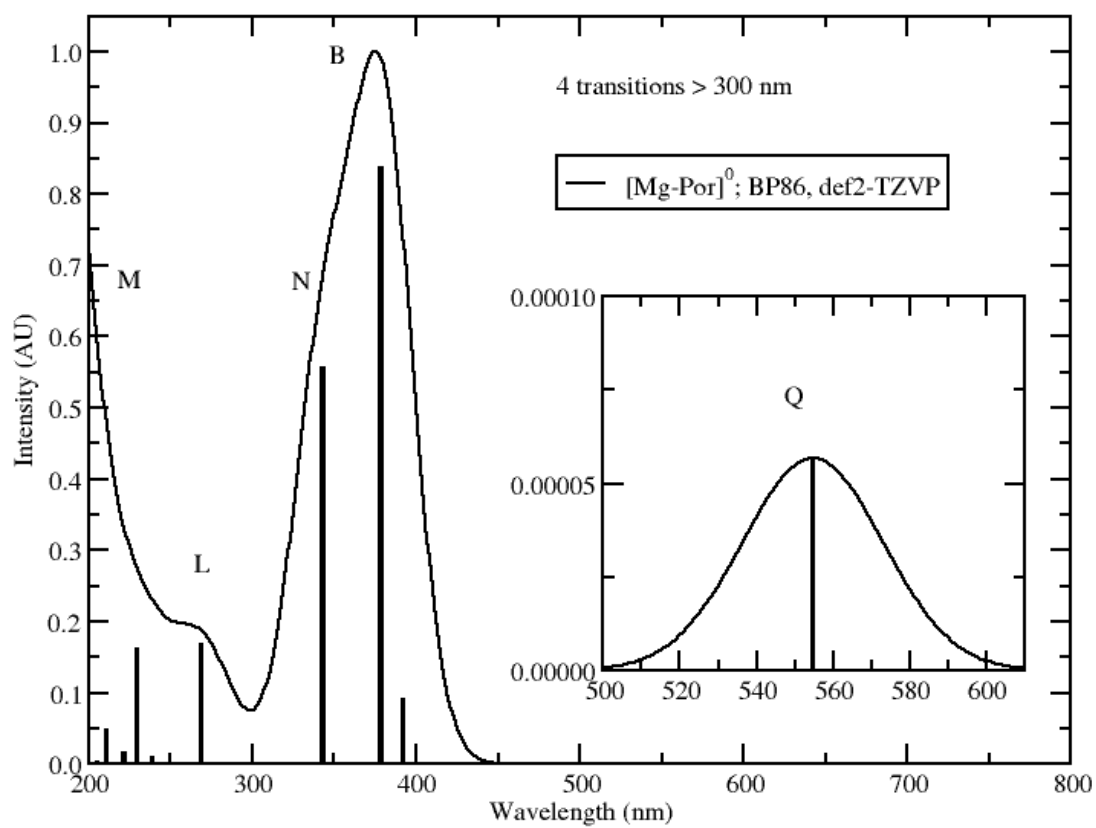


Fig. S5a:
TD-DFT/BP86 UV-Vis absorption spectrum of $[\text{Mg-Por}]^0$.

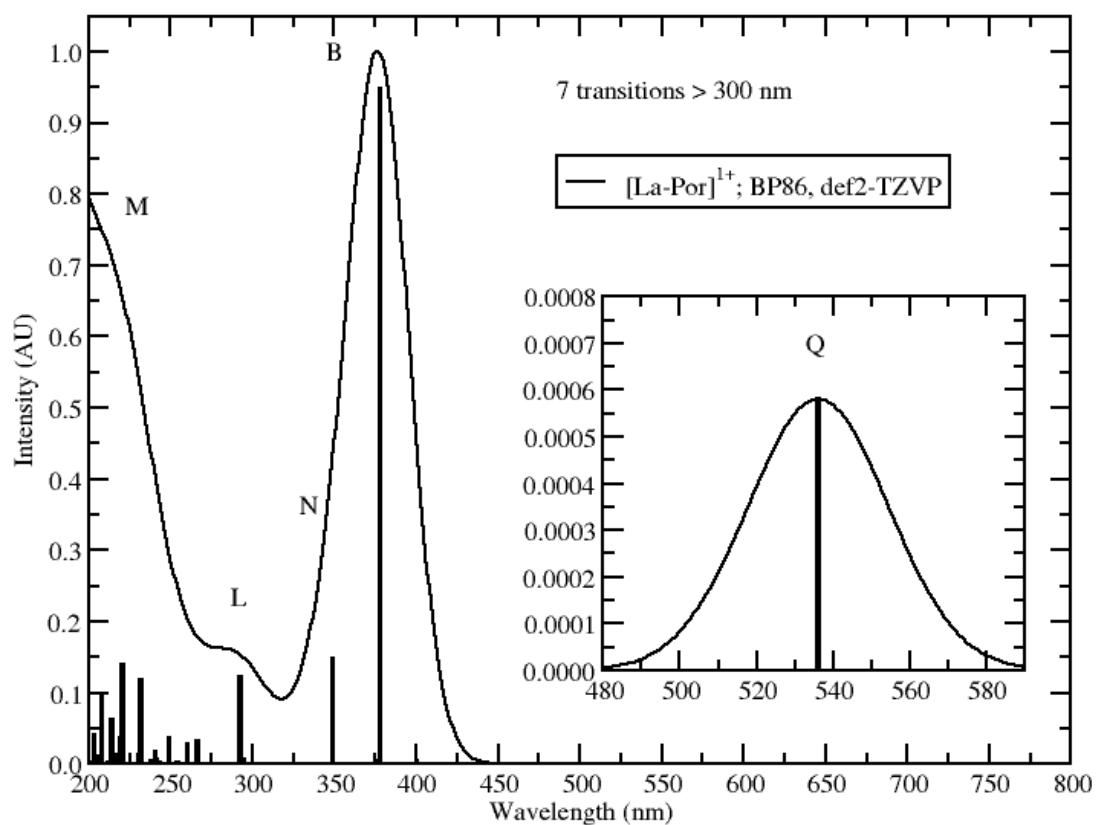


Fig. S5b:
TD-DFT/BP86 UV-Vis absorption spectrum of $[\text{La-Por}]^{1+}$.

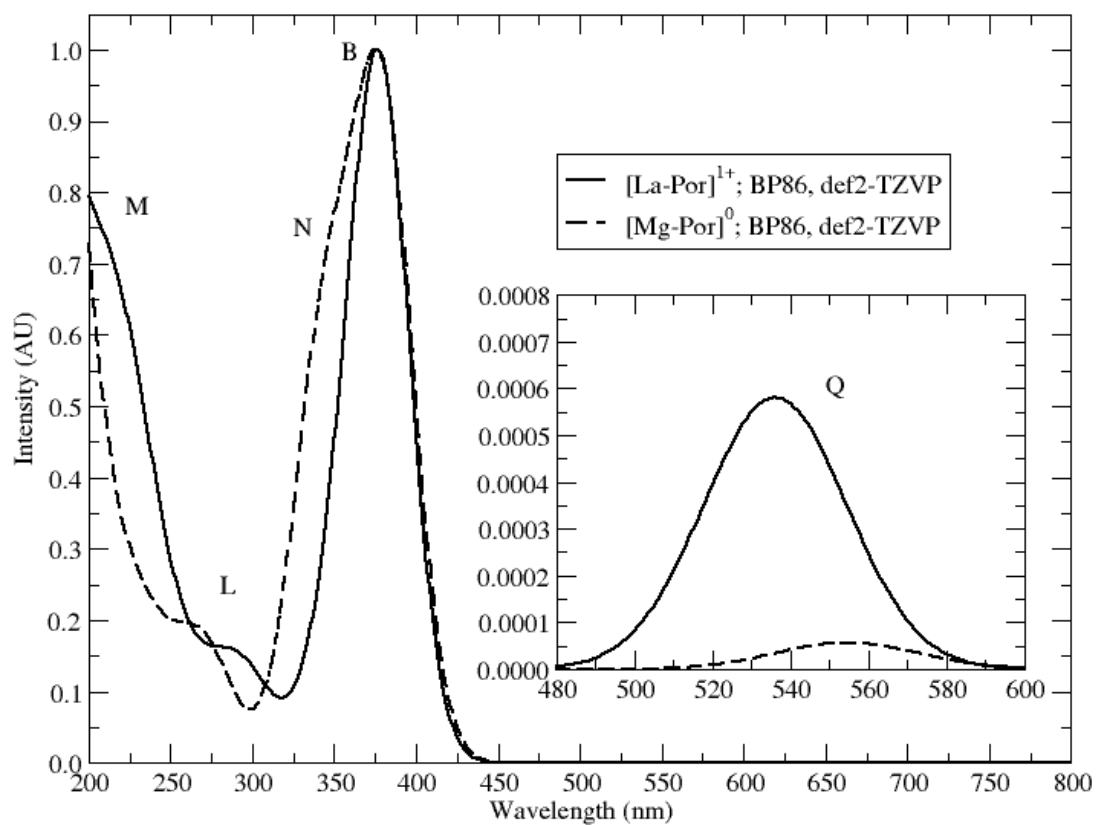


Fig. S5c:
Comparison of TD-DFT/BP86 UV-Vis absorption spectra of [La-Por]⁺ and [Mg-Por]⁰.

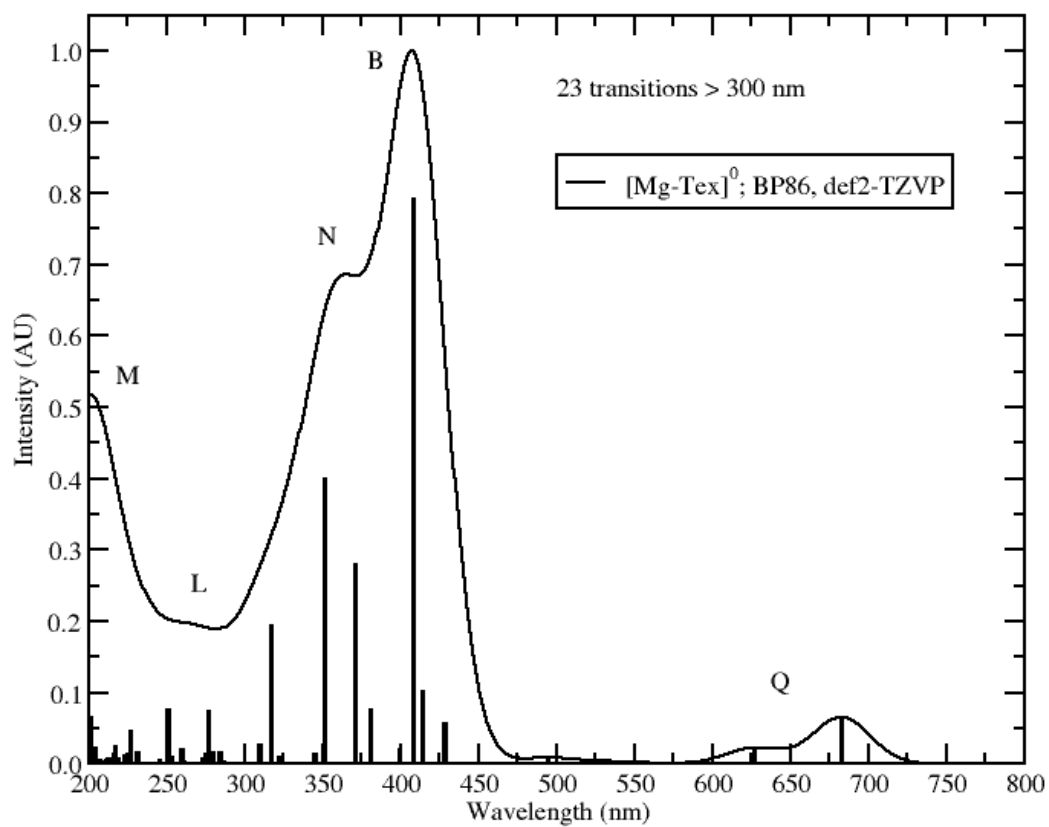


Fig. S6a:
TD-DFT/BP86 UV-Vis absorption spectrum of $[\text{Mg-Tex}]^+$.

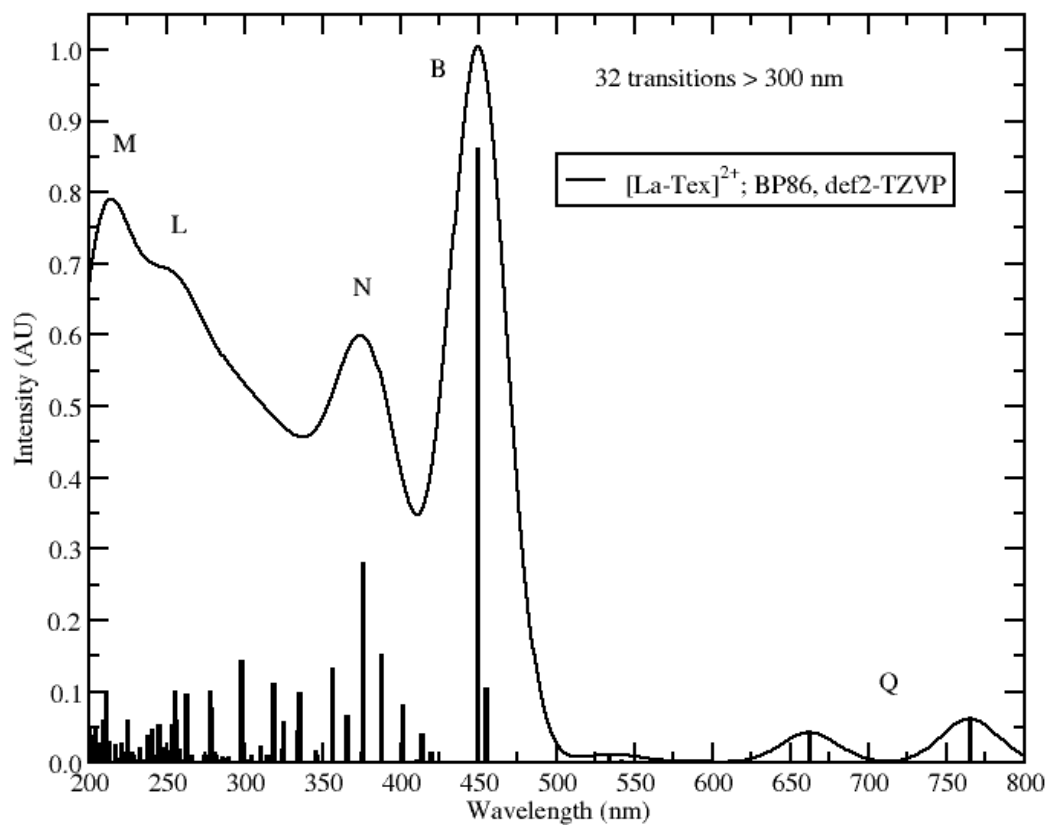


Fig. 6b:
TD-DFT/BP86 UV-Vis absorption spectrum of [La-Tex]²⁺.

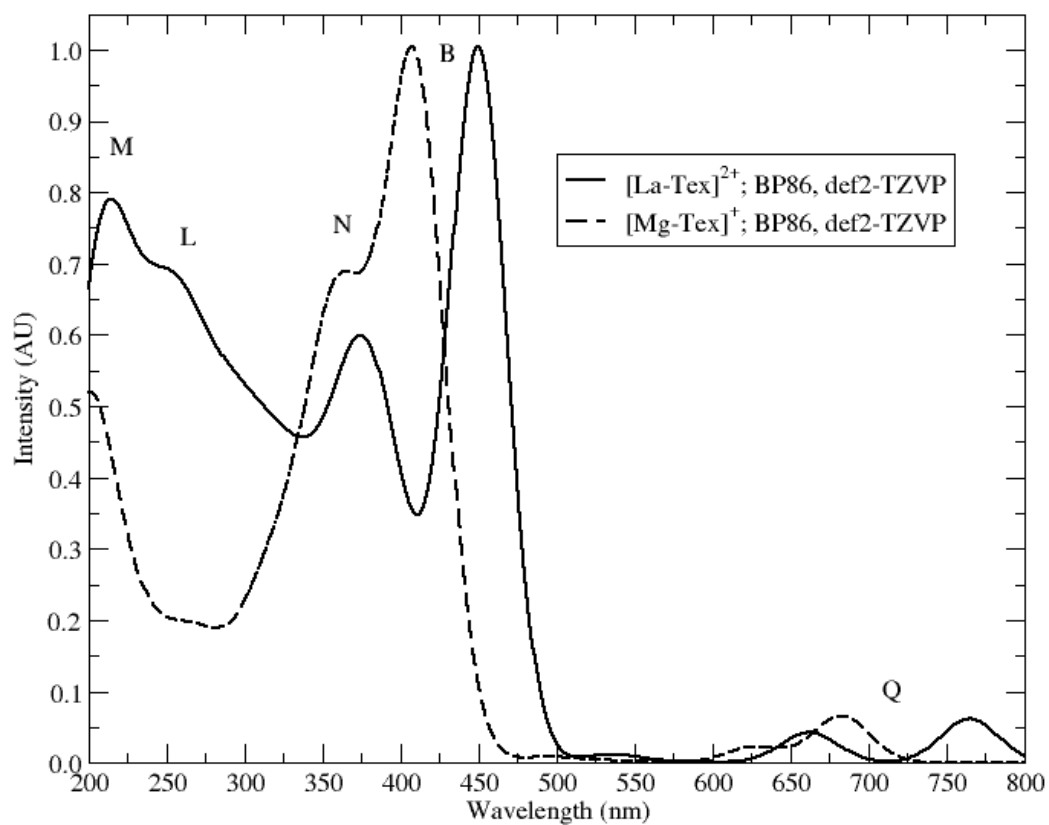


Fig. S6c:
Comparison of TD-DFT/BP86 UV-Vis absorption spectra of [La-Tex]²⁺ and [Mg-Tex]⁺.

II.e Effects of Metal-Coordinated Water Molecules and Substitution at the Ring System on the UV-Vis Absorption Spectrum of $[\text{La-Tex}]^{2+}$

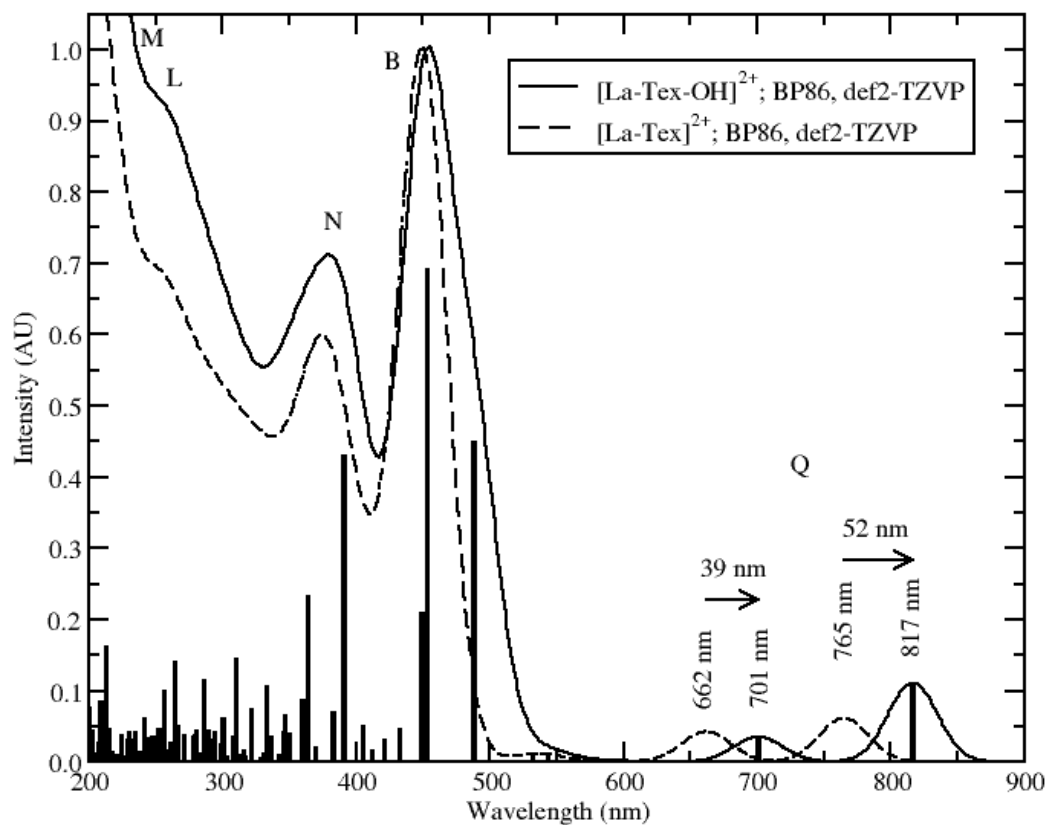


Fig. S7a:
TD-DFT/BP86 UV-Vis absorption spectrum of $[\text{La-Tex}]^{2+}$ with one $-\text{OH}$ group at the R^4 position (cf. Figure 1 in the main text).

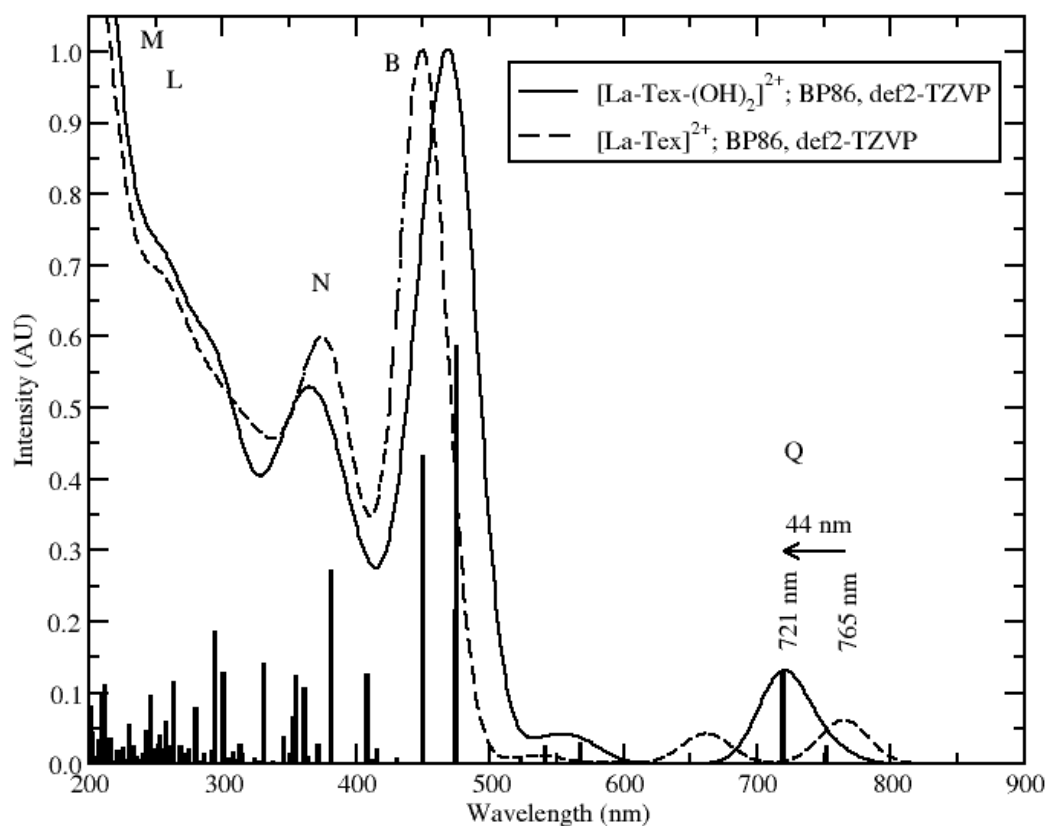


Fig. S7b:
TD-DFT/BP86 UV-Vis absorption spectrum of $[\text{La-Tex}]^{2+}$ with two $-\text{OH}$ groups at both R^4 positions (cf. Figure 1 in the main text).

Substitution with $-\text{OH}$ groups in position 4 causes a red shift of the B-band, but a blue shift of the Q-band. The relative intensity of the Q-band is increased.

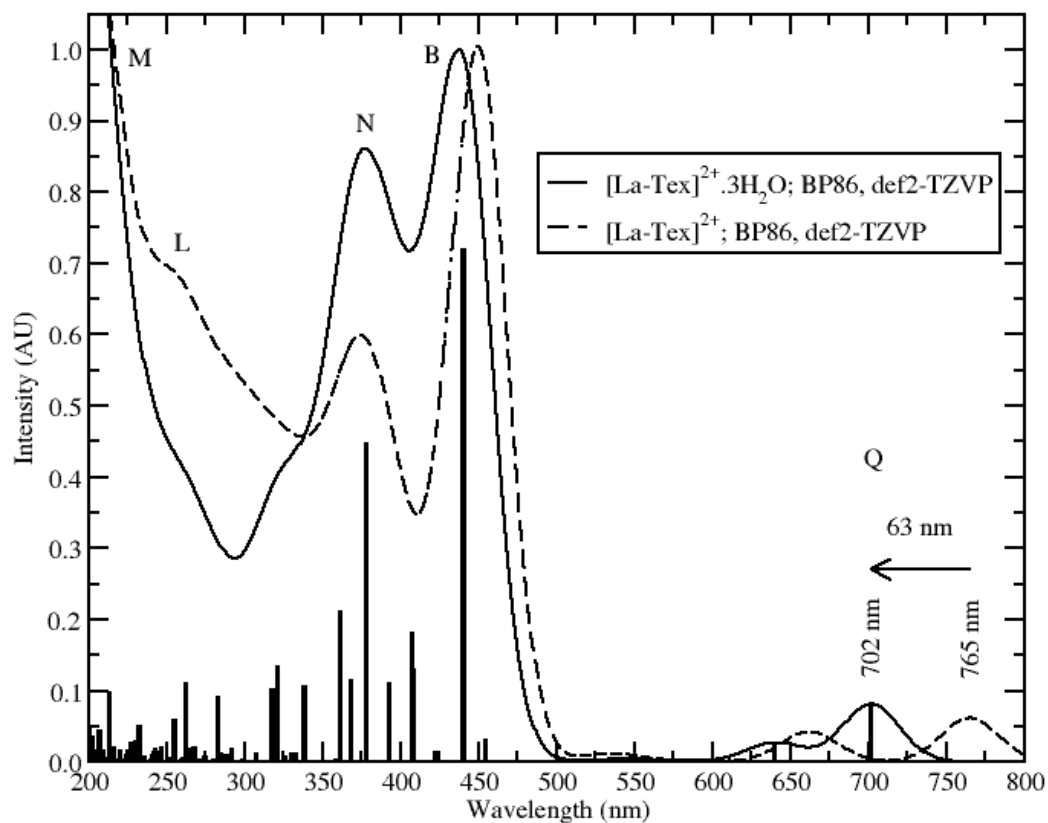


Fig. S7c:

TD-DFT/BP86 UV-Vis absorption spectrum of [La-Tex]²⁺ with three water molecules directly coordinated to the La³⁺ central ion.

The intensity of the N-band relative to the B-band is increased by almost 50% when three water molecules are directly coordinated to the La³⁺ ion. At the same time the Q-band undergoes a large blue shift of 63 nm.

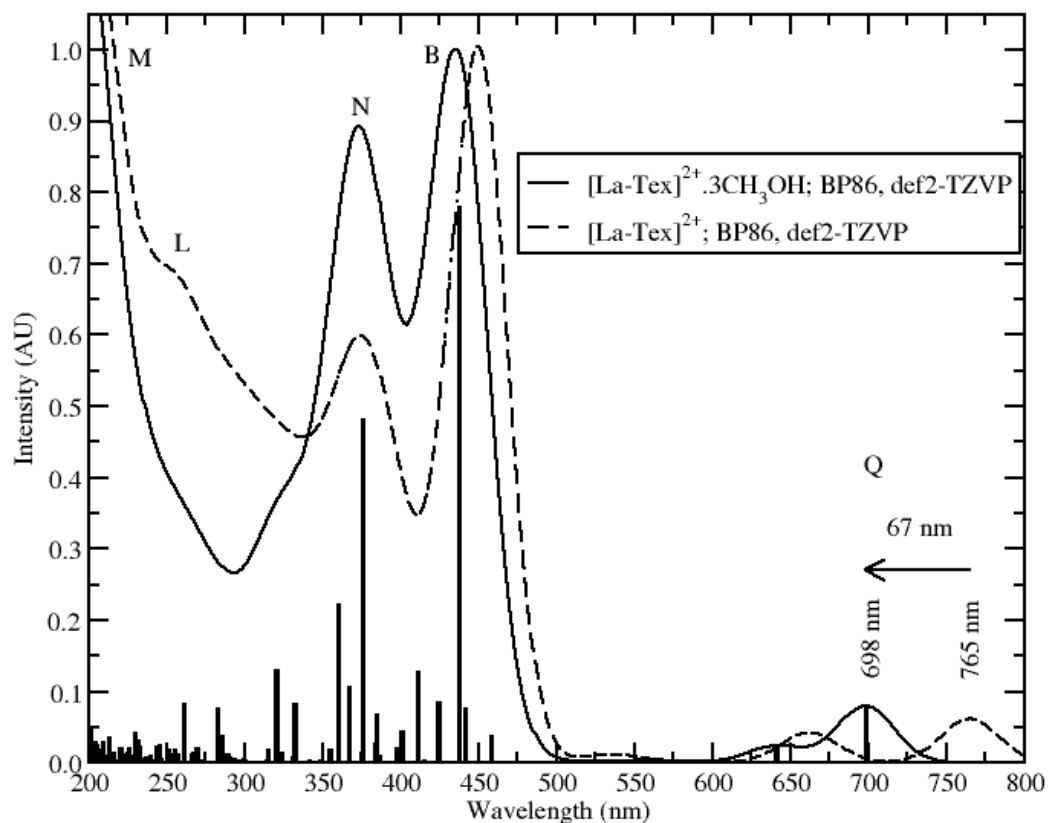


Fig. S7d:
TD-DFT/BP86 UV-Vis absorption spectrum of $[\text{La-Tex}]^{2+}$ with three methanol molecules directly coordinated to the La^{3+} central ion.

The spectrum of $[\text{La-Tex}]^{2+}$ complexed by 3 methanol instead of 3 water molecules is almost unchanged. The change of the solvent leads only to minor shifts of the band maxima, i.e., λ_{max} at 374, 435, 560, 643 and 698 nm for methanol compared to 378, 437, 544, 641 and 702 nm for water.

II. Lanthanide Motexafins [Ln-Motex]²⁺ (Ln=La, Gd, Lu)

II.a Cartesian Coordinates of Optimized Structures of Lanthanide Motexafin Complexes (Ln=La, Gd, Lu)

Program used: TURBOMOLE V6.6

All energies are given in units of Hartree

All cartesian atomic coordinates are given in units of Bohr

Relativistic large-core (4f-in-core) pseudopotentials were used for La, Gd and Lu (ECP46MWB, ECP53MWB and ECP60MWB, respectively)

Solvent effects were calculated with COSMO (epsilon=80 for water) for the gas phase structures

The input coordinates given below are for the optimized structures for basis sets A (cf. text).

[La-Motex.6H_2O]^{2+}:

input coordinates and input keywords

Energy: -3382.373266282

\$symmetry c1

\$dft

functional b-p

gridsize 5

\$coord

2.54475609212951	0.55304364469365	6.72186602932475	c
-0.21394012314231	0.53931407552916	7.06453073630435	c
-0.76881152927241	0.72510150833922	9.58181431051532	n
1.45459442408670	0.93752110301380	10.86726760960915	c
3.58888818761644	0.79812206669242	9.12931069334477	c
-2.07269404028522	0.48664302094050	5.15262531263263	c
-4.72729253019541	0.90033670837917	5.28524777698776	c
-6.09948898701792	1.50007314628846	7.41632126429245	n
-8.52049462058809	2.03747856604427	6.61444810425580	c
-8.73908401516800	1.65426516029039	3.87065155224051	c
-6.35512091074489	0.95334204028520	3.03372873595924	c
-10.53900385520831	2.99870560320964	8.09952259226694	c
-10.67115365402507	3.63390480168806	10.69138287651993	c
-8.73180885626019	3.25509788102879	12.35092768434900	n
-9.45098708873162	4.15493743052742	14.65441323872947	c
-12.01573490993073	5.15560925431887	14.53469782752393	c
-12.80591726774473	4.81755114052736	12.03074700387616	c
-7.70964783971114	4.11318794704349	16.74165836112126	c
-5.41878205287769	3.13402402264688	16.36906594715257	n
-4.76907528637670	0.66573178838769	12.08392205019372	la
-7.87794189287643	-2.98282944075260	11.55294823856438	o
-15.31883118299369	5.58177043927452	10.91382674141338	c

-17.57092175757033	3.81155677182500	11.54896122878880	c
-17.20867448677129	1.06716942620914	10.72880258560028	c
-15.30463287854024	-0.21779500636747	12.20781264523579	o
-13.46214735145951	6.33217640737673	16.67137940900225	c
-5.55967875446717	0.29338000917293	0.38245706950118	c
-5.41153720269177	-2.57620747232313	-0.13069950135513	c
-11.13272217436567	1.87374326638261	2.35176417300950	c
-12.77549247417378	-0.53906840374131	2.46129240758835	c
1.45704908784062	1.39649982634275	13.54295085714688	c
-0.71085974844710	1.64859473038948	14.77042200479571	n
-1.00384486189023	2.23861802633098	17.28635589062151	c
-3.49107828439408	3.09232132987846	18.13171918743338	c
-3.79211835763942	3.87793378041893	20.68267565417200	c
-1.80636258593689	3.72323479788471	22.40953596044528	c
0.62195147845177	2.69741194226376	21.60654809174274	c
0.98315280215311	2.06370626780890	19.07948340575759	c
2.32822395529445	2.46631290733040	23.47591662800688	o
4.67056105951408	1.14761294536357	23.10515821931152	c
4.35955939317915	-1.69164515988689	23.49121838278073	c
2.72447592196918	-2.65856586883056	21.60997709568354	o
1.88770374049290	-5.16767593075591	22.00397491765997	c
-0.45923559900562	-5.64319414677637	20.39293277339833	c
-0.02469081015837	-5.54746449458261	17.71989554555386	o
0.87020743723589	-7.87223387135326	16.67513311162953	c
1.30914125802777	-7.66263690382457	13.84478609941408	c
-1.02999426555946	-7.57664632093050	12.49497609492310	o
-0.73937839212931	-7.90301442610911	9.83373093937643	c
-1.89272721958384	4.32173247793210	24.86863371102237	o
-4.15131757328554	5.19161750254823	26.11608798481619	c
-4.17395648482803	8.04752326201135	26.44685032147895	c
-4.87803890527617	9.24703309898530	24.14887035520461	o
-4.97011039028735	11.94621558003415	24.29663281911310	c
-7.09131937700586	12.90188374309637	22.61182464224543	c
-9.38801584456911	11.97431083421292	23.62287621179757	o
-11.57267821334008	12.61202517382233	22.21780894136831	c
-13.86108301773599	11.39350388197219	23.45030193712217	c
-13.77793718535633	8.72019133579659	23.13207838115746	o
-15.74256646238806	7.43470184006492	24.43839824779436	c
6.33277415807603	0.96007468120990	9.83818625613801	c
3.93431315375701	0.44844976295186	4.24171686739160	c
5.01103417175165	2.99573876770701	3.26958591521880	c
3.07369383775578	5.09885025118145	2.82985361007451	c
1.97971735525826	6.04310725128208	5.12919299797412	o
-3.44127056991707	5.35738250437327	11.37236084954038	o
-12.27097547976967	-3.10572378146471	9.49689499993567	o
-2.80831481258143	6.81047310555784	6.74349998739076	o
-9.09427387489036	6.54258019222331	22.12403081027400	o
-1.34995253511066	0.19810124686866	3.22120784709838	h
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2.77400402204053	1.20975607697143	18.48449339325486	h
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-8.29456428368500	4.96796522314187	18.57568244095806	h
-12.27413850805075	3.38187051453012	7.01557835249791	h
-10.66083636213222	2.30053481686265	0.34875015117325	h
-12.26364716397729	3.51788264822718	3.01872792395342	h
-14.58594878518146	-0.25190741718457	1.43444264378180	h
-11.78321687894067	-2.16261237279757	1.57055996143915	h
-13.20260826655184	-1.08234842989842	4.44714872589678	h
-3.69256576892038	1.16741440495664	-0.04834150467463	h
-6.90633302985718	1.16211891746637	-0.97659829317391	h

-4.82776712057141	-2.94215102600343	-2.11527769262199	h
-4.02433741635688	-3.51939204978081	1.13660142548881	h
-7.27499964498766	-3.49652046281005	0.17353058696925	h
6.93453420709518	2.94214748934927	10.22552543593473	h
6.76493651704793	-0.15144593767590	11.56932560891752	h
7.56973941974261	0.23160398517156	8.30688717854336	h
-4.07803033130861	4.29889368546665	28.01274074698001	h
-5.89247310822475	4.55908528186516	25.12639052549699	h
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-5.55820019324546	8.51588894930410	27.97596748466050	h
-15.15250807901930	5.73642479868174	8.82375880640311	h
-15.80741872581659	7.51485983151772	11.58864314024367	h
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-17.97264626532629	3.85416454870363	13.61523269183510	h
-18.98912457752317	-0.01609892423313	10.98387836178564	h
-14.11903142770482	1.08134230181463	12.84251275527219	h
-12.21733996969181	6.89281527191264	18.26331651168495	h
-14.51650568165070	8.03560980446459	16.03083556147219	h
-14.89317130626144	5.00483335815168	17.46363320676610	h
-5.36075433183101	12.55179316150304	26.27724084506723	h
-3.12557681903030	12.77808123177191	23.70006753996817	h
-7.05523713637225	15.01753056741806	22.57677997290199	h
-6.81180176182468	12.2240691620442	20.62570038974964	h
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-2.65752510280851	-7.83140318313107	8.99162900625383	h
0.45429242617088	-6.38140303516015	8.98932120781202	h
0.12744458970069	-9.77603231819353	9.40621494579480	h
-15.62027145970091	12.17111655075111	22.57474670462188	h
-13.88676812106578	11.88584217393659	25.50460581076048	h
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-15.64730093100870	7.78423173562650	26.51836389365192	h
-17.64261519355516	8.03471630584039	23.74169625185665	h
-7.90998202114896	7.83886498879867	22.79132730580442	h
-10.79484615109069	7.17978739599164	22.63197705775315	h
-9.63366387826199	-3.12929576510944	10.67301074987134	h
-7.75255678250503	-4.29920014837727	12.85228002496808	h
-13.05321991721259	-4.69104425529073	8.94119954610491	h
-13.56204384780646	-2.14419064831509	10.56184727850222	h
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-3.14964932428065	5.95022652985623	9.52862270476476	h
-4.53448159283666	6.62735957627006	12.16100363138565	h
-1.05545140576041	6.55140920780144	6.05140037825877	h
-3.93462913095062	5.78589330300356	5.68444432414161	h
3.27858589692305	6.92815811509548	6.11395558568193	h
3.95240016553395	6.67752688983536	1.74399315730766	h
1.45133266147545	4.40086758132989	1.69175182472130	h
6.00280785258501	2.63653718184463	1.44750190834653	h
6.49338254237895	3.70070227817586	4.59253440083290	h
5.54532778104027	-0.89611522538633	4.41205379896676	h
2.68754531597629	-0.36237656174413	2.75445884145402	h
-3.43314763946028	-3.54099271206551	14.34627030704658	o
-2.81948895526624	-5.05810003059460	13.35860248798200	h
-2.33062555785234	-3.70557671913952	15.87073682666871	h
5.50178304743771	1.59246182490464	21.22650383294776	h
5.95632412634824	1.90424702492871	24.57770408283666	h
6.27496338780731	-2.59378290209656	23.41654117807238	h
3.56591076924904	-2.04237917279736	25.41997863112914	h
1.34094942463721	-5.47202187344771	24.02615509323615	h

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3.42372518880483      -6.55821287786176      21.57073964865556      h
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-1.86535912586097     -4.13954211209191      20.80294385818634      h
2.70725414628958     -8.40956578319136      17.56178017941549      h
-0.51000023205232     -9.42587810957071      17.05661567008453      h
2.38881241026621     -9.37031747644321      13.23835156725551      h
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[Gd-Motex.6H_20]^{2+}:
input coordinates and input keywords
Energy: -3386.706650373 ==> CN(Gd):8

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$symmetry c1
$dft

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functional b-p
gridsize 5
$coord

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-0.82464090587969     0.69604629725285      9.68288259483469      n
1.40408109775921     0.86307487080225      10.97180442342184      c
3.54495837118556     0.57997331818250      9.26679632094503      c
-2.08031033817091     0.29287859661721      5.25821684016866      c
-4.71696085611620     0.76651662767450      5.38382420290984      c
-6.06204348929461     1.49697415306524      7.49321104466486      n
-8.48273088297253     2.00353420776135      6.66224953176184      c
-8.71885887534025     1.48425920189584      3.94456561534318      c
-6.34809971724852     0.71731477654029      3.13758785958706      c
-10.50064114959321    3.02198519009043      8.09692282796922      c
-10.62971663237767    3.69774533988497      10.67200973364612      c
-8.68644330278437     3.34353990019604      12.33206576020324      n
-9.45049676649933     4.21491909155729      14.63115492153339      c
-12.02400259069119    5.18597604804892      14.50432011070760      c
-12.78868906813378    4.85302293700002      11.99412622216381      c
-7.74122409499264     4.14707312097957      16.73056870947919      c
-5.44777888537975     3.18090138117315      16.34850955136843      n
-4.69968822348319     1.08933751879659      12.05047004440944      gd
-7.66561625539699     -2.36881142955653      11.66426969141205      o
-15.29798080206614    5.59029220549597      10.85110033527057      c
-17.54831333151462    3.81836230546446      11.48799106847143      c
-17.15103083428245    1.05770595552589      10.74238635891586      c
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-13.49633727596020    6.32460577510440      16.64424997054376      c
-5.56679738594428     -0.08334600616992      0.52088264547637      c
-5.44378898529810     -2.97510026466479      0.14467957458848      c
-11.11684216537662    1.64558270228841      2.42539296932104      c
-12.77091853954469    -0.75170590508055      2.64553469222087      c
1.39578767487566      1.37474924787754      13.62680568643896      c
-0.78693437636366     1.73778797644146      14.79794145680530      n
-1.07407105700808     2.28737886905164      17.32045432576238      c
-3.56157096638594     3.12012521209313      18.15129985498784      c
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-1.93789898871085     3.65762760671223      22.45729386446895      c
0.50437933010231     2.65622062636209      21.66016009919304      c
0.89734235677257     2.07402754723531      19.12645226493450      c
2.18950424146597     2.39247837117231      23.54402040716583      o
4.57618175585774     1.16077855072684      23.15262609327557      c
4.35296150858990     -1.70332124957074      23.38901031036029      c
2.79881980223722     -2.62231962678254      21.41745562111269      o
1.99606131237982     -5.16207328627271      21.65653008753337      c

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0.03693505471743	-5.25836235864593	17.37675871075658	o
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1.32968611759972	-7.08953639922916	13.34684093805772	c
-1.02619403524821	-6.86847744275125	12.04280857210267	o
-0.78209065640504	-7.01184302301108	9.36018990041686	c
-2.05240429675746	4.20429162776485	24.92638839196283	o
-4.32006564842475	5.06759474975019	26.16256773740779	c
-4.30643069661479	7.91308633500962	26.57250918996357	c
-4.95201236834864	9.18553366392463	24.29662548777218	o
-5.02077635571683	11.88025245359436	24.52186044258002	c
-7.10753083797721	12.90720038853289	22.83598399591244	c
-9.42626993315200	11.97087832016182	23.78533921925198	o
-11.58515696093261	12.65942854913482	22.36450482371314	c
-13.89682061095658	11.42593104823546	23.53686488135602	c
-13.82437368898781	8.76044001489132	23.15519874721765	o
-15.80099074708823	7.45381022788300	24.42145242631043	c
6.28615700541588	0.67718043166579	9.99616576243084	c
3.91134478083902	0.07812782263382	4.39358885516862	c
5.03750702907590	2.57814247919059	3.35438392966621	c
3.14525920317365	4.71323110787875	2.87241007481165	c
2.11137659134535	5.76313600120443	5.15664481441757	o
-3.43578126300145	5.47191883521247	11.28438412475388	o
-12.06269138999320	-2.96699222927158	9.69935337696549	o
-2.62017261925844	6.84442440101708	6.70255178851490	o
-9.15733327160153	6.57171158622942	22.11532088002106	o
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3.23275583640041	1.55317005201334	14.61735912493911	h
2.69251116417471	1.22464794237735	18.54200207642169	h
-5.75677549595408	4.57113982221773	21.31902852965287	h
-8.33890770259457	4.96552683717102	18.57553249172243	h
-12.23408101557910	3.37238183348270	7.00048152425460	h
-10.64786852991284	1.97895041965939	0.40402103347009	h
-12.23816805042432	3.32387560641332	3.01880558193747	h
-14.58670710836896	-0.49701292193215	1.61985502558612	h
-11.79286661848090	-2.41567895554397	1.81562912814992	h
-13.18676071400988	-1.21100376267233	4.65456661511422	h
-3.69495169950799	0.75338556033616	0.03954978671833	h
-6.91200426969478	0.72802176671564	-0.87470540824497	h
-4.88095732792405	-3.43872843582135	-1.82543028284044	h
-4.05217483132858	-3.86861891604042	1.44284315359697	h
-7.31101830232067	-3.86573861868768	0.50748746763304	h
6.96026155324831	2.65411554739229	10.27481703709190	h
6.66038953451136	-0.34718494740855	11.79302466509150	h
7.50740589210293	-0.18418006426722	8.52208061829244	h
-4.29100657838566	4.12055112323411	28.03375815624803	h
-6.05339454806137	4.49000280929272	25.12720172706923	h
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-5.71008263186231	8.36051912681900	28.08994770837291	h
-15.11608083949202	5.72289096985280	8.76110286948354	h
-15.79994171665554	7.52907633488139	11.49963830426176	h
-19.25729528210446	4.53424258258048	10.49274401941186	h
-17.98997094334510	3.90770690044854	13.54472703055980	h
-18.92893936773145	-0.03216691909896	10.98630701835232	h
-14.11977872778680	1.15184209342781	12.93847587361866	h
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-14.60415382763087	7.99350552902639	16.00392925897923	h
-14.88266840226136	4.95667826223416	17.44741204724167	h
-5.43592941371998	12.43135769820868	26.51331778832090	h
-3.15963089182493	12.71131150946509	23.97787113286133	h

-7.05086436623438	15.02256261311075	22.86639788614964	h
-6.80554575049124	12.28634362861054	20.83406864452860	h
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-11.38600232313240	12.05759115478178	20.34472219609054	h
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-2.71017587667506	-6.83386346599646	8.55849729913147	h
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0.03250257019096	-8.87050920813630	8.79058655309390	h
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-13.94350937426805	11.86735609615148	25.60224689353772	h
-15.55093189098378	5.41071319110965	24.02351379662369	h
-15.72230316465939	7.76502212206277	26.50812580616087	h
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-10.85406197878371	7.21333388903116	22.63176995207236	h
-9.42237274414602	-2.67126456257333	10.82905415929540	h
-7.37683773134050	-3.63178387570910	12.99285210745955	h
-12.70286443241352	-4.65070042540208	9.26429565856249	h
-13.42416899784295	-2.05524668287149	10.72053516555340	h
-16.59444538139288	0.92045830334379	8.70932070295360	h
-3.06638213172950	6.05800118821129	9.43865130053163	h
-4.36085196156542	6.83925623227562	12.12150943023009	h
-0.87851811065263	6.45066401977070	6.03476476600373	h
-3.81303308490126	5.92266609678501	5.62149182543316	h
3.44072133615361	6.67506282028646	6.07424807732998	h
4.04442928739516	6.23328792741831	1.72236115808010	h
1.48821493169252	4.01878382090718	1.78345624194179	h
6.01087554143376	2.15291251353024	1.53668128065667	h
6.54248184021670	3.28253411569284	4.65144575436069	h
5.49785049438205	-1.28807111342419	4.61085414951200	h
2.65723268937802	-0.75228776941649	2.92361391619134	h
-3.47242467875869	-3.02069407612142	14.18834916133623	o
-2.77985091192866	-4.44193863452472	13.10571940309950	h
-2.34920542559882	-3.19923544929255	15.69019531950221	h
5.42299277078360	1.72695749474909	21.31334617855874	h
5.81207742610599	1.88155409034619	24.68469713371097	h
6.29977342644262	-2.53575700125524	23.32005309996366	h
3.52379826963198	-2.17850392580838	25.27542963920614	h
1.47328602941284	-5.60394218732623	23.65898766191092	h
3.54320424506994	-6.50196464066446	21.11778584076728	h
-1.17542950551662	-7.46146117173263	20.44220461930007	h
-1.78726089354455	-4.10958652133242	20.57670087789077	h
2.77271749762668	-8.09769514561626	16.98260935437473	h
-0.44995095324327	-9.07855535001749	16.44494018488306	h
2.37193358395099	-8.76506388850330	12.60142541823106	h

\$user-defined bonds
\$end

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[Gd-Motex.6H_20]^{2+}:
input coordinates and input keywords
Energy: -3386.698838421 ==> CN:7
$symmetry c1
$dft
functional b-p
gridsize 5
$coord
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2.13348677114642	0.22466848242489	6.45110898351171	c
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-1.11320028936182	1.16421663943073	9.23026613672966	n
1.07746330370029	0.89943168594897	10.56413915464542	c

3.16440280858370	0.28038772713889	8.87692469263756	c
-2.41894402946805	0.90715113260752	4.81703469177781	c
-5.02171527548236	1.55995036492762	4.94222060965503	c
-6.35888192273661	2.29727031691263	7.05919780885099	n
-8.77590838674437	2.86192299096691	6.24249476589427	c
-9.00354759006781	2.43328805575942	3.50996041508114	c
-6.64921454418465	1.61586725623630	2.69469157322303	c
-10.81669009515662	3.76187976548601	7.73155109087558	c
-10.94042674697947	4.34970404188918	10.33364344659483	c
-8.90547591951628	4.19537069278731	11.91316728431656	n
-9.66893835273340	4.89092296769523	14.27822754860257	c
-12.34288534237053	5.54713440514734	14.26790124077659	c
-13.16705950112182	5.16470806001168	11.77948098889378	c
-7.92946439557718	4.78188575045133	16.35750665346704	c
-5.60079587502548	3.92048174270398	15.91801765117510	n
-4.82322426538569	2.33230182531628	11.50489520235976	gd
-6.17149486086241	-1.62283107650894	12.73270815750799	o
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\$end

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input coordinates and input keywords

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\$symmetry c1

\$dft

functional b-p

gridsize 5

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2.30147431374639	-0.02061380502046	2.40827969777213	h
-2.00869854541470	-4.30810819803318	13.73532391199613	o
-1.89026929467820	-6.08677793224355	13.09683658340258	h
-1.53622819297188	-4.57143448797345	15.54057660206260	h
5.11906375676416	1.07364550276522	20.84413068588693	h
5.72759170593864	1.62836153312561	24.14041138483828	h
5.64590545495995	-2.96650665945345	23.36093357974994	h
3.07089528589764	-2.02274210032039	25.39190769667369	h
0.28588886798316	-5.19831098532715	24.37324823414017	h
2.53048519251331	-6.76706318985674	22.35353393499841	h
-2.21386896270544	-7.58222383110945	21.43976886860104	h
-2.45645681669929	-4.31430093806989	20.51691021997445	h

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1.68283994039111      -9.77431809690897      18.96592281209113      h
-1.55061266514227     -10.28055329187990     17.99007353933748      h
1.86653156847024     -11.51154323569241     14.87924479039921      h
$user-defined bonds
$end

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The input coordinates given below are for the optimized structures for basis sets B (cf. text).

La-Motex^{2+}:

input coordinates and input keywords

Energy: -2927.345224264

\$symmetry c1

\$dft

functional b-p

gridsize 5

\$coord

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-0.91244550955021      0.26214185705453      7.56343363058542      c
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2.37506384182956      -0.18860729512564      4.29633996925854      c
4.23379735324443      -0.13592040117262      6.21100197109045      c
3.57363252696316      0.08129600700722      8.73995796526379      c
0.92256359389187      0.28094380914965      9.43721556153706      c
-1.96140813062471      0.02176797404622      3.02009291649578      n
-4.40961712752685      0.55513588677047      3.26764261463211      c
-5.93819896237545      0.58918760208579      1.08668705364353      c
-4.85418978597928      0.11463862716603      -1.23537100865968      n
-6.77482474714232      0.22784488220360      -2.97316173098298      c
-9.15802566356284      0.79003324806744      -1.71414093001464      c
-8.61260695437000      1.03919714619846      0.84207067235084      c
-6.43162633322790      -0.13067283039059      -5.57308075468462      c
-4.17778617266030      -0.50141378174172      -6.91775046134924      c
-1.76762115624303      -0.69867684912430      -5.90231127745952      n
-0.15750997059101      -0.80751591483623      -7.96978044341365      c
-1.58289810046679      -0.80113585528616      -10.32528468782223      c
-4.09745609148193      -0.60644282035623      -9.66821247894052      c
2.49105156592634      -0.80018315691462      -7.91516941445606      c
4.12506327514564      -0.58400238201848      -5.84307637505006      c
6.87006472948429      -0.40683492869197      -5.92906148844799      c
7.68362162197699      -0.22758641047438      -3.43512683193949      c
5.44070653004949      -0.30238967726449      -1.90265812711348      c
3.30524075116085      -0.50798741867501      -3.38328086958029      n
8.49722085141597      -0.41426207113378      -8.24656814259153      c
9.60397907371055      2.19155505259150      -8.98559824739540      c
7.59207562625959      4.14436142762586      -9.68590503677247      c
8.63261232924593      6.41018045416270      -10.69101726114100      o
-0.64686904294451      -1.70763634380940      -1.37727208831699      la
2.88244621275655      -0.36191854863725      1.74796179737694      n
5.18745522316043      -0.21352533308460      0.74851658077736      c
10.34006942188035     -0.02358532551968      -2.49260688775824      c
-6.33479888065767     -0.45262181436976     -11.39736035625716     c
-7.15235856982797     2.27407379502179     -12.01922160427419     c
-0.47125218444480     -0.91626468733959     -12.92810080329710     c
0.40380638567826      1.66713759478844     -13.95269405280439     c
-10.38702505304517     1.64576594549949     2.95589825657648      c
-11.64315645334334     1.07147717011388     -3.01952760513502      c

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-13.51430109200985	1.95230560268782	-8.13361447473866	o
5.17183210315920	0.11032963762348	10.68506033184215	o
7.86722897134314	-0.07915658907525	10.21990024652044	c
9.19663593265788	-0.26964201868868	12.73890555739421	c
8.76843678567427	-2.70778360051208	13.73945541945915	o
9.94360456815370	-3.05662006002588	16.14982203014255	c
9.40439533901788	-5.74585321657966	17.00719546662121	c
10.60551966729024	-6.06267042834319	19.37856685596491	o
10.30618098321130	-8.54618224010178	20.38001290673170	c
0.50484651137364	0.45021444350051	11.91398052840392	o
-2.06602905648869	0.63288317694778	12.84727867820578	c
-1.99495216072513	0.41530880644267	15.69467259757254	c
-1.44903083956330	-2.13245389453517	16.30567664069762	o
-0.84364949202520	-2.56654969169065	18.90803727241070	c
-3.19042924399159	-2.74522483942607	20.58109271627471	c
-2.34490635769048	-3.35973721719496	23.04667122667085	o
-4.37329459173454	-3.63750395152324	24.80204319169885	c
-8.13947829851656	-0.01948599442086	-6.72291036731252	h
-5.25839682866375	1.01776056569269	5.09601789734680	h
-2.88871659489618	0.40194386756101	8.10579297391701	h
6.21982826223043	-0.30302612889504	5.71393713689472	h
6.88034759944187	0.03204071705907	1.91100427358616	h
3.39665622492847	-0.89358077519765	-9.76220575882104	h
-1.88790708205734	-1.71524217829211	-14.22319009994661	h
1.12756320322550	-2.24947242678519	-12.95367452677828	h
1.18853618800723	1.45803703120926	-15.86159865649443	h
-1.17483097163265	3.00897397511514	-14.05148096916986	h
1.86427820065399	2.51448627614110	-12.74352409306970	h
-7.94550747089029	-1.47727857890640	-10.56994546769086	h
-5.87761833269714	-1.44716968263782	-13.16537659723487	h
-8.77307500624373	2.25687384192163	-13.31296709695533	h
-7.71824167126260	3.30459889241211	-10.30925404564434	h
-5.61431587077414	3.33232925243081	-12.92452476442927	h
-13.18922522155463	0.71246480825579	-1.67620115548069	h
-11.81925120988324	-0.36579161419741	-4.51285668120262	h
-10.29211471457403	4.27307058855577	-5.24652010183197	h
-12.39489662540670	5.13384699963836	-2.80116557715254	h
-14.47253710590821	5.60250687988296	-6.90735851959429	h
-15.96918497490667	3.08287445271779	-5.22777815646897	h
-14.93785447808536	1.79631520086034	-9.28368610497667	h
-12.35630719248294	1.63089327634780	2.31134505385758	h
-10.23071008974973	0.27803340743487	4.51355385838887	h
-10.00981447099454	3.53307041966345	3.74652026156651	h
-3.19785836054934	-0.92543762515167	12.05716126021124	h
-2.86747008325030	2.46425024502061	12.26216929300711	h
-3.85753240844670	1.02677804722264	16.42727742464617	h
-0.54773384737775	1.70766181183301	16.47542748927873	h
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8.25204929494036	-1.78513323652555	9.09029395600475	h
8.49811384022992	1.22237734275633	14.02953613033781	h
11.24000410024596	0.07329891001587	12.42490364561623	h
7.43749268576186	-1.17965581938388	-9.86439381548483	h
10.08275097677170	-1.72894908226392	-7.93894317453026	h
10.87291111743983	1.93217187466103	-10.61206447278313	h
10.77202023543666	2.92283168492892	-7.42257612612248	h
6.35765250278746	4.54184108517676	-8.04171658030725	h
6.37831099957473	3.39169245690822	-11.20026118276335	h
9.65669311961013	7.21946420389797	-9.39568865142791	h

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10.63857669345772	-1.14444994433676	-0.76970904405753	h
0.17317002731123	-4.37500719908986	18.96079960035856	h
0.43530198639282	-1.07894106996803	19.62198008054036	h
-4.24557414690090	-0.93448221302638	20.60126684141773	h
-4.47568764995017	-4.22012083400608	19.83585083867722	h
-3.23660354291680	-4.34132528785591	27.34598132595290	c
-5.45259014595361	-1.85509773021648	24.97063173691622	h
-5.69132506617197	-5.13325938122169	24.17398873108550	h
12.00690752637572	-2.75846624718941	16.01109428041284	h
9.18378637556925	-1.69360596859719	17.53878532675967	h
7.33753571293462	-6.05030534959766	17.15464204076625	h
10.14950596257604	-7.10603397484019	15.60239901762910	h
11.88472485776039	-8.80026527128680	22.74639745942878	c
8.29533963805012	-8.90191675603746	20.84224213845367	h
10.91460492195182	-9.97292443303209	18.97769230473773	h
-5.26850203098167	-4.63299562873676	29.06803281928300	o
-2.14106204660643	-6.11709916442912	27.17671829263085	h
-1.92182867181658	-2.84516501059533	27.98938680215057	h
-4.44851924246716	-5.28213575699859	31.54479863064666	c
-6.14544558492363	-5.46313168550745	32.71763838923363	h
-3.40916797522441	-7.09384041657560	31.54372181683535	h
-3.20875479869643	-3.80209853207630	32.34134310992295	h
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14.47239130370678	-8.97899387976668	22.06104810502218	o
11.56682491440474	-7.15064781193243	23.99523160673132	h
16.09657403270136	-9.17123057372876	24.19354380160568	c
18.03289369945671	-9.30769009749280	23.47257612686633	h
15.92987327849503	-7.49151065321021	25.42358338828686	h
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\$user-defined bonds
\$end

Gd-Motex^{2+}:
input coordinates and input keywords
Energy: -2931.659381771
\$symmetry c1
\$dft
functional b-p
gridsize 5

\$coord			
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2.39168436747091	0.05601466529124	4.28346278939459	c
4.25360732078152	0.07843136658754	6.19477459550661	c
3.59506874812091	0.25171908432603	8.72756585180628	c
0.94366035292248	0.43405447063559	9.42966330956648	c
-1.93678889688065	0.25691072597761	3.00722524008545	n
-4.41046790686260	0.65923525013415	3.29306724656097	c
-5.94968751258246	0.68861487388593	1.12592503521915	c
-4.84583822765659	0.32797332774415	-1.20856128703600	n
-6.78106111157624	0.36993345586182	-2.93437665897790	c
-9.18283955032673	0.77906514599792	-1.66379667506803	c
-8.64409616780086	0.99655902541828	0.89875706612189	c
-6.42293204638629	0.03469581388948	-5.53229183672807	c
-4.15649702224817	-0.30429817926016	-6.85672365651204	c
-1.73804242232692	-0.44770396558962	-5.83360568633023	n
-0.13949051852649	-0.62531242978476	-7.91484187405645	c

-1.573210011111107	-0.69309421378919	-10.26067555151174	c
-4.08444659246689	-0.48508440580040	-9.59982673777941	c
2.50579189271219	-0.65695658237074	-7.88927536361338	c
4.15255082235886	-0.44873634576154	-5.82970104856741	c
6.89715969654966	-0.41083145301755	-5.91544967845891	c
7.71685261778284	-0.22984916865298	-3.42101313588101	c
5.47141264664991	-0.16606186835458	-1.89508445201554	c
3.32779691103287	-0.28423562800021	-3.37475394026118	n
8.52286199045230	-0.56534631408840	-8.22854362432484	c
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7.87546527375075	3.98920745960164	-9.81114209635793	c
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-6.33017762993857	-0.39328533066291	-11.32153669299555	c
-7.18899866960446	2.31269291594435	-11.97895756802363	c
-0.47438131955953	-0.90083055100269	-12.86307406870835	c
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-12.21630780340639	3.55529332348813	-4.16105263151608	c
-14.37083170546362	3.43931562453523	-6.06244716502823	c
-13.58995100028520	1.77918184519009	-8.06232801902267	o
5.19512857278109	0.25531138266183	10.67080001886115	o
7.88958028637497	0.05683166489308	10.20180090068137	c
9.21951060206577	-0.16820290740336	12.71772464374770	c
8.75958504091247	-2.60676599260945	13.70234167061920	o
9.91477229204580	-2.98244119543248	16.11839710096659	c
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-2.04815779575595	0.71296494868912	12.84136804641252	c
-1.97941353860690	0.45237581178241	15.68505698351434	c
-1.41331085491340	-2.09981607745675	16.25727857673310	o
-0.79889247882390	-2.56724613181437	18.85137464111015	c
-3.13901765666875	-2.78132068757447	20.52972834271943	c
-2.27857742310883	-3.42107754590470	22.98361850219501	o
-4.29517292014461	-3.74285217468662	24.74520429675159	c
-8.12791908742122	0.08960295313416	-6.68960667276055	h
-5.26623561973267	0.99274656673032	5.14440021643123	h
-2.86675990319682	0.57653117617435	8.10632970075577	h
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6.90079769885977	0.07653646139151	1.92737544892849	h
3.39292227941574	-0.81681461323808	-9.74031942476515	h
-1.89944811781730	-1.74132505233097	-14.12163298379151	h
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-1.17504745173296	2.98210842137683	-14.12789366529985	h
1.86841996384348	2.53102831406351	-12.81176191067057	h
-7.92182889923585	-1.42888430358817	-10.47121522805111	h
-5.86634382121119	-1.40709037620558	-13.07631381949775	h
-8.81970147881051	2.25368993304568	-13.25879745334146	h
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-5.67247193055769	3.37636051410346	-12.91382241734784	h
-13.20401923158137	0.48078939365105	-1.61571746806548	h
-11.78555478004994	-0.48394651293337	-4.46936291131036	h
-10.51306474041924	4.24397865574392	-5.13941349924426	h

-12.66607375013695	4.95183584825400	-2.68799697319191	h
-14.75727138742584	5.35410210990229	-6.79520424102379	h
-16.11319975968475	2.73351510401466	-5.15119807164546	h
-14.99986850980299	1.55323734121368	-9.21766368886807	h
-12.41088598607161	1.38239150297090	2.37472766863922	h
-10.24298336437687	0.00843929429626	4.52219767506776	h
-10.13995574546610	3.30142704413188	3.90740313509359	h
-3.16525093385516	-0.84279398976970	12.02553012640690	h
-2.86430710858966	2.54602472323215	12.28262349110792	h
-3.84841665942076	1.03652696668807	16.42351595386042	h
-0.54457896732073	1.74486383228497	16.48815566295731	h
8.52455842122205	1.76067132729781	9.18571876604619	h
8.26242155731396	-1.63918142156113	9.05321234601079	h
8.54284945942345	1.32407636495168	14.01967590725639	h
11.26653636524260	0.15030893910571	12.40119491135865	h
7.42228745639178	-1.30920394293548	-9.82924702775765	h
10.03114131775378	-1.95960995079981	-7.88539876309023	h
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10.96430776744134	2.66953344215630	-7.47577334447863	h
6.65296610946476	4.50712777742030	-8.19132008980622	h
6.63342332811752	3.25315216589960	-11.31070538412085	h
10.10439404509407	6.95489718794155	-9.60630848122526	h
11.69228768678882	-0.94840071555565	-3.86648130229953	h
10.99498412488133	1.80149565374974	-2.09641268412700	h
10.60568675661643	-1.22167667140233	-0.71090885261635	h
0.22677442915933	-4.37126815242442	18.87603620469912	h
0.47495710595436	-1.08347045580237	19.58233443131473	h
-4.20518362732247	-0.97755232539565	20.57722827053087	h
-4.41781498365793	-4.25481708636302	19.77087576820002	h
-3.13095449727736	-4.44530869812107	27.27714988754306	c
-5.40124800438126	-1.97875126253824	24.93134001098226	h
-5.59259551803921	-5.25448132545397	24.11231406649713	h
11.98493401591123	-2.73096411355476	15.99077712610711	h
9.17837687353807	-1.60292866096883	17.50372044555543	h
7.23532161309837	-5.91460768644822	17.11079082139289	h
10.02765873909117	-7.03571048967505	15.56920281915585	h
11.66936440078747	-8.77775040265413	22.72797490602207	c
8.09324275105195	-8.77650489231850	20.79836285683974	h
10.69297288870824	-9.92363488627884	18.95203854769888	h
-5.14249337332446	-4.78080870178379	29.01472676984399	o
-2.00831972897994	-6.20208266060709	27.08787018371322	h
-1.83502554193267	-2.93222473942250	27.91921598457983	h
-4.28724900682020	-5.41719848407961	31.48311515169801	c
-5.96881252020035	-5.63518393646624	32.67161044945607	h
-3.21038905648126	-7.20681756441379	31.46959198622051	h
-3.07088664308244	-3.91300001802384	32.27040421503876	h
11.01206347018528	-10.47194012176227	23.77046259077856	h
14.25574771070823	-9.03761212657752	22.06401941787763	o
11.39224094762630	-7.11728330041693	23.97219114507884	h
15.85416759747671	-9.29861662827506	24.20896840328819	c
17.79067986709098	-9.49658062325161	23.50296086423547	h
15.73464370352934	-7.62239949021686	25.44922388837963	h
15.34968616975835	-10.98970428315289	25.32772639231217	h

\$user-defined bonds

\$end

Lu-Motex^{2+}:

input coordinates and input keywords

Energy: -2935.745519236

\$symmetry c1

\$dft

functional b-p

gridsize 5

\$coord

2.39476652392991	0.31423426238442	4.24769661341074	c
-0.23848366015384	0.61996044229819	4.95400325436018	c
-0.48770098590589	0.73631872854108	7.53478264962036	n
1.93191436461343	0.50709042214425	8.48213566345481	c
3.76093083583007	0.23494448147628	6.49008420045259	c
-2.28366997948067	0.79044834078336	3.29780343786996	c
-4.83589255826906	1.10923186780261	3.89400254619078	c
-5.88585518843541	1.37530145797749	6.29737773694296	n
-8.46076246065595	1.71195083982016	5.84068048636624	c
-9.02301815504083	1.63723747820222	3.15229367813528	c
-6.75666477001452	1.25092231443456	1.93460755352592	c
-10.35867002947978	2.10662533464382	7.63078948386988	c
-10.13794477141523	2.21124230215935	10.25763995442881	c
-7.86542385927551	1.93488900197033	11.48504147266218	n
-8.40331791330586	2.19650596118846	14.02416611978790	c
-11.04621615509101	2.64063962335081	14.43848556289461	c
-12.16190742770898	2.64179357228978	12.05518120199493	c
-6.41379265295287	2.02511119821341	15.76609359251528	c
-4.09173706280360	1.60548247351689	14.87839646256430	n
-3.76874167333545	1.28248235410213	10.28256480111835	lu
-14.90249195193925	3.03965190278091	11.46494316785941	c
-16.63842720982930	0.76630080599203	12.07877226074241	c
-16.04223277164875	-1.59472404285287	10.52223972783721	c
-17.86348664703936	-3.54649624182405	10.83254334960392	o
-12.30366769597859	3.03126262511861	16.93657191769757	c
-6.30792142311914	0.96670998182711	-0.84562650069382	c
-6.20173675770026	-1.81218719545617	-1.71673720970076	c
-11.59193446573165	1.90074954171026	1.99059005851822	c
-13.12830861659351	-0.57514074983628	1.96919192186329	c
2.27268076046858	0.58972779826442	11.10726969383543	c
0.23236765374816	0.89333047797687	12.55970022802879	n
0.35932298121809	1.01331351256733	15.15678663116680	c
-2.00821673265776	1.40129601212129	16.42679928189646	c
-2.05899103052512	1.55377743019097	19.09030725230029	c
0.14686436785178	1.36029540153441	20.49487998688886	c
2.54661339045689	0.97957475240124	19.208274993926197	c
2.59886365530846	0.79964561367334	16.59292671446032	c
4.53906756014222	0.83321102216431	20.73855574294358	o
7.04291021639799	0.49124239421716	19.67593155556504	c
8.94862659226409	0.78791123540684	21.78271276134140	c
9.05339063299001	3.38187799443206	22.43114622085824	o
10.38752170721139	3.91859164256249	24.72407199089514	c
13.25171008208549	3.96088751035795	24.36218750595840	c
14.32179878229876	4.66235458632472	26.71453179516025	o
17.01204131284232	4.82695104602828	26.62548331907031	c
17.92404090610593	5.61177063248028	29.23518208254546	c
20.59587513661963	5.77962810014712	29.12453304411835	o
21.69104135016790	6.48800543343691	31.47544768337603	c
0.31367099940119	1.48776428417667	23.00309980174191	o
-1.95887198751663	1.87742800717343	24.48677858286429	c
-1.19762807533617	2.20515898707647	27.21848670050404	c
-0.08687775668550	4.61571651304606	27.50499001788059	o
0.74285792416511	5.07710444174485	30.03721143763191	c
1.84375120920347	7.73007684322360	30.12970973625957	c

2.66449534092851	8.14391940242676	32.64402915006577	o
3.66759441351606	10.61558237094989	33.02567402483054	c
4.21350910596104	10.98492332260732	35.80475067782736	c
1.89631374910742	11.30174940022343	37.11929480103257	o
2.23877945576820	11.59344581770787	39.76901157215809	c
6.54803639287910	-0.06538969968788	6.83332101999634	c
3.33365507899179	0.12179747620164	1.59465597754966	c
2.97286356174016	-2.52966674147837	0.40699500381468	c
3.09301936578775	-2.44027147296552	-2.46496860413664	c
1.01343699600617	-0.91060868327239	-3.30699430134386	o
-1.84140073030395	0.66355414798109	1.28883913875176	h
4.17325887096295	0.41917735529063	11.89589446248113	h
4.40223773797002	0.49315117942336	15.66093748811724	h
-3.83707298472878	1.82838881507713	20.07899712284928	h
-6.80152809578709	2.24278889968364	17.78245528719189	h
-12.25032568042765	2.36922903310797	6.86377040323669	h
-11.37457795304126	2.58217942449050	0.03909266995650	h
-12.67037673519755	3.38004795615997	2.98138197234436	h
-14.97607917401135	-0.26867749347893	1.07720925041550	h
-12.14267031142579	-2.05905155367993	0.90597247489237	h
-13.45169664246278	-1.29375508227652	3.89066864907566	h
-4.54250136038804	1.92301431854278	-1.39005934055848	h
-7.82611428438806	1.94784229554149	-1.87193271847915	h
-5.90072002874286	-1.90967978990074	-3.76631779130877	h
-4.64735160179482	-2.83519705735620	-0.79773302520624	h
-7.97020348611425	-2.80457228260924	-1.27611764257649	h
5.34348532775938	0.64626624629937	1.51497499410369	h
2.32083381901338	1.49215011404120	0.40148048147178	h
1.12295732826238	-3.30855637433292	0.95817400774894	h
4.41304392718925	-3.84655267852521	1.12347200988186	h
2.94708138435046	-4.37496922287696	-3.23113477188887	h
4.91121920314719	-1.63012449169920	-3.09839057578357	h
1.15333624364970	-0.68499044657399	-5.12455855895564	h
7.53683042073783	-0.03392314845235	5.01306564405726	h
7.34763657162730	1.45412453638090	8.00539645397158	h
7.00887580300525	-1.87123621860111	7.75804038740775	h
7.37529909178646	1.94357825270099	18.22166365141900	h
7.16310796841566	-1.40746571971261	18.82796456071834	h
10.78605856451842	0.06764820961561	21.08625332939719	h
8.38674780272246	-0.38029108532245	23.42397664121539	h
-3.20064273421889	0.21991038272458	24.26501597246790	h
-2.92976537527206	3.59176060893754	23.81310475795403	h
0.12282859368608	0.68084584001344	27.77799738732468	h
-2.91785032749561	2.01587864933898	28.40030471446919	h
-15.13882608199586	3.54694393781247	9.46179602384087	h
-15.57992340543777	4.68526206165799	12.54689709357537	h
-18.60810076887301	1.32277852850822	11.71325845736557	h
-16.50890100462324	0.31584326763484	14.10935349067234	h
-14.11200164251792	-2.28373212256804	10.95637801553015	h
-16.09018470261383	-1.13221939028077	8.49327057379034	h
-17.86721440497574	-4.08342797663402	12.59134313208035	h
-14.07378480357714	4.09157534599649	16.72414043180143	h
-12.78119871053279	1.21837615651517	17.84128600958026	h
-11.09644342098133	4.08323776177302	18.25799811132620	h
9.74605136720322	5.79732014110424	25.32888773693320	h
9.87388180958390	2.54490288584634	26.21001386825630	h
13.96754803199604	2.08344395885161	23.76590850070945	h
13.75330704596812	5.33571861820148	22.86538527420311	h
17.84716721314520	2.98309180383581	26.10271331305221	h
17.61783088856949	6.23600936954141	25.20538123137034	h

-0.85606981325814	4.92557231838744	31.37353056422422	h
2.19113044205979	3.67998158651974	30.59848047578772	h
3.43176506910105	7.89339609797779	28.77415838287282	h
0.38866417238213	9.12840469957319	29.57699964031440	h
5.4355530492817	10.85641948952631	31.93023195784243	h
2.30067396605591	12.06110699097398	32.38227940914972	h
17.08241663587502	7.45309990204146	29.76756540361925	h
17.32322482502765	4.20447460122913	30.66351326404448	h
23.74069346390446	6.56558840442984	31.19162146219765	h
21.00402976094711	8.36156017476291	32.09223356475926	h
21.24843187947264	5.09184844057145	32.96444355254117	h
5.42802270234356	12.67404871578591	36.05114471645065	h
5.26136600168311	9.33294967356474	36.54956346159894	h
0.35751292168456	11.82750836303821	40.60208169230025	h
3.16309127893975	9.91490143241140	40.59998559505600	h
3.40110533405452	13.27470738005977	40.20260537845233	h

\$user-defined bonds
\$end

[La-Motex.6Water]^{2+}:

\$symmetry c1

\$dft

functional b-p

gridsize 5

\$coord

2.47393672546720	0.60730507862878	6.73936159021950	c
-0.27601130156025	0.57501476477311	7.04573860900477	c
-0.86776052162276	0.78695801020233	9.54707670813283	n
1.34084538215894	1.02317607517809	10.84761100080182	c
3.48085995795877	0.88520018207271	9.14046022982314	c
-2.10180052147696	0.47623405541630	5.12761424148717	c
-4.74636617914885	0.83406264771291	5.23448730665460	c
-6.15620171778471	1.37689596886916	7.34975628801232	n
-8.56501873766712	1.89271474559685	6.50556810146104	c
-8.72237826396981	1.55144450357933	3.76492051688344	c
-6.33275431747074	0.88765614765138	2.97044121095189	c
-10.61083254212601	2.80441651881337	7.95258984148650	c
-10.77029397588550	3.45856059577940	10.52177039189104	c
-8.82608919282417	3.15574694799551	12.18505368273887	n
-9.56741121060944	4.11948845245670	14.45276086187931	c
-12.13065060691914	5.08104423517814	14.29067542649668	c
-12.91284735919456	4.64344868152549	11.81818280796140	c
-7.85539278969665	4.13633626406924	16.54049921411374	c
-5.57107137447375	3.14619719880393	16.21210718024879	n
-4.86751757894362	0.62681887739719	11.99107366209233	la
-7.96493938268937	-3.07581434468630	12.14703989122475	o
-15.42524937829746	5.31765358004697	10.67051871897626	c
-17.68166556319166	3.64180232765788	11.49091136336053	c
-17.35322457835523	0.82996914176442	10.96779054014480	c
-15.57395207701944	-0.35440372689566	12.68923137147998	o
-13.58711994469928	6.31648203399454	16.37380875812383	c
-5.47950070311676	0.30046389914489	0.33211392071871	c
-5.27159559159995	-2.55093022809906	-0.22367103476449	c
-11.05463594640261	1.85631161387560	2.18413867614030	c
-12.77825310096482	-0.49165430241915	2.18760907083145	c
1.30486445036528	1.48880748995727	13.50118568891004	c
-0.88687405139446	1.71582488069629	14.67969200171735	n
-1.20195853696686	2.27227081303536	17.19500725436093	c
-3.69026097803609	3.08486546240524	18.01589106714929	c
-4.03793008573860	3.79463084302456	20.56867770095284	c

-2.08739283912996	3.60724898887365	22.30870559086062	c
0.35627484534071	2.64688370812041	21.51185386201887	c
0.75381037226677	2.07321561570321	18.99611348639299	c
2.04043380007368	2.37271834029476	23.40010412320894	o
4.43957461408917	1.14347407348359	22.96650592190833	c
4.25971618683480	-1.69691193101441	23.32807648312395	c
2.68572533384654	-2.73139135970953	21.40722041596414	o
2.06678689297253	-5.32616943780387	21.77340587652419	c
-0.23175600082720	-5.96616348304110	20.17378952451791	c
0.21867858499892	-5.87170948257948	17.49039652167335	o
1.17601396193320	-8.21200226411046	16.49984841712683	c
1.76393997585175	-7.99767100857385	13.70985118125419	c
-0.51607718794225	-7.87631721702356	12.23690553505065	o
-0.04692572499735	-8.27330415691879	9.59534995703764	c
-2.20053842537588	4.14319638509913	24.78342293207386	o
-4.51460666884183	4.91890046737329	26.02715014490360	c
-4.45831007773409	7.70271861818263	26.68658155663841	c
-5.00305616249043	9.18553462743077	24.49791620257619	o
-4.91919917330205	11.86487074533854	24.97982008284866	c
-6.87902642672375	13.17849305428639	23.36448964830604	c
-9.30123267187137	12.41124853883243	24.24260282142437	o
-11.34766905777719	13.38192960487681	22.78618035195369	c
-13.78196264973407	12.25003838918269	23.76470559584382	c
-13.90663217903650	9.62380384002210	23.11572765112318	o
-16.04128329202684	8.40564323743214	24.23678470506515	c
6.20744103128893	1.06631176058620	9.86964353673074	c
3.89022940997169	0.42825200902461	4.28979542863199	c
5.06678262891946	2.90843702184965	3.28067915103368	c
3.21138058702035	5.03920947572600	2.69834555277014	c
2.24282440712398	6.26680366286475	4.94106167706366	o
-3.60505416514603	5.38945473013238	11.19988874171809	o
-12.62589586780710	-4.07184946328782	10.86514303844882	o
-2.46113875626088	7.49755469235128	6.76520799143954	o
-9.31326902824579	6.98388933900635	21.96005488262105	o
-1.36479513714849	0.20239992703905	3.22085756476063	h
3.11191068766122	1.77600459135720	14.47692117821551	h
2.54560057196314	1.26066653298110	18.41295531462425	h
-5.88466485679729	4.47932067705119	21.16811295060160	h
-8.44858006749935	5.02760151887233	18.32282038197975	h
-12.32268992477813	3.15107480786061	6.85622656008377	h
-10.50084757103071	2.28884641047992	0.22733925618479	h
-12.14075969728570	3.51000412208730	2.83309985372682	h
-14.46564142195050	-0.15772667841223	1.02573960161005	h
-11.78739138455381	-2.14418085407828	1.41617936096446	h
-13.39682124715474	-0.97854830258727	4.10953686549963	h
-3.63957996352118	1.20458635359961	-0.03880391373475	h
-6.80512900873837	1.15992479471279	-1.01894840457877	h
-4.65605741624462	-2.86996558744244	-2.18017579959303	h
-3.90546433057488	-3.47415088937516	1.03996944454647	h
-7.10159224339495	-3.49542828379923	0.03436370349519	h
6.78401051493223	3.03628199684195	10.21998942590738	h
6.61783841654361	-0.00257809754182	11.60337428757100	h
7.43995403402730	0.32346111054699	8.37479607216100	h
-4.55283246574164	3.81752198804596	27.78707270121606	h
-6.19432939563168	4.44390986262657	24.90445640226784	h
-2.58704814027936	8.19791152276661	27.46891409636754	h
-5.89407014010743	8.05090037326765	28.16664626815397	h
-15.28209889431040	5.26577135433276	8.59636679981873	h
-15.88457482499823	7.29063747349997	11.15578200152332	h
-19.37455679637304	4.29825475751016	10.47466153929765	h

-18.07854756735500	3.90251687859603	13.51726037547662	h
-19.14896753232474	-0.17468166463857	11.23920009759412	h
-14.29720178215495	0.92106840436301	13.09982557157697	h
-12.33636363134607	7.25479373589817	17.73702118798834	h
-14.91144307375950	7.73054471223888	15.62561812558506	h
-14.71358678801935	4.93002534841725	17.44304854413600	h
-5.33818608852852	12.23547642860273	26.98770183302469	h
-3.01493687940673	12.59955117118476	24.55147526201386	h
-6.63146512443853	15.24945609303872	23.53503998437647	h
-6.62847133148644	12.66576754698093	21.35018799591264	h
-11.45274884488169	15.46419754409552	22.95550364246423	h
-11.09481143152900	12.91141856916426	20.76302597256551	h
2.95527217244719	-6.32350745835436	13.33267967340420	h
-1.88162904667799	-8.20170842549543	8.63702578758870	h
1.20794526653084	-6.80061817101325	8.81911025826925	h
0.81400446414461	-10.14313170347939	9.28418017518309	h
-15.40642550873814	13.26309193081776	22.92636259326020	h
-13.87444930343060	12.47504631197006	25.83948578362133	h
-15.98557558532418	6.41672237614973	23.65982690022838	h
-15.96523202925671	8.52024688326906	26.31758442081333	h
-17.82363113952229	9.26516296476346	23.57810778739494	h
-8.04734769523762	8.04811874137185	22.81061465078785	h
-10.92962292337432	7.76882180305429	22.45625740565587	h
-9.77086704432166	-3.53993423534017	11.67173968668696	h
-7.24375746070304	-4.45059815616419	13.13504939532145	h
-13.36723324974626	-5.73571759863700	11.08557383573483	h
-13.86504554482850	-2.82282003889900	11.56919689138751	h
-16.73209154270774	0.51101446279831	9.00005657517514	h
-3.19570187590118	6.07493245684228	9.47488788301903	h
-4.61384719653920	6.68560118628856	12.01647154773756	h
-0.82783353498586	7.03497023022058	5.96969151696639	h
-3.69689149881086	7.54488783316876	5.41098196637036	h
3.54598138955638	7.37778708529911	5.60783134211113	h
4.10832617860631	6.45418021752276	1.46218677925178	h
1.53826339301420	4.31836017173595	1.69783909309867	h
6.08562685617665	2.45616946051054	1.52128540140191	h
6.50714688890118	3.61324749265122	4.60994191424524	h
5.43453436755123	-0.95343241561964	4.50620338911239	h
2.64806011159073	-0.35648414928579	2.81604114846201	h
-3.10728733563522	-3.78273944951902	13.93424887627940	o
-2.37249548500537	-5.21301421176103	12.94643248060037	h
-2.13468981943545	-3.99624912517331	15.51376577873072	h
5.20364223777965	1.63886237294944	21.09883625682963	h
5.70032386244529	1.93340858516931	24.41212970892440	h
6.19431435114335	-2.49476613357951	23.24963757834298	h
3.46965067238582	-2.11237774004359	25.21840434879740	h
1.57335223427927	-5.68522365473758	23.77492628792964	h
3.69908057611330	-6.54798686237297	21.30571720758564	h
-0.94779792332006	-7.85148806451567	20.70898453856712	h
-1.72276599892743	-4.57133727841923	20.55726062766819	h
2.94441434837999	-8.73101337107983	17.47875464471254	h
-0.21551139565894	-9.73684016585423	16.81744559183195	h
2.83847416202589	-9.69760272160956	13.15262335525468	h

\$user-defined bonds

\$end

[Gd-Motex.6Water]^{2+}:

\$symmetry c1

\$dft

functional b-p

gridsize 5
Energy: -3390.668419356
\$coord

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-0.49200597457116	1.63426859251653	6.50852020013938	c
-1.02442464390832	1.86784897484252	9.01825230958304	n
1.20754127282115	1.79633726073281	10.29847648976210	c
3.30019388021228	1.48654309843335	8.55846100317915	c
-2.37231174226733	1.59427861055953	4.64216230590869	c
-5.02005735216768	1.85383856074490	4.85317613892331	c
-6.38207152945697	2.29956797977552	7.02755612569440	n
-8.87343057079353	2.51651605727544	6.28749264374136	c
-9.10749795374483	2.15044226899455	3.55980977515696	c
-6.69781371877801	1.74218801551783	2.66288016464313	c
-10.96570616992638	3.06215867597135	7.84375140582953	c
-11.08723959973685	3.60799968891773	10.43951202606553	c
-9.00184509609129	3.74005026604689	11.94713806066595	n
-9.77511907898927	4.37502195400796	14.32202865130134	c
-12.49757934865982	4.67763098675066	14.38155188231154	c
-13.34014312634195	4.14383371571323	11.94585849850374	c
-7.98455090975965	4.49897863915964	16.33515085409718	c
-5.60186554914437	3.86734342705127	15.83918546595820	n
-4.77113494620902	2.39567994843522	11.40580611070570	gd
-5.47119106364365	-1.77390760062690	12.66352176062084	o
-16.02800859918983	3.98492095034724	11.04779571366428	c
-17.43499195351583	1.54315756520704	11.86482877547401	c
-16.07371811357165	-0.92383484985916	11.24950880848697	c
-14.01425382204821	-1.44569672506539	12.98422209887786	o
-14.05169824587531	5.37900252893343	16.63649417799009	c
-5.89957477618737	1.22936162762968	-0.00783272947548	c
-5.41113546814648	-1.58762846640568	-0.56539698613904	c
-11.52538470989389	2.19640712351225	2.08267612019217	c
-12.97050334756097	-0.33184289480810	2.12644234151539	c
1.21035301568107	2.07271801696606	12.97475295396646	c
-0.96067950670545	2.48270955835979	14.15864260004211	n
-1.25937125350763	2.79984138256488	16.71713555543695	c
-3.71067988156266	3.64128099259571	17.61366400215552	c
-4.04005422105949	4.11776432844891	20.22272044703309	c
-2.10679313969926	3.68365863065960	21.93362499214265	c
0.29490929790577	2.68548826327227	21.05160229183361	c
0.66667545512016	2.30694694151041	18.49454542406454	c
1.97175294955213	2.22926388183371	22.90207063031708	o
4.23938059865179	0.78027190843472	22.43983526081652	c
3.87415994391078	-1.94534115960220	23.23819774159894	c
2.03350139441785	-3.12535674012905	21.67362863502958	o
1.43266566269550	-5.60114715364924	22.56509236375424	c
-0.77583449009708	-6.71088537874133	21.12634294542788	c
-0.05689394774441	-7.39017917339098	18.59735520378801	o
-1.29522245441550	-9.63438798407540	17.70512450961018	c
0.01445337134739	-10.65200568315085	15.37497725924397	c
-0.62771236238384	-9.19529462044405	13.18251322690254	o
0.60163240101615	-10.11117238735736	10.95323811024366	c
-2.19621279196966	4.00927759838405	24.44446795588540	o
-4.48169051761426	4.74609356072615	25.76230716206621	c
-4.36401541813527	7.47512203453022	26.61231268500557	c
-4.92625098404003	9.10887625431329	24.54105328359523	o
-4.77446473487516	11.74125499239453	25.20469853720435	c
-6.45106713544040	13.24392887316565	23.44491771165938	c
-9.00199816412838	12.61606287780582	24.01609918760820	o
-10.79369545027786	13.71002345810112	22.33100682556062	c

-13.41073043937282	12.85270203056765	23.09171031146852	c
-13.72867824429156	10.22166278051010	22.53656883510585	o
-16.05922645642675	9.26195406030181	23.50854848221456	c
6.03268433569096	1.31209166780824	9.26241034958053	c
3.59458291305739	1.20769265969554	3.68234088463012	c
4.85318104545752	3.65971442330979	2.70009750830951	c
3.09998950329345	5.91838381003343	2.31509327029315	c
2.39994041739421	7.14584808669931	4.66031813981468	o
-3.75186687754942	6.84835392143552	10.76314679728283	o
-9.79085504439662	-4.18080008699884	11.81224416530224	o
-1.97186803394622	8.95504601480062	6.67793596923094	o
-9.31632255341883	7.11740594003227	21.94510636284905	o
-1.70252665393239	1.32219003688505	2.71141743378134	h
3.02169844202689	2.00927984447103	13.97821213909106	h
2.43748087057093	1.50619061439943	17.83286715255938	h
-5.85224982506256	4.83748521591064	20.88363234807406	h
-8.62480307633954	5.07114229944691	18.22658238146340	h
-12.76955746735538	3.11125075072847	6.84766920308939	h
-11.10647039780242	2.70166204530361	0.10972747948499	h
-12.76112387680148	3.71316937420600	2.79502647671206	h
-14.71520506577709	-0.19316079240423	1.01085913099533	h
-11.82005077073453	-1.86321691410654	1.32766096778163	h
-13.48142966860139	-0.88393627325776	4.06269379848039	h
-4.18537737492468	2.32475557352330	-0.45796544109553	h
-7.36599669466279	1.93417789777690	-1.30176915733536	h
-4.85339734844212	-1.85242030104300	-2.54704637216536	h
-3.90072099336392	-2.35262927406629	0.63784546491986	h
-7.11502761311874	-2.72158400879340	-0.22218629472316	h
6.80311320297143	3.16196950685503	9.82763714258578	h
6.33302377221976	0.01315459096092	10.85702163169856	h
7.17938575396410	0.62541523616449	7.67635477237597	h
-4.52595909976389	3.52298292733757	27.43924847503686	h
-6.18063261913738	4.38395563312933	24.62507817210206	h
-2.46972420189078	7.88874956935994	27.38809840127209	h
-5.76255272353210	7.74679948503251	28.14369502280496	h
-16.08096491138030	4.12169129877256	8.97359547381018	h
-17.10312797986771	5.62149733779545	11.75499173826919	h
-19.29015481280188	1.52308409980701	10.92354512956301	h
-17.82009994027967	1.58770654528370	13.90990420328828	h
-17.37399863519926	-2.53144546760549	11.42843910275183	h
-13.28180124991613	0.18811337788042	13.44501167552000	h
-13.09350526714413	6.79657677851253	17.81200334686845	h
-15.89078873052060	6.15214955625751	16.06537354728765	h
-14.42332463256567	3.73153129807865	17.85427565278579	h
-5.42896244323070	12.01536191946592	27.16635928602443	h
-2.79832808726943	12.39699068072361	25.06506804057080	h
-6.09544711524883	15.28634070546456	23.73113372653510	h
-6.00535193967987	12.78566463854549	21.45124198175622	h
-10.71892393498516	15.79858286585188	22.42563845288885	h
-10.38646040891287	13.13832130207900	20.35926723582398	h
2.08273237498637	-10.64425769396743	15.66655091601344	h
-0.02455391939043	-8.91751424986987	9.38072566803996	h
2.67508737115262	-9.99516059260720	11.13556742982946	h
0.06002666908225	-12.08729757307962	10.57458186183136	h
-14.83651480037029	13.97128997274732	22.05035331999310	h
-13.68714196406506	13.18424796016086	25.13547138794513	h
-16.14493613096820	7.25097862229511	23.01862323786021	h
-16.14988106878226	9.46779027832167	25.58140318395836	h
-17.68800779000864	10.24995624257125	22.65923309641000	h
-8.04312918708477	8.13447098727106	22.83953513913272	h

-10.89249058888815	8.06317799390758	22.24907608486551	h
-7.06436676560569	-2.79846387582734	12.43819622853350	h
-4.08229462534668	-2.86898223398770	13.40845840502650	h
-10.04515440160830	-5.94032792495295	12.26204441391886	h
-11.40700857757567	-3.29623565124818	12.21771126034693	h
-15.34655520788883	-0.90458906614861	9.29225626029011	h
-3.06390399470323	7.62518690504624	9.14548348975475	h
-4.17239524003505	8.23526206817148	11.88501029178891	h
-0.44128123178417	8.27193336114930	5.82515762688988	h
-3.12357758436408	9.48040101881024	5.35092731915698	h
3.86380606918138	8.05746217806532	5.29689266202487	h
3.98596626705854	7.30925005124315	1.04410889866970	h
1.30405193027446	5.33841852696016	1.44585982271289	h
5.74482670295452	3.22631819676435	0.86870648979581	h
6.40618184397939	4.22543518031551	3.96841665197540	h
5.07717937250039	-0.24669766441795	3.83470907866198	h
2.28301244047587	0.51432476964809	2.22322849102300	h
-1.52387845272842	-4.25026782692506	14.33096070529553	o
-1.19705749213658	-5.94246579613472	13.58700783391268	h
-1.05910943102286	-4.55022811611479	16.10095289445338	h
4.85234924005916	0.92466407539615	20.46352475534712	h
5.69338771729217	1.65210469025555	23.63681378029136	h
5.72398407683347	-2.91920259164144	23.10158008890622	h
3.27054125246498	-2.00735064351570	25.23996819587881	h
0.90446490868859	-5.51086766742482	24.58882319172173	h
3.09119132348056	-6.86182336254753	22.38842418402591	h
-1.40089932923442	-8.41358591899441	22.15726977590597	h
-2.37245490926799	-5.36504505822588	21.09111628450141	h
-1.20127589170911	-11.10596730821239	19.18266063278766	h
-3.31145133268554	-9.26457955199284	17.29458304527879	h
-0.59602496433536	-12.62805140889754	15.08021623487868	h

\$user-defined bonds
\$end

[Lu-Motex.6Water]^{2+}:

\$symmetry c1
\$dft
functional b-p
gridsize 5
Energy:-3394.767536066

\$coord			
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-1.16712374358722	1.59756411289895	9.23230322328454	n
1.03946378453103	1.38203199193302	10.54307050004736	c
3.14259415517170	0.91592225867111	8.85947430724937	c
-2.40772176952479	1.32284108235168	4.82828022393417	c
-5.02997642311740	1.72327304609623	5.00609155048451	c
-6.38587990110634	2.29768899292336	7.15810470411842	n
-8.85593900655263	2.57676925629672	6.36054312903007	c
-9.07631742769244	2.13962323844050	3.64436479293494	c
-6.67646342216910	1.61161831506311	2.79465389796392	c
-10.95023298125331	3.23195905954374	7.85377013094616	c
-11.06413529020788	3.79686553954047	10.43534925178540	c
-8.99153035685640	3.80168758276694	11.97123919434750	n
-9.78776231526571	4.52044071203103	14.31766288905937	c
-12.48086392975298	4.99751066918385	14.32934403308787	c

-13.30701612378501	4.49175994292422	11.88542401313004	c
-8.03840662631357	4.57990191801151	16.35094243615380	c
-5.68615849422198	3.83957579994205	15.87620109078699	n
-4.82373250682088	2.53307401872080	11.47038158025294	lu
-5.75724591829659	-1.47629924198911	12.44632368563166	o
-15.97831081087439	4.50167289135833	10.92792533258492	c
-17.56279567799519	2.16662392213810	11.73135001796108	c
-16.35428896918383	-0.38982954093780	11.16597323846122	c
-14.34393088495125	-1.01464821422632	12.92479308418308	o
-14.02156858250297	5.82878647640108	16.54831727492099	c
-5.86706978110884	0.98617508398617	0.15122673439103	c
-5.59250426983293	-1.86962944674401	-0.35132812059581	c
-11.47304437844894	2.22453907147037	2.13438049237214	c
-12.99246522859450	-0.25914537988871	2.20775993165456	c
1.00971919900899	1.68258339297538	13.20248360820419	c
-1.16338606779983	2.23577266056429	14.31784753911082	n
-1.43861176672071	2.63004451261636	16.86702309630950	c
-3.85827628495435	3.57568053780237	17.70618437024251	c
-4.21993175967356	4.11904014808170	20.29812329488191	c
-2.31273920205103	3.69567533879835	22.03936293622162	c
0.08830154538410	2.64544848051993	21.20800167612366	c
0.46811852011316	2.14894991313642	18.67212964024162	c
1.74638080723979	2.25108930404605	23.09147040962273	o
4.12585420382732	0.98419583326481	22.65657330149303	c
3.92365947413460	-1.81619587047670	23.23023589485627	c
2.28026307655891	-2.97124570409285	21.44604000056646	o
1.65112575149650	-5.51527189893545	22.08521011970220	c
-0.51045007752882	-6.39455411855495	20.41527310491785	c
0.19291148271617	-6.76578773396666	17.81908160532836	o
1.01807320549141	-9.29648005735570	17.28478568290558	c
1.74899563295193	-9.59299779208617	14.53517003288691	c
-0.44151936162134	-9.55187206966245	12.93992164118288	o
0.10336007280407	-10.45063888440969	10.44405119496403	c
-2.42278653116147	4.09191773525554	24.53956814766464	o
-4.72936202149436	4.83312775167182	25.81916618150902	c
-4.62915838539067	7.56626177187858	26.65907921707094	c
-5.14797230017082	9.19669572817249	24.57231269855433	o
-5.01577130425683	11.83297189277900	25.23279031352298	c
-6.76886800940142	13.31446607124738	23.52897883609852	c
-9.28945100006696	12.62304129474770	24.15704662085757	o
-11.15427101358118	13.73094752880239	22.56171943519823	c
-13.72460067467255	12.76994164136134	23.35786398556633	c
-13.98201299345882	10.15321105885023	22.70888378783593	o
-16.25346263611021	9.08648179027565	23.71037386376839	c
5.84222552693065	0.57038031187450	9.62346277876368	c
3.51431261332695	0.57083304256520	3.99544086366441	c
4.94109804175665	2.93250415822382	3.02119256276122	c
3.33796692602699	5.29365112517858	2.59702519674416	c
2.67797187343502	6.57700282036712	4.92589107271091	o
-3.65044846235271	6.73138128441625	10.85750505291775	o
-10.15431382719072	-3.75711295788307	11.67647473470538	o
-1.53278084367130	8.73827088203312	6.92520540539412	o
-9.49163997579683	7.21335451713062	21.89754732489101	o
-1.71890971218285	0.96970792142973	2.91802594641901	h
2.78439626211447	1.52084306911350	14.25492615427968	h
2.21464112751127	1.25589415329413	18.06922744354290	h
-6.02127597323289	4.89463423710872	20.92107269958402	h
-8.67339631295002	5.19307825317200	18.23026119812698	h
-12.73487397670746	3.35283071866245	6.83025630565970	h
-11.01095941455296	2.67570731885614	0.15793403485406	h

-12.67467604473235	3.79034258342692	2.79614435861479	h
-14.72749355000662	-0.08507117127859	1.08206681294867	h
-11.88482530942502	-1.83576053336819	1.43714682710581	h
-13.52800491906176	-0.76710053831599	4.14934789934823	h
-4.06514921061325	1.93617038138545	-0.28318284604128	h
-7.24966726754468	1.77844577157942	-1.18410488079891	h
-5.00180364371267	-2.21083447626015	-2.31173128678300	h
-4.18342684158710	-2.73252376305614	0.90736681788604	h
-7.39189368550032	-2.85676140740620	-0.04412522436289	h
6.74274121438156	2.37952844157345	10.12501147758209	h
6.01902407534575	-0.67673780779668	11.27585587671461	h
6.95883979401154	-0.26793397703571	8.08906246730823	h
-4.79775484635751	3.62063349808292	27.50352885310981	h
-6.40961928103864	4.46040713459111	24.65872533413506	h
-2.75195007812395	7.98137298717238	27.47404197125705	h
-6.06144188068698	7.84034008065965	28.15832458183861	h
-15.97808268329252	4.62476160745429	8.85249314135256	h
-16.95664757770499	6.21164853711686	11.59981279899695	h
-19.39303262562052	2.26002600261714	10.74670237774802	h
-17.99019875678448	2.25498176972934	13.76667323484590	h
-17.75604189745799	-1.90839250776580	11.35561312696210	h
-13.54913831247289	0.58020621643065	13.41658731682439	h
-12.97097990579327	7.14816712439777	17.75722868280239	h
-15.76820841138557	6.76604868006194	15.93409353834124	h
-14.57206219272758	4.21736063924271	17.74623572925770	h
-5.61113117993994	12.09698505203672	27.21386704562389	h
-3.05556876284612	12.51822235473080	25.03155309598310	h
-6.45080501538607	15.36102621561362	23.82729203123370	h
-6.36283151273862	12.88725073927713	21.52005489006984	h
-11.13184317551183	15.81540031387232	22.73664908994532	h
-10.78613310285004	13.24722507907351	20.55924938013203	h
3.09245936470158	-8.09690443617207	13.96379130141800	h
-1.67119114864149	-10.38710164332819	9.37752892679273	h
1.52792010658428	-9.25622908448882	9.49760782004582	h
0.79454988619304	-12.41492778415522	10.50577177166275	h
-15.20999501857224	13.88569501388970	22.40058444782720	h
-13.95265345146170	13.01487471289242	25.41974775762126	h
-16.29400102835590	7.09225600379364	23.15122644480511	h
-16.28938839175318	9.21620453018916	25.79107963327952	h
-17.93502507226821	10.05270382550317	22.94355774385773	h
-8.23208569010456	8.22241648601624	22.82034017712271	h
-11.08896647634536	8.09798130340220	22.26999339963091	h
-7.43399146243922	-2.36231665068099	12.20694743850287	h
-4.43863747402371	-2.78671825103201	12.93062351549099	h
-10.36384793586002	-5.47764542716705	12.27894932221605	h
-11.76278974723561	-2.86284577119353	12.09446616436312	h
-15.61165543908300	-0.44723946129834	9.21553078288055	h
-2.83151923510904	7.47439689436541	9.27506498557188	h
-3.90567816496712	8.11082245792037	12.03713191345267	h
-0.07508079983502	7.91715941158781	6.06311698692481	h
-2.56293392602553	9.50796266751795	5.61740714381133	h
4.18860086917761	7.39240065321909	5.58390902115285	h
4.33048691594636	6.62017137803101	1.33629458495649	h
1.52396482293199	4.82184291925367	1.70087400060596	h
5.83353085192660	2.43446287336550	1.20674766519814	h
6.50564177783296	3.40733057300997	4.31245214452528	h
4.90155797064148	-0.97015120723992	4.18721334274882	h
2.19014178428219	-0.05268284282485	2.51683409749259	h
-2.14389415043646	-4.62078802199623	13.61642863312878	o
-1.88134169147214	-6.32040680063167	12.89127570764561	h

-1.50359729744475	-4.89511309667107	15.34375468463413	h
4.82278901525865	1.33076713553975	20.73187767619239	h
5.44729164832495	1.86129977312619	23.99476381559911	h
5.84533800453372	-2.64633320066074	23.15431939720490	h
3.19199509187942	-2.07601359540012	25.17175585713461	h
1.02639956459545	-5.62171349403471	24.07991272215872	h
3.32117405892968	-6.75895970815009	21.88328648023221	h
-1.31675609547283	-8.15318791105251	21.19529569005663	h
-1.99908463462065	-4.94380403244501	20.42181315367273	h
2.69131118477950	-9.76242457065939	18.44359055516944	h
-0.50237800160544	-10.64735940452181	17.75873348071565	h
2.71310456707076	-11.43446184774443	14.33344483884719	h

\$user-defined bonds
\$end

[La-Motex.6Water]^{2+}:

\$symmetry c1

\$dft

functional b3-lyp

gridsize 5

Energy: -3384.150089949

\$coord

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-0.96205037868230	0.79568438436132	9.58287751519384	n
1.22894631749803	1.06382901722098	10.85893330672116	c
3.35153959578694	0.91963707258944	9.14795212128251	c
-2.22648309966100	0.42551658912539	5.19671014507833	c
-4.86758137369272	0.75483039037403	5.31337753469985	c
-6.26850769395953	1.27572262950263	7.41579574135438	n
-8.66921590441035	1.77897084296782	6.59350550207129	c
-8.83363293017200	1.43616567322739	3.86427779414499	c
-6.45746488666161	0.79712008298022	3.06529991719056	c
-10.70110989560635	2.68925391190651	8.04463926542735	c
-10.85700542790508	3.35020981390134	10.59894524862552	c
-8.92844361914464	3.04301457936393	12.26205458024522	n
-9.64310140958645	4.03329635682643	14.50212850482191	c
-12.18636364745186	5.01555712972228	14.33456632161516	c
-12.97339117643807	4.56504719352017	11.88532139239781	c
-7.91942708535428	4.06975763266232	16.58204303155715	c
-5.65660786211741	3.08836079217258	16.26518067840967	n
-4.94426373738578	0.55368158321488	12.04382511406293	la
-7.95786839139081	-3.27020448324818	12.13137690900403	o
-15.48325751408432	5.24692825420805	10.74273668106468	c
-17.74315521412910	3.57715070978957	11.54257550310755	c
-17.49456834940735	0.78298712454792	10.91274585880162	c
-15.74986086406136	-0.52789050336754	12.54700687629500	o
-13.62097030000582	6.28598375542271	16.41145809403982	c
-5.60872865167530	0.23102879430461	0.42266375602986	c
-5.39700905448682	-2.60808255961720	-0.16074652070581	c
-11.17320928186404	1.72315690669755	2.29347940474005	c
-12.87648245252174	-0.63196900366077	2.29800968657358	c
1.20738424860106	1.54557362648221	13.51213462823283	c
-0.95344443934704	1.74785410671040	14.70037440590492	n
-1.28134294291138	2.27992283268543	17.21541766381574	c
-3.76084257894243	3.02923788981895	18.04823707680224	c
-4.11460268664884	3.67264016216173	20.60980171142652	c
-2.17303264733422	3.48389682139427	22.33623642588778	c
0.28101709240444	2.61747147024658	21.51527615390325	c

0.67770734429408	2.09864895180070	19.00441211995156	c
1.98098909431236	2.36010089955914	23.37557081768629	o
4.40480414855060	1.22483561117629	22.95105733835238	c
4.33012374876956	-1.61577278777037	23.30425353218756	c
2.78968408464792	-2.70735090084164	21.40775836033511	o
2.30933029973690	-5.32120928260965	21.72642277256002	c
0.04726026933774	-6.06168757245880	20.12843836564237	c
0.47169070182719	-5.89614180700584	17.46210745035404	o
1.53270740575775	-8.13519155154144	16.39433878426932	c
2.12352274639791	-7.78485491947439	13.62397786263355	c
-0.13526919328523	-7.66533700314987	12.15177556154977	o
0.32040242219498	-7.93696112845833	9.50920038900093	c
-2.30554946398822	3.95545528286071	24.81074499703479	o
-4.61900071547262	4.51915613808676	26.12333015377604	c
-4.62891095898077	7.21630381120225	27.05954242760335	c
-5.15820168196724	8.89214708153700	25.03468628321666	o
-5.02180930517966	11.49668436471288	25.73636415802026	c
-6.57799773075717	13.04966670429093	23.91883942446268	c
-9.15118612829991	12.43906049111592	24.30615898706250	o
-10.85131637927783	13.66546781289743	22.64388942311519	c
-13.50533338154037	12.80902235093401	23.24299915693266	c
-13.82673248435143	10.23015334416965	22.54495857701856	o
-16.20866281099251	9.24332843449637	23.29575313133608	c
6.07789135774580	1.12863725631893	9.86832415631319	c
3.74961258569714	0.38921232838962	4.31933289293891	c
4.98453079657777	2.82700560012445	3.29607581718483	c
3.19851722320111	4.99422324909505	2.66011767197834	c
2.22789915780312	6.27189439334491	4.85367088077110	o
-3.77994982018515	5.41478469199597	11.18321924845480	o
-12.64688306689549	-4.18508050388804	10.66282582031305	o
-2.68888638663383	7.11385425688859	6.44398930697606	o
-9.38192520281671	7.04868363528927	21.95400999806607	o
-1.50410755666893	0.15651987514537	3.30331601705600	h
3.00754340290915	1.83912784732360	14.46208371135769	h
2.47293715470619	1.34889173114825	18.40778870951592	h
-5.95661343510839	4.30247416482978	21.21825650456298	h
-8.50158043992501	4.97638074687114	18.33760299477162	h
-12.40121144288275	3.03253668818156	6.96271707533604	h
-10.63571439883185	2.15856697797299	0.35008397912553	h
-12.26279796109737	3.35449050736515	2.94243221497391	h
-14.56039298592686	-0.30606334878078	1.15346502853098	h
-11.88543193981697	-2.26351576560609	1.51931663315587	h
-13.47893644850574	-1.12655601572551	4.20824301977182	h
-3.78666808279832	1.13726258853969	0.05957825824021	h
-6.92743601691102	1.09135554446569	-0.90952100425987	h
-4.78238387271232	-2.90172733278963	-2.10691544498237	h
-4.03971478549967	-3.53799403952514	1.08467456028955	h
-7.21389999309535	-3.55186367661076	0.08125670589851	h
6.64323020310018	3.09504822026231	10.16773651705072	h
6.48793705946489	0.10877570091514	11.61438744481767	h
7.30258846973058	0.35701774205217	8.40253640246778	h
-4.63754599788863	3.25112756351973	27.74921709577500	h
-6.27570326156354	4.12906637497754	24.96707434026936	h
-2.79196548124011	7.65626079227867	27.91130093408918	h
-6.08160888126916	7.39385866850213	28.53057011255930	h
-15.34261833639803	5.21582953899120	8.68386319653892	h
-15.93683478938359	7.20066326185312	11.24261422689418	h
-19.42735230512446	4.29465113291103	10.58496072820442	h
-18.10033687442020	3.77277364327352	13.56884978299455	h
-19.30961296401871	-0.16258461989907	11.15159569905432	h

-14.52407516556138	0.67605267998544	13.16388296044668	h
-12.37878516981412	7.37403716900838	17.64182785504901	h
-15.04839213796853	7.56558465487892	15.65457118461228	h
-14.59916880048450	4.91131204688010	17.60671965440756	h
-5.76957427776207	11.75067801048134	27.64973207682025	h
-3.04985396017702	12.12963351130292	25.71024306835075	h
-6.23156324111871	15.06436889048729	24.28039124254613	h
-6.01435412422005	12.64414398160233	21.96175912971215	h
-10.74635292212358	15.72492062706444	22.88156164232020	h
-10.38436482983583	13.22343161030560	20.66999786869673	h
3.25364212916216	-6.07143563135851	13.33305293042087	h
-1.50712436062958	-7.88149982833986	8.56657682918269	h
1.51440468839675	-6.40493179629897	8.79396320863904	h
1.22901156922854	-9.75027749396243	9.11200584826584	h
-14.85725578777624	13.99113018810202	22.20514585496460	h
-13.86458584476476	13.04062631289610	25.27083853181662	h
-16.27420136956036	7.27439878027640	22.70178010290486	h
-16.44151240675077	9.33874111531170	25.35012009165905	h
-17.75969696490125	10.27943300379856	22.39697767589758	h
-8.14183825161321	7.94423550210486	22.97126735908425	h
-10.93929523420723	7.98399952288080	22.24843080554608	h
-9.71213101108587	-3.68387395349566	11.57834105239164	h
-7.31627315122936	-4.66737691034229	13.11025657009939	h
-13.40777564085761	-5.83106645204741	10.51914802023505	h
-13.93673985792154	-3.02896011975449	11.34563752756498	h
-16.90265633207265	0.52897830823535	8.94396534897116	h
-3.39611505554125	6.03416193082478	9.46597116377771	h
-4.82895328147399	6.68151703024499	11.95950020107481	h
-0.96403874393435	6.89199092304918	5.81453551858683	h
-3.31608496381394	8.66141959831898	5.72350025041761	h
3.56639894471288	7.23411385446523	5.62788534512007	h
4.15542750669582	6.35867637061228	1.43819896215656	h
1.53779896719260	4.31631659120326	1.64249942537856	h
6.00128055682557	2.32955018593675	1.56560137319586	h
6.41935447377305	3.50967237110198	4.62000899953336	h
5.25124300847712	-1.01564899081341	4.53980507148575	h
2.49920186109222	-0.36836637910286	2.86132418074458	h
-3.04151337056708	-3.79249048173882	13.99635306270154	o
-2.25525887563901	-5.14920441053188	12.99461372173789	h
-2.07135005806471	-3.95419136519581	15.55567151571236	h
5.15595259118818	1.74333561848590	21.10226392405433	h
5.62896337772329	2.04449101381160	24.39000342003640	h
6.27484094452391	-2.33999872417270	23.20726117371066	h
3.57593338381864	-2.05654093897801	25.18495037509188	h
1.84759970220578	-5.73668676478978	23.70713113018423	h
3.98919625103161	-6.43576040590543	21.23422599876105	h
-0.54876249182255	-7.97982811144876	20.63063253103135	h
-1.50853016725662	-4.77505022571422	20.54903178063461	h
3.30363912717558	-8.61201566613247	17.35539334069681	h
0.21909561936732	-9.71947972942077	16.63619108314017	h
3.24703550101927	-9.41133549267169	13.00682478645213	h

\$user-defined bonds

\$end

[Gd-Motex.6Water]^{2+}:

\$symmetry c1

\$dft

functional b3-lyp

gridsize 5

Energy:-3388.483039584

\$coord

2.05630021038554	0.70557687523614	6.32436233941231	c
-0.64729621302765	1.13052640678037	6.62789103386785	c
-1.17713512641263	1.44420418781058	9.11831165289612	n
1.00805370589820	1.24038957081308	10.41889142212709	c
3.08281267609820	0.74893120725903	8.71604801293679	c
-2.48948273634275	1.22296585498734	4.74687540045384	c
-5.10089263064865	1.71084610958352	4.90964444212014	c
-6.45093445488999	2.27821577286078	7.04122635668764	n
-8.88731841892487	2.70921751750258	6.26975158931973	c
-9.10378749617156	2.35791330399039	3.54916115609886	c
-6.73958152542220	1.73923905013627	2.70022945345066	c
-10.94177666109890	3.43767676492387	7.78565574836170	c
-11.06888594968110	3.97510792634268	10.36918274190342	c
-9.02956368392698	3.89140687762369	11.92201073521049	n
-9.77916190931236	4.58595532117068	14.26445545099600	c
-12.44839645697805	5.15323364475548	14.26645013507379	c
-13.27902797729400	4.72590282887967	11.82518674811248	c
-8.01635964419036	4.57940307268502	16.30479594387689	c
-5.69164133975143	3.79868605535186	15.86035345668113	n
-4.91365977229078	2.22234651483916	11.44589086833991	gd
-6.00135408794489	-1.94887180416615	12.52196060923599	o
-15.94579650510645	4.86306753879422	10.86979688317168	c
-17.64642802470437	2.61165197070890	11.64860306899663	c
-16.64030864593314	-0.00278998683360	10.97998826643347	c
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functional b3-lyp
gridsize 5
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-1.41178066447455	-4.98483142429304	15.27512312374007	h
4.75768560282706	1.30538730945849	20.78386180458812	h
5.33536189827954	1.83373268283765	24.02771141665961	h
5.81840377540176	-2.64147130445351	23.17986440232496	h
3.15832570241565	-2.12926812698522	25.16200011168025	h

1.06418537782050	-5.74494897905715	23.98858653511260	h
3.44733811277575	-6.76322777034047	21.86762012140664	h
-1.08231498041061	-8.30902736124520	21.01526764093612	h
-1.85970027603975	-5.14168798451276	20.27473607857360	h
3.07263414451121	-9.68882807628897	18.35243469367024	h
-0.02236533008242	-10.71200579635802	17.54534361859583	h
3.30697926850429	-11.24561138044594	14.22242425616843	h

\$user-defined bonds
\$end

[La-Motex.6Water]^{+}:
\$symmetry c1
\$dft
functional b-p
gridsize 5

\$COORD

2.37627951837409	0.55264018772309	6.92315426424645	c
-0.35467976410139	0.48083356726222	7.18831244127932	c
-0.98155577303991	0.70523237906417	9.67254888776103	n
1.21842059025266	0.97053109500019	11.02375850256186	c
3.35798819258775	0.85727654939439	9.35262885557002	c
-2.17826988254456	0.30839668043261	5.22972969035714	c
-4.80669800940998	0.67491823313653	5.31495174538778	c
-6.23020917371665	1.35267253067852	7.40310118791872	n
-8.65396276009013	1.81884419068516	6.53756252820058	c
-8.79742609404522	1.30950769882950	3.81859640812724	c
-6.41551873534172	0.60017798014472	3.06112205336994	c
-10.69701166676350	2.78369540480305	7.92482191649759	c
-10.86235181558644	3.52855423325105	10.49705868899082	c
-8.93415520540648	3.24898035717391	12.17567530211067	n
-9.69978634454329	4.23033749782212	14.45308220752783	c
-12.23216768263243	5.18933995293327	14.24834510036671	c
-12.99491252477734	4.72507238418550	11.75489565544016	c
-8.01161589378838	4.18146148552987	16.55977666679742	c
-5.76764562893544	3.10980452723928	16.27764555887000	n
-5.02332680012447	0.64638478479298	12.06724692929585	la
-8.10539511219256	-3.06712125082148	12.57867360467435	o
-15.49932020119557	5.39138735072725	10.57809601460603	c
-17.75573329744838	3.70589021775624	11.37292741088061	c
-17.32533939102312	0.87965268202988	11.00506730351904	c
-15.59957049354691	-0.14537888025638	12.86694801945917	o
-13.73203363766396	6.44604033933133	16.29240674156753	c
-5.56857932403593	-0.13365566961168	0.45702579752396	c
-5.36096888554152	-3.01009699462396	0.05748983539015	c
-11.12880370149142	1.52710228368138	2.22079184394065	c
-12.86657901115853	-0.80451608661105	2.36530704306057	c
1.10748730652450	1.43535126333083	13.67431944500330	c
-1.10177502141039	1.59917837415840	14.81800638134733	n
-1.45774555372612	2.11811891112894	17.36834385566723	c
-3.91728096706403	2.95059108937234	18.14811414135893	c
-4.32068150266879	3.53609636988252	20.71962143021069	c
-2.42112593504742	3.22587291254364	22.50995455737860	c
0.00206062853065	2.29488707764096	21.73768233615635	c
0.44368736872006	1.80375756209972	19.20246416024212	c
1.68707435539002	1.93156408405444	23.65486306313802	o
4.13712039150601	0.89041923140642	23.14237070305873	c
4.18359475319883	-1.97757216012512	23.28919640383429	c
2.75925602231027	-3.00462475971769	21.25391822811693	o
2.49974009519149	-5.67522535520191	21.32942478205091	c

0.32036026921586	-6.44058876433874	19.61638823324103	c
0.68559703234094	-5.83091834030367	16.99807556787900	o
2.19454522147303	-7.63969963778009	15.66514531637398	c
2.52871701063916	-6.86637271492515	12.93152878817654	c
0.22787093421856	-7.22144828176770	11.53953792195213	o
0.60074297147379	-6.90323439824282	8.87186958156892	c
-2.61783486405333	3.65288402245832	25.03502437830853	o
-4.96953687425086	4.34453714318772	26.20882653254398	c
-4.90824567398456	7.05892964325812	27.11993083457925	c
-5.29830747121074	8.73930162554663	25.04391048876154	o
-4.99104824370519	11.34524704664656	25.71928959057940	c
-6.41018951115539	12.97010963244429	23.84376284240465	c
-9.04236923944650	12.63394217407073	24.28557633867393	o
-10.60664966608032	13.80320413461112	22.43623188400540	c
-13.33798228508396	13.22102523938448	23.04548118827766	c
-13.84836056548151	10.61111061130048	22.57466343396412	o
-16.32616209797904	9.89962450034063	23.35977657679150	c
6.08446584929000	1.08458235257692	10.09045688702691	c
3.84169410819444	0.41760676702990	4.49674672031898	c
5.01900160339459	2.92070085765297	3.55322364091007	c
3.17581559756744	5.02701510544352	2.85084558508289	c
1.94452128116146	6.18117072248019	4.98663466006412	o
-3.71716417748856	5.47012650168228	11.38291307146669	o
-12.89474024958811	-4.37070605203169	11.99813685045777	o
-3.09097113269576	6.73448559175237	6.50529833232904	o
-9.63979116082778	7.05731628174009	22.17016467144823	o
-1.42414221808305	-0.04773663331553	3.34366898717341	h
2.88777892151445	1.75788831234777	14.69425221158884	h
2.23123989541850	0.97671972464688	18.62441307680451	h
-6.17051353904094	4.23247935712623	21.29254916099637	h
-8.60641574668297	5.07591812057041	18.33949192195102	h
-12.40895255077031	3.08347324387711	6.81600443788780	h
-10.57594619208366	1.83887101772433	0.23968213010386	h
-12.20582712049864	3.22114492309443	2.77488183129820	h
-14.55939181303784	-0.53593927550883	1.19155342402290	h
-11.88471642148829	-2.50658877181283	1.69448600911673	h
-13.47916768196025	-1.17003008753556	4.31567991276208	h
-3.72605954343528	0.74506480420849	0.03898632591086	h
-6.89469223715681	0.65099220008962	-0.94016218014685	h
-4.73684796352102	-3.44338489391775	-1.87598377319074	h
-4.00165309180001	-3.85731821031987	1.37991404556924	h
-7.19355018348551	-3.93683504066662	0.363808936834487	h
6.69965819334308	3.07029614967530	10.23255540898968	h
6.46310484816160	0.20919255615291	11.93636463311356	h
7.32408027265225	0.16402867813889	8.70021101619912	h
-5.14810865186902	3.09976829735744	27.86554851436457	h
-6.60231314660461	4.01562065278715	24.96953090530792	h
-3.06787113097314	7.44087233870538	28.03070684924224	h
-6.41293953365351	7.32713175035862	28.54953910739028	h
-15.32331206728135	5.32601130450786	8.50613420164558	h
-15.97863685233171	7.36657065687655	11.04030887051006	h
-19.42360719944001	4.26722899975687	10.25957054141258	h
-18.23940726133542	4.04020408914584	13.36978965397139	h
-19.10004298585484	-0.17054054931737	11.24743035804302	h
-14.25937063964997	1.12519601945822	13.07972351508217	h
-12.50602513852270	7.25025033310560	17.75911451620940	h
-14.90776418578624	7.97932630051051	15.52432984864019	h
-15.01858483187613	5.10759524543329	17.23640539620914	h
-5.75688270326348	11.68610054990280	27.63153923734050	h
-2.96351661717790	11.84627400390512	25.71907187070675	h

-5.85934742497762	14.97299034180102	24.10438320587545	h
-5.91027914961360	12.41171472401861	21.89053627516966	h
-10.34272227652579	15.88014180226747	22.44738161268648	h
-10.12984224355469	13.10203435668322	20.52377207957875	h
3.14610685399779	-4.87451368689943	12.80217174810949	h
-1.22551112819336	-7.26098123572096	7.96265835208742	h
1.23933198219929	-4.97027828867158	8.42235155457933	h
1.99812912303391	-8.27921519399480	8.16725392435900	h
-14.58156520112371	14.41532741321234	21.86101090274089	h
-13.71917918994126	13.67340516951065	25.05058402753974	h
-16.54381699641930	7.88179159826327	22.94489780000526	h
-16.58785929838300	10.21268754544270	25.40639362128771	h
-17.78203936957648	10.97696615200508	22.32211567516445	h
-8.30252866327170	7.91657753309164	23.13079281665538	h
-11.12001069834794	8.14888951692106	22.42282199439844	h
-9.92416203865969	-3.61900460341188	12.37157226151948	h
-7.11894160227698	-4.46489703818148	13.26575389872464	h
-13.57709581393490	-5.70669817670280	13.05433500926047	h
-14.01648743893832	-2.86899148790210	12.28343174914277	h
-16.60501796334886	0.48663680543782	9.08455271596193	h
-3.39128648380309	5.98880497322119	9.58136403005882	h
-5.13879685186796	6.50172169713166	11.92225135658497	h
-1.33316015789812	6.55352877501269	5.89778589039995	h
-3.97884075110599	5.28660800949874	5.78926124253530	h
3.22898308157026	6.79918489866867	6.14600562308160	h
4.17139833059729	6.49106851111298	1.74674246239261	h
1.63162849631015	4.29854191120343	1.66573390694372	h
6.15769560018218	2.50428403449717	1.85740239475970	h
6.36606236547760	3.64985530808810	4.96938293554790	h
5.39852064739340	-0.95364551626210	4.71153952792456	h
2.63214769529721	-0.34840302637748	2.98521326181058	h
-3.18974295216716	-4.00166788419210	13.73563512829065	o
-2.18539408747775	-5.15100311916954	12.63446042707439	h
-2.17261325598300	-4.10519753248808	15.28793930550065	h
4.87720455390741	1.56599264429221	21.31914847099643	h
5.35911420783750	1.64036102497439	24.64569881439127	h
6.18081271325420	-2.61053759378185	23.21262786464726	h
3.38294152459538	-2.59698384624556	25.11990393241874	h
2.03915347294221	-6.32236195785072	23.26713248936912	h
4.29074888974260	-6.60853709424941	20.77620843533238	h
-0.04477769381513	-8.48619850567588	19.83385030119473	h
-1.38140990883673	-5.40437658460228	20.20296030350014	h
4.09350626552826	-7.77344627326746	16.52355579490272	h
1.30076667101228	-9.52670397199269	15.76530926230260	h
4.01938797948481	-8.06763190788809	12.09611414192769	h

\$user-defined bonds
\$end

[Gd-Motex.6Water]^{:+}:

\$symmetry c1

\$dft

functional b-p

gridsize 5

Energy: -3390.918764991

\$coord

2.08602231978519	0.95677121224706	6.32009707331678	c
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1.00554993898655	1.25992214095016	10.44715093367335	c
3.10466803798284	0.95201266382240	8.75247237573294	c

-2.47642263329118	1.31796333238524	4.67112161060199	c
-5.09116028846905	1.74252300986904	4.83679076067404	c
-6.47644670402966	2.28360404479262	6.99146866054598	n
-8.93825591161322	2.69997333407954	6.20115511808883	c
-9.12681995643642	2.35294185910373	3.46169582552196	c
-6.74340293423131	1.76698538790956	2.61475175827675	c
-11.00857617590524	3.40499983486556	7.69299386039837	c
-11.14818792893574	3.92331053569867	10.31965006083974	c
-9.10022976093195	3.85358607065701	11.87589813049334	n
-9.89681192675079	4.45365907588203	14.27609411939143	c
-12.56398522858069	4.95220485860099	14.27332426592236	c
-13.37671944256543	4.57821304396576	11.77880115223643	c
-8.14548150444386	4.34588150199099	16.32216807587734	c
-5.81154963023999	3.55802895816464	15.86402004221375	n
-4.99368596447938	2.11025178598614	11.43118919124310	gd
-6.18835633189680	-2.03551648414776	12.52903907296030	o
-16.04638008890131	4.68266467875503	10.80948727616991	c
-17.69599851551332	2.36510157917686	11.51733674674742	c
-16.49898609861573	-0.19722170556688	10.93848752243952	c
-14.54940923030815	-0.85945711296608	12.74295633130418	o
-14.14766638391583	5.67877662751063	16.50359424657297	c
-5.93659997120842	1.20011552600009	-0.04348909141016	c
-5.72177231765369	-1.64528485128693	-0.62459517518689	c
-11.50061553386720	2.58356234854345	1.92864032414065	c
-13.14645130261583	0.18172015885019	1.94381306992671	c
0.93795375918386	1.51409026912010	13.11775020412933	c
-1.25242839349079	1.90995577881761	14.26766814788994	n
-1.55350313428901	2.28653810523930	16.85235272670946	c
-3.95542711580664	3.21480610159270	17.70052393523835	c
-4.30361844195520	3.70327922198112	20.30032796111082	c
-2.39342351612306	3.25976604314550	22.04530449836621	c
-0.00707593326805	2.28039784999017	21.20412732709558	c
0.35386313338282	1.79821764472332	18.65034470613661	c
1.71112726474480	1.91838628239516	23.07521193754417	o
4.20502948611886	0.98602027813410	22.54598038283655	c
4.51930060552866	-1.72148291415706	23.42130608749970	c
3.02184510649883	-3.36867154925021	21.92165569870652	o
3.28271598736702	-5.93017103801440	22.72155508932287	c
1.39134778652494	-7.61050712119585	21.39564577065286	c
2.02033145458990	-7.86056227917745	18.79030589292743	o
0.52843725291730	-9.74019351016313	17.57801786570307	c
1.18637325889030	-9.84241137946483	14.80050356234699	c
0.27187211699325	-7.62277264358990	13.55141464798331	o
0.77931434952143	-7.63229259792866	10.90137771013779	c
-2.52813553944417	3.63413680006991	24.57992547236690	o
-4.85664920002019	4.29231668355370	25.82045696004629	c
-4.82389620604333	7.00854358160510	26.72782511406713	c
-5.31272568447774	8.68000166598525	24.66462741846242	o
-5.02111499692823	11.29126907184757	25.32559596749227	c
-6.46093637506373	12.89390791759272	23.44671253408263	c
-9.08854805117580	12.55516806251823	23.91222020322390	o
-10.66989857473472	13.68470626176204	22.05248893931778	c
-13.39710847581278	13.14288404222930	22.71494397847420	c
-13.93534971055711	10.52388504604480	22.33244748109625	o
-16.40160337057591	9.85558776382469	23.19152459826111	c
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3.51314812282398	0.78614086968302	3.87488993848402	c
5.01522502746088	3.17235181713761	3.10531194089602	c
3.47761792465037	5.55652128465144	2.58193227615663	c
2.38616965957844	6.69007452730554	4.80849444822497	o

-3.72157792594600	6.56106111487030	10.85425378715779	o
-10.69939337113225	-4.18860782209055	11.92957804755547	o
-2.60688928405069	7.60505658412855	6.12391445605679	o
-9.77329016890458	6.92175748849394	22.05183222389632	o
-1.77295575951602	1.02905284979684	2.75505503774359	h
2.72899074467182	1.45739558213486	14.16305744309245	h
2.11681699754274	0.95626555368712	18.01426273370710	h
-6.10358438694958	4.47478958991859	20.93053021963355	h
-8.79315871206218	4.89304577588186	18.21834378050668	h
-12.77837114474214	3.61660382665050	6.65810706406680	h
-11.00105917386601	3.04751475910956	-0.03673223469055	h
-12.62823011351692	4.19356882513353	2.61589837126533	h
-14.86744353354871	0.46177573281630	0.81492638071006	h
-12.11339263123858	-1.43461172253764	1.14991061550747	h
-13.71455209743706	-0.33267077821782	3.87422163602766	h
-4.10744668329868	2.11622679446137	-0.43810034919219	h
-7.29181461288687	2.06146805469854	-1.36568867161198	h
-5.11515664312917	-1.95164914311399	-2.58752254462338	h
-4.34895701722646	-2.57097306958537	0.62903525338786	h
-7.54775894894066	-2.59725593871395	-0.36098844872997	h
6.72509647561421	2.54050660513659	9.85295089505278	h
6.06042813713184	-0.44194849134186	11.20501762039042	h
6.93007130250713	-0.22401005712400	7.98008831083460	h
-4.95912878705382	3.04757584324775	27.48311884537569	h
-6.51641443915137	3.92257754590099	24.62841912172165	h
-2.96490688612374	7.42995784288727	27.58144860239723	h
-6.28873720200913	7.24630252980195	28.20319318282616	h
-16.02058087712374	4.87127498475772	8.73810419482178	h
-16.99386376551676	6.39528335747345	11.52345472895947	h
-19.49969751981810	2.49960798661425	10.48580060868413	h
-18.17188342047680	2.41401065642582	13.54338687894509	h
-17.91617225816600	-1.70853932582271	11.07038303999404	h
-13.59983065846706	0.70105025876033	13.07008301762625	h
-13.04059231337136	6.71931403899491	17.91558564408734	h
-15.74391136227340	6.87721737555843	15.92613710311300	h
-14.94769116302673	4.01069653799633	17.46021960850646	h
-5.77960151744114	11.63711638347527	27.24006081758897	h
-2.99727592349027	11.80689482269802	25.31227742066257	h
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-5.97399681986004	12.31727885865052	21.49540002141977	h
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-10.22452298613394	12.92696194089204	20.15385563001165	h
3.25669548339872	-9.97661829373237	14.55917615652189	h
0.02292543083359	-5.86750132263497	10.12547796315372	h
2.83135832529336	-7.72145575061035	10.54272855010535	h
-0.14489938211824	-9.25313474564713	9.96767179785815	h
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-13.74772962620285	13.66031899983282	24.70971094551014	h
-16.64277577604179	7.82799531989900	22.84270216115693	h
-16.61607654346233	10.23224010932979	25.23268967287371	h
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-8.41800159682855	7.81894391342437	22.95063884466448	h
-11.23917336771484	8.04153597099899	22.26472841714284	h
-7.88625025837415	-2.88502824221409	12.33570816502602	h
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-11.04016663801906	-5.65890208740512	12.97308429712517	h
-12.18944526994367	-3.04961204677235	12.15683357359698	h
-15.70876187894973	-0.22617429886843	9.00567760372032	h
-3.21406420737637	7.05173329386689	9.06446700073428	h
-4.88645396225869	7.85583361441627	11.43317932068638	h

-0.81432316681281	7.32939276764164	5.65012844642099	h
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3.70651993815393	6.90555786110217	6.06804794173816	h
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1.86455380535959	5.14616239729048	1.33739651992888	h
6.08525939848762	2.73836445699452	1.37003339792719	h
6.45209736711984	3.60404816410545	4.55537309148962	h
4.86865435723010	-0.79480022414414	3.97666283287565	h
2.20863614687663	0.30003691248522	2.32774308025136	h
-3.26653621660153	-4.55831736195507	15.76399620616411	o
-1.95355239375045	-5.63771272779230	14.96312696123660	h
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4.69512026300780	1.18549099676945	20.53964489197855	h
5.49800215163042	2.18797827899593	23.64534229557106	h
6.55179387808902	-2.21809735588370	23.27960933617575	h
3.96956323498893	-1.87137777060766	25.43566068806116	h
2.94240061155533	-6.07192612490881	24.78274995420359	h
5.22431776698613	-6.61190482094330	22.34296248636290	h
1.43222342885449	-9.48450293813459	22.33142771894764	h
-0.53878518499874	-6.83224834682074	21.61181321593761	h
0.89937496850055	-11.62348212854479	18.41790130574041	h
-1.51119392399069	-9.33287583791463	17.81214888411960	h
0.31236356733070	-11.54169628045360	13.95188883346288	h

\$user-defined bonds
\$end

[Lu-Motex.6Water]^{+}:

\$symmetry c1

\$dft

functional b-p

gridsize 5

energy: -3395.016139119

\$coord

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3.07943842366778	0.68742049003993	9.24200198243275	c
-2.40690795616692	1.00551504266157	5.06451754243233	c
-5.01094157335982	1.45162306137491	5.19955038468145	c
-6.40059568611579	2.10100023448523	7.32361627863173	n
-8.85390437025931	2.46199252674622	6.47781054136668	c
-9.02490852829005	1.98599326859395	3.75878821739247	c
-6.63723451770171	1.36442652640392	2.96288999079131	c
-10.94138006660291	3.22681814676463	7.89911074460853	c
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-9.05428573751204	3.74297421716611	12.07764709028685	n
-9.88093626434181	4.48374306547651	14.42907008081207	c
-12.52431768343909	5.07281678252947	14.37075472040530	c
-13.31153924326232	4.62513033903465	11.88375633843466	c
-8.16495870781137	4.43649635991229	16.49071570037176	c
-5.84353315126135	3.60601311902065	16.06692990422910	n
-4.93944767588692	2.23748319407476	11.70506641331449	lu
-6.17053804639766	-1.74990098269451	12.53891335173165	o
-15.95622454285946	4.80260740288941	10.85827146605728	c
-17.70647143983794	2.56913363923653	11.59298978278850	c
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-14.69040610222467	-0.73447740763224	12.92544436193282	o
-14.10453658135190	5.95215602405948	16.54753788416642	c
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-11.38705372166975	2.13929687274276	2.19837202921355	c
-13.02580394227130	-0.26480712599507	2.30378006014683	c
0.84518670034206	1.38913594596650	13.53541425951950	c
-1.36480166184696	1.86294993295375	14.60408809403132	n
-1.66711788646742	2.28990181674498	17.17664875598057	c
-4.04733733921838	3.28791721638016	17.96189352152087	c
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-0.20194025024338	2.30115079520966	21.54243555591193	c
0.19775234679932	1.77569454254482	19.00648889694674	c
1.46933047903481	1.87208450112770	23.45318852041774	o
3.93807224066732	0.88118462462550	22.93037628013068	c
4.06455252991213	-1.96656998681252	23.24990271504457	c
2.60507218268690	-3.15685912823472	21.33407311933719	o
2.41456634585951	-5.82033781931292	21.63861563121170	c
0.27941001863676	-6.80240034004729	19.98776835070245	c
0.70431667970228	-6.50795279949708	17.32511032890291	o
2.19170964375146	-8.49165935981671	16.23734800829162	c
2.51971820642515	-8.08200335970059	13.42441748475264	c
0.24356103554278	-8.67763120712146	12.09140599911494	o
0.59175948132843	-8.58528536330723	9.41210095642570	c
-2.72351481594666	3.80998470737814	24.85201098437200	o
-5.04022464847452	4.59380768538358	26.03786738340726	c
-4.92754659497260	7.33893356590249	26.84822088002417	c
-5.37124229156133	8.95329993233966	24.72928785687772	o
-5.01792232009165	11.57774886670932	25.30378915261058	c
-6.50349648591392	13.15176420867617	23.43573615832657	c
-9.11630877981532	12.85510713466824	24.00092756067484	o
-10.75111609238543	13.97006113281248	22.17903777677471	c
-13.45788014279433	13.44484073098802	22.93265514177347	c
-14.01912325608120	10.82669189360351	22.58153583767032	o
-16.45822638079295	10.17279708515890	23.52456144345589	c
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3.56050522185463	0.38374413137175	4.37772317326517	c
5.08983014295982	2.73545452704895	3.55684718243461	c
3.57825734925697	5.11151640092852	2.93045560630347	c
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-3.70134025967098	6.45589107293016	11.00499272523649	o
-10.70802453417479	-3.86485454835434	11.94813646548375	o
-2.53060574669571	7.31391223012152	6.29389912596461	o
-9.86469655693433	7.22409790129505	22.14506467545344	o
-1.68179501042187	0.63431683996890	3.17154136259107	h
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-8.81656797198498	5.05469308797688	18.36174109686041	h
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-10.87094701252491	2.51829570333169	0.21891317831287	h
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-14.73856764975431	-0.03928788465922	1.15031232075704	h
-11.98162180577645	-1.91002960771134	1.58763831863358	h
-13.60636100205542	-0.69869940082972	4.24996214869959	h
-3.97295619692746	1.55936485629659	-0.08159322364361	h
-7.14978273177383	1.45478244791508	-1.03059192902118	h
-4.96475945474726	-2.61523957633992	-2.02869998235712	h
-4.22068585452040	-3.06639902801410	1.22155716170784	h
-7.41223422595108	-3.14602880975092	0.21212249746467	h
6.73048144986971	2.26863474642278	10.25065819988454	h
5.97503172932296	-0.56780472995039	11.84128222277666	h

6.88149087303620	-0.64535375648644	8.61763006753227	h
-5.20227356614584	3.41596353623805	27.74388144313853	h
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-6.38317061392473	7.67144980759115	28.31427766990760	h
-15.88556322149665	4.93565057875483	8.78367638206261	h
-16.84958434839784	6.56801333082041	11.51057500581109	h
-19.48865885825748	2.74925854947999	10.53153810041390	h
-18.20886128426559	2.68302589687275	13.61019950379160	h
-18.07137120491493	-1.50403860076539	11.23875537812999	h
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-15.57983658571189	7.27227723489135	15.91449097842481	h
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-5.92661010030499	15.15732603945284	23.60338821410198	h
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-10.46503672784374	16.04237387363002	22.09676827934755	h
-10.36901165694864	13.18877006785031	20.27624140003865	h
3.08914203518151	-6.10623936251261	13.04549315704180	h
-1.21689750755697	-9.10669511378764	8.54734487396992	h
1.13583458583459	-6.67222398207696	8.78338899672534	h
2.05505940098994	-9.94491479693767	8.81215203523045	h
-14.74113887641911	14.61135203354728	21.76308430579353	h
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-11.32852167258199	8.33713174966049	22.40199319493992	h
-7.92058642047906	-2.47506926440701	12.30516284043988	h
-5.07899783775965	-3.18031943695273	13.17738887987911	h
-10.91070561382609	-5.32811448358645	13.03746605398671	h
-12.24728440802212	-2.80870625427025	12.23119805638222	h
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-3.17043099400497	6.88904699205648	9.19620434773141	h
-4.80662523739224	7.80663165632653	11.57194699779918	h
-0.73065120606520	7.01010307258035	5.86067331863476	h
-3.43358644854449	5.92699691054793	5.47659078048463	h
3.76368950988735	6.54763116350786	6.38507237959647	h
4.79962614001995	6.47383687850099	1.92876559445378	h
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6.18658736943953	2.23974590898295	1.85509269490289	h
6.50555952202211	3.20500633886365	5.01618923391946	h
4.90590929744086	-1.20021600948890	4.54842134453719	h
2.27596976204110	-0.14233552367360	2.82682386996111	h
-3.59702927447977	-5.66057921815695	14.25450675481396	o
-2.64875375105544	-6.76776194902996	13.09733855333623	h
-2.36283712397285	-5.48907470549088	15.63197445978295	h
4.60067345305624	1.46318269369681	21.04731480261295	h
5.18403044811236	1.75353107595179	24.34685670987201	h
6.07436673827813	-2.55554679220400	23.14883348094959	h
3.33984412794067	-2.48805722581005	25.14202446367259	h
1.95728607999382	-6.30032864385518	23.62526692169021	h
4.23607376681145	-6.74683104969830	21.18127543990279	h
-0.07818811271724	-8.80967619811723	20.44163928765363	h
-1.44245569729722	-5.72007252688403	20.41125587874543	h
4.09007138794618	-8.52929985687611	17.10673939193510	h
1.28074462149918	-10.34090397498881	16.58162074986839	h

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$end
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[La-Motex.6Water]^{+}:
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$dft
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functional b3-lyp
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gridsize 5
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1.14418622152424 0.98871272461998 10.93324215660809 c
3.24582229052415 0.75506594911725 9.25342509863949 c
-2.33227620016084 0.31104245630233 5.21637889549076 c
-4.94080909723509 0.70256793674460 5.32174800141215 c
-6.36166062916642 1.28853011819641 7.40934871058631 n
-8.76443395255106 1.80213394365794 6.57294576530675 c
-8.90752418795911 1.38800833690267 3.83964963922378 c
-6.54662304588647 0.71008603717958 3.06766005532271 c
-10.79323485689931 2.72928557730339 7.98087816268912 c
-10.94946098101075 3.43997353853468 10.56059861160690 c
-9.01162231871851 3.17470103519843 12.20988285092898 n
-9.75140342876125 4.13404867165138 14.48975180319740 c
-12.27977356129026 5.05686738283769 14.31896102383929 c
-13.06392828765936 4.60053810633591 11.84358163799848 c
-8.02417249857279 4.11672501817306 16.56487201754414 c
-5.79861562958967 3.07150186172946 16.27178695179832 n
-5.06603575415177 0.61481996253489 12.04218383073915 la
-8.04520127154016 -3.27003871308356 12.36402502428285 o
-15.59103644924605 5.24736412398248 10.71153829278098 c
-17.81422106856076 3.51954803628522 11.48510234661778 c
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-15.68247510992873 -0.43903265620333 12.69901267248585 o
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-5.69537636492482 0.08193355543282 0.43962268944759 c
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-11.23881109576119 1.66705729891015 2.25441615240294 c
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1.06555868881709 1.49633317154915 13.57636951341155 c
-1.10524722675578 1.68930377684434 14.73713887978285 n
-1.44721963916947 2.22494594096187 17.28838858894753 c
-3.89653412302100 2.98150303241239 18.09736940537431 c
-4.27291260578241 3.56249479495563 20.66325193730390 c
-2.34819486430712 3.32908269690420 22.41602159444395 c
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0.48385367846196 1.98491910169094 19.08941886272058 c
1.81079013445100 2.20753597928140 23.48687160840155 o
4.26002917474522 1.20913856521510 22.99181605207476 c
4.36540227269658 -1.64362873095635 23.24931936839085 c
2.92431203535984 -2.77953691710709 21.30507236067128 o
2.69224884801793 -5.43233548883789 21.48433285680051 c
0.50438595732085 -6.29199674346920 19.83891969667074 c
0.83754881722457 -5.81584817929238 17.20682084642993 o
2.26320942146861 -7.69117385951949 15.91210456411435 c
2.57933594522992 -7.00068630658757 13.15992999704394 c
0.24755928422169 -7.24692626075533 11.83352885883664 o
0.53937809965563 -7.03819527727392 9.16190266347563 c
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-2.52698850169734	3.79615713737604	24.92508951356993	o
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-5.45904512798226	8.62401896062873	25.36999011289388	o
-5.22008533443977	11.17492218893991	26.18723966025367	c
-6.46861304403961	12.89439253147461	24.28369403850563	c
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-10.51786703062519	13.85329055566285	22.58536793762279	c
-13.29406789657263	13.31625534037442	22.96639456550123	c
-13.82762534651543	10.75801558629055	22.35638765839408	o
-16.36892051612113	10.07004295536817	22.85393591727307	c
5.98611648010379	0.88801714237708	9.95754002348309	c
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gridsize 5
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-14.88158720737860	-0.64019858046149	12.84613590497872	o
-14.06150869678211	6.12799531547957	16.48189959923300	c
-5.88920735690411	0.53530538086230	0.38071251023589	c
-5.73712227395363	-2.33658864312422	-0.03550498456014	c
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4.71331943018012	5.87842929292040	1.66766946351776	h
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3.43054630749118	-2.38092132740896	25.11665256671084	h
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4.48392396458616	-8.31826408998719	16.98473375379021	h
1.76552376151635	-10.18685002661774	16.35606825016108	h
4.47557308362140	-8.93454323636648	12.61253074892660	h

\$user-defined bonds

\$end

II.b Explicit Hydration of Lanthanide Motexafin Complexes (Ln=La, Gd, Lu)

Table S3. Calculated change in the Gibbs energy contribution ΔG_g^{elec} and $\Delta G_g^{\text{vib+rot+trans}}$ (kJ/mol) , in the reaction $[\text{Ln-Motex}(\text{H}_2\text{O})_{n-1}]^{2+} + \text{H}_2\text{O} \rightarrow [\text{Ln-Motex}(\text{H}_2\text{O})_n]^{2+}$ (Ln=La, Gd, Lu; n=6,7)^a

		ΔG_g^{elec}	$\Delta G_g^{\text{vib+rot+trans}}$	ΔG_g
[La-Motex(H ₂ O) ₆] ²⁺	DFT/B86	-97.61	42.87	-54.74
	DFT/B3LYP	-97.92	46.97	-50.95
[Gd-Motex(H ₂ O) ₆] ²⁺	DFT/B86	-94.47	65.38	-29.09
	DFT/B3LYP	-97.27	70.54	-26.73
[Lu-Motex(H ₂ O) ₆] ²⁺	DFT/B86	-97.92	69.74	-28.18
	DFT/B3LYP	-90.47	70.91	-19.56
[La-Motex(H ₂ O) ₇] ²⁺	DFT/B86	-34.86	53.74	18.88
	DFT/B3LYP	-36.43	51.47	15.04
[Gd-Motex(H ₂ O) ₇] ²⁺	DFT/B86	-42.71	50.86	8.15
	DFT/B3LYP	-43.61	47.09	3.48
[Lu-Motex(H ₂ O) ₇] ²⁺	DFT/B86	-40.10	47.11	7.01
	DFT/B3LYP	-43.31	47.65	4.34

^a basis sets B used, i.e., 46-, 53-, 60-core-electron PPs are selected for La, Gd, Lu respectively. (8s7p6d3f2g)/[6s5p5d3f2g] basis sets are used for lanthanides. For the lighter elements def2-TZVP basis sets were applied, i.e., H (5s1p)/[3s1p] and C, O, N (11s6p2d1f)/[5s3p2d1f].

II.c Reduction Potentials of Lanthanide Motexafin Complexes (Ln=La, Gd, Lu)

Table S4. Calculated absolute reduction potentials for $[\text{Ln-Motex}(\text{H}_2\text{O})_n]^{2+/+}$ ($n=6, 7$; Ln=La, Gd, Lu) in the aqueous phase, $\Delta G_{\text{EA}}^0(\text{aq})$ (kJ/mol), and its components $\Delta G_{\text{EA}}^0(\text{g})$ (kJ/mol), ΔG_{s} , and $\Delta G'_{\text{s}}$ (kJ/mol)^a

			$\Delta G_{\text{EA}}^0(\text{g})$		ΔG_{s}	$\Delta G'_{\text{s}}$		$\Delta G_{\text{EA}}^0(\text{aq})$	
			I	II		I	II	I	II
n=0	La	BP86	-728.27	-738.48	-660.41	-336.43	-339.42	-404.29	-417.49
		B3LYP	-728.05	-744.33	-688.88	-348.52	-352.03	-387.69	-407.48
	Gd	BP86	-729.23	-738.84	-674.28	-347.20	-350.73	-402.16	-415.29
		B3LYP	-730.13	-744.02	-700.54	-356.80	-362.35	-386.38	-405.83
	Lu	BP86	-730.22	-737.75	-680.80	-351.08	-355.15	-400.49	-412.09
		B3LYP	-730.92	-746.47	-706.85	-360.91	-365.96	-384.98	-405.58
n=6	La	BP86	-632.97	-659.00	-464.09	-209.77	-207.09	-378.65	-402.00
		B3LYP	-620.82	-650.94	-467.10	-210.95	-211.68	-364.67	-395.52
	Gd	BP86	-634.73	-664.23	-460.85	-212.58	-206.83	-386.46	-410.21
		B3LYP	-626.79	-654.83	-462.85	-211.15	-207.81	-375.09	-399.80
	Lu	BP86	-632.03	-659.81	-462.28	-213.55	-207.12	-383.30	-404.65
		B3LYP	-623.80	-650.66	-465.90	-212.86	-208.79	-370.76	-393.55
n=7	La	BP86	-629.23	-658.19	-466.35	-211.95	-208.81	-374.83	-400.65
		B3LYP	-615.60	-648.57	-470.30	-215.90	-213.13	-361.20	-391.40
	Gd	BP86	-633.74	-664.83	-469.52	-220.69	-211.83	-384.91	-407.14
		B3LYP	-623.82	-652.43	-470.24	-219.20	-214.40	-372.78	-396.59
	Lu	BP86	-630.71	-661.81	-472.88	-223.86	-213.88	-381.69	-402.81
		B3LYP	-620.09	-650.96	-473.10	-221.94	-215.55	-368.93	-393.41

^a basis sets B used, cf. Table S3;

I: geometry of the $[\text{Ln-Motex}(\text{H}_2\text{O})_n]^{2+}$ is used to calculate the energy of $[\text{Ln-Motex}(\text{H}_2\text{O})_n]^+$; II: optimized geometry of $[\text{Ln-Motex}(\text{H}_2\text{O})_n]^+$ is used; $\Delta G_{\text{EA}}^0(\text{aq}) = \Delta G_{\text{EA}}^0(\text{g}) + \Delta G_{\text{s}} + \Delta G'_{\text{s}}$, where $\Delta G_{\text{EA}}^0(\text{g})$ is the calculated EA in gas phase; ΔG_{s} and $\Delta G'_{\text{s}}$ are the solvation Gibbs energies of the $[\text{Ln-Motex}(\text{H}_2\text{O})_n]^{2+}$ and $[\text{Ln-Motex}(\text{H}_2\text{O})_n]^+$, respectively.

II.d TD-DFT/BP86 and B3LYP UV-Vis Absorption Spectra of Lutetium Motexafin $[\text{Lu-Motex}]^{2+}$ in Comparison to Experimental Data

The absorption bands of the $[\text{Ln-Motex}]^{2+}$ complexes are denoted as Q (≈ 600 - 800 nm), B (≈ 450 - 600 nm), N (≈ 400 - 450 nm), L (≈ 300 - 400 nm) and M (≈ 200 - 300) nm.

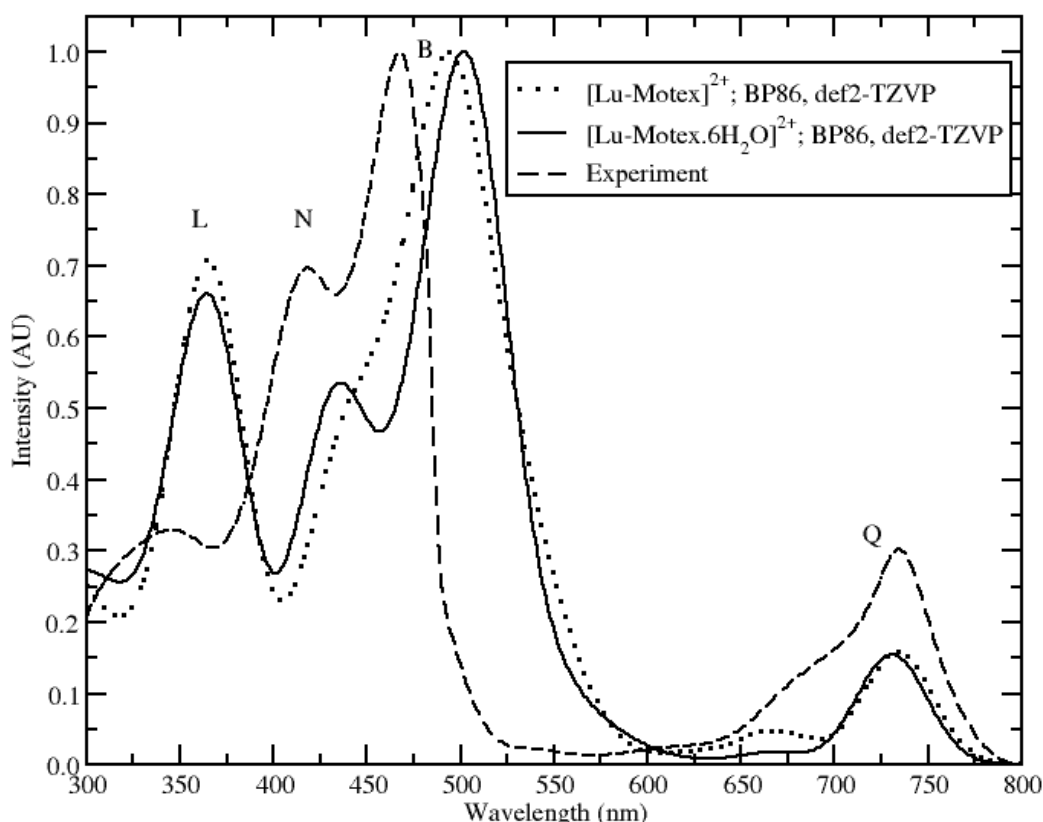


Fig. S8a:

Calculated TD-DFT/BP86 and experimental UV-Vis absorption spectra for $[\text{Lu-Motex}]^{2+}$.

The theoretical spectra were evaluated by time-dependent density functional theory (TD-DFT) for the $[\text{Lu-Motex}]^{2+}$ complexes in aqueous solution modeled by COSMO. For $[\text{Lu-Motex}.6\text{H}_2\text{O}]^{2+}$ the most strongly bound six water molecules have been taken into account explicitly. The location of the Q-band in the “therapeutic window” is accurately reproduced, and the two-peak structure of the Soret-band (B-band) is obtained when strongly bound water molecules are treated explicitly, although the position of the Soret-band is slightly red shifted compared to experiment.

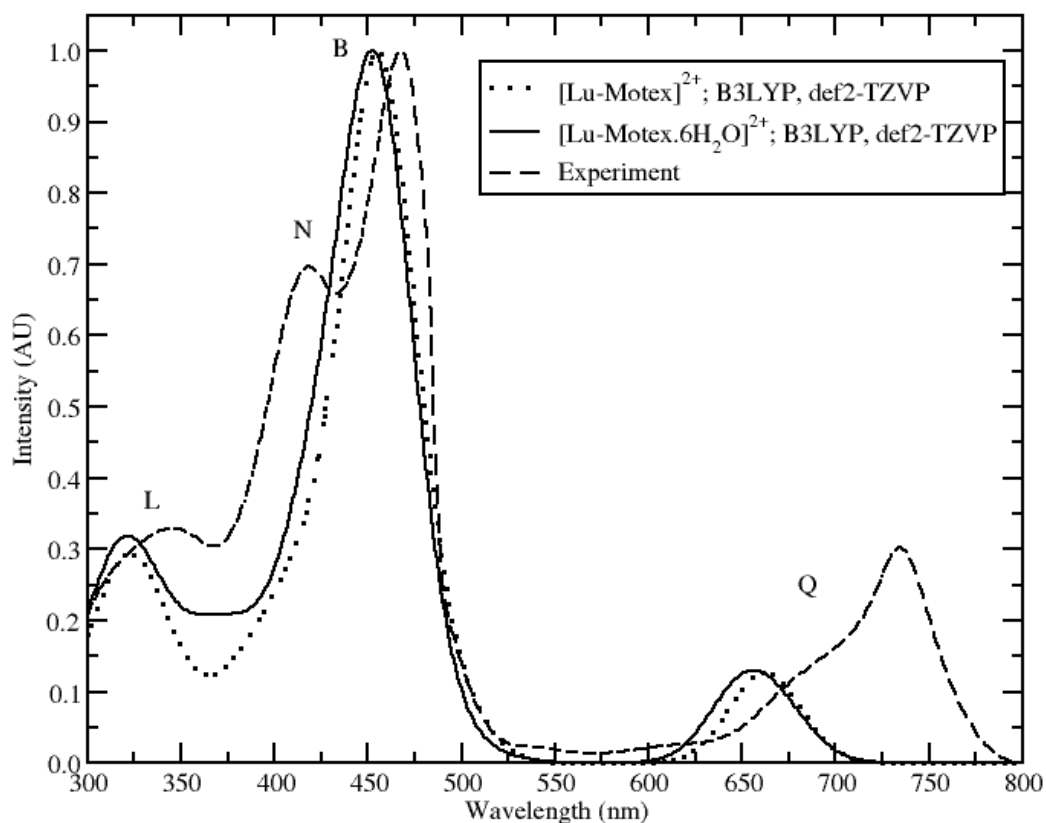


Fig. S8b:

Calculated B3LYP and experimental absorption spectra for $[\text{Lu-Motex}]^{2+}$.

The theoretical spectra were evaluated by time-dependent density functional theory (TD-DFT) for the $[\text{Lu-Motex}]^{2+}$ complexes in aqueous solution modeled by COSMO. For $[\text{Lu-Motex.6H}_2\text{O}]^{2+}$ the most strongly bound six water molecules have been taken into account explicitly. In contrast to BP86 the location of the important Q-band in the “therapeutic window” is blue shifted compared to experiment and the two-peak structure of the Soret-band (B-band) is not reproduced.

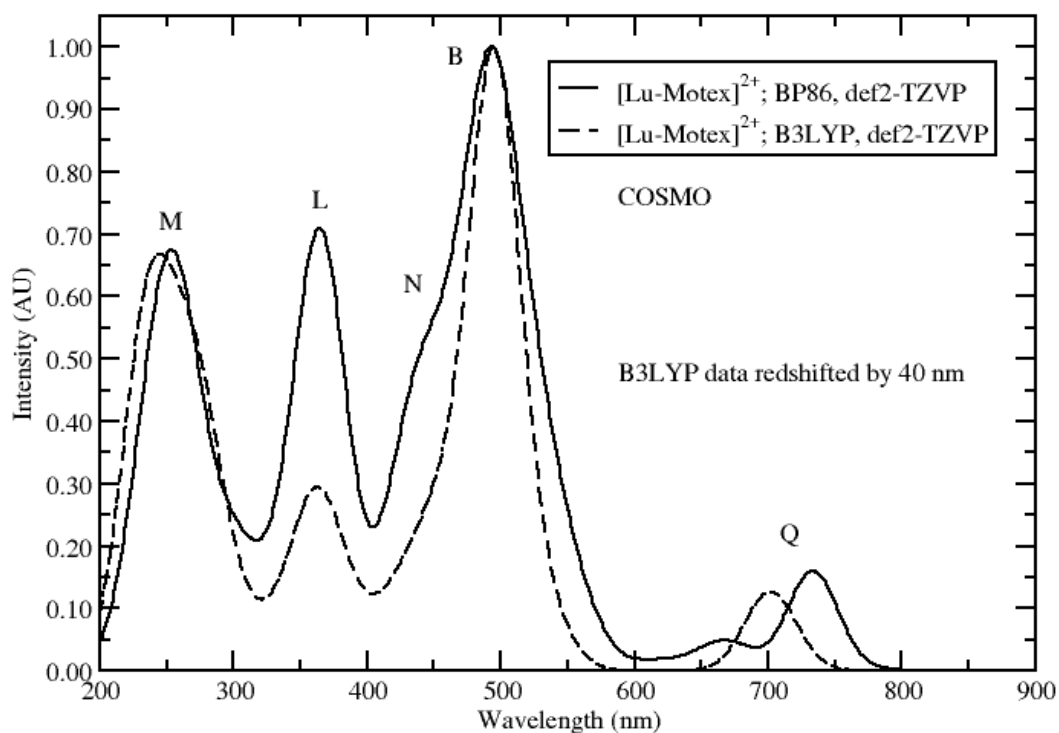


Fig. S8c:

Comparison of calculated BP86 and B3LYP UV-Vis absorption spectra for [Lu-Motex]²⁺.

The effects of bulk water was taken into account by COSMO. The B3LYP spectrum was shifted to larger wavelength by 40 nm for comparison.

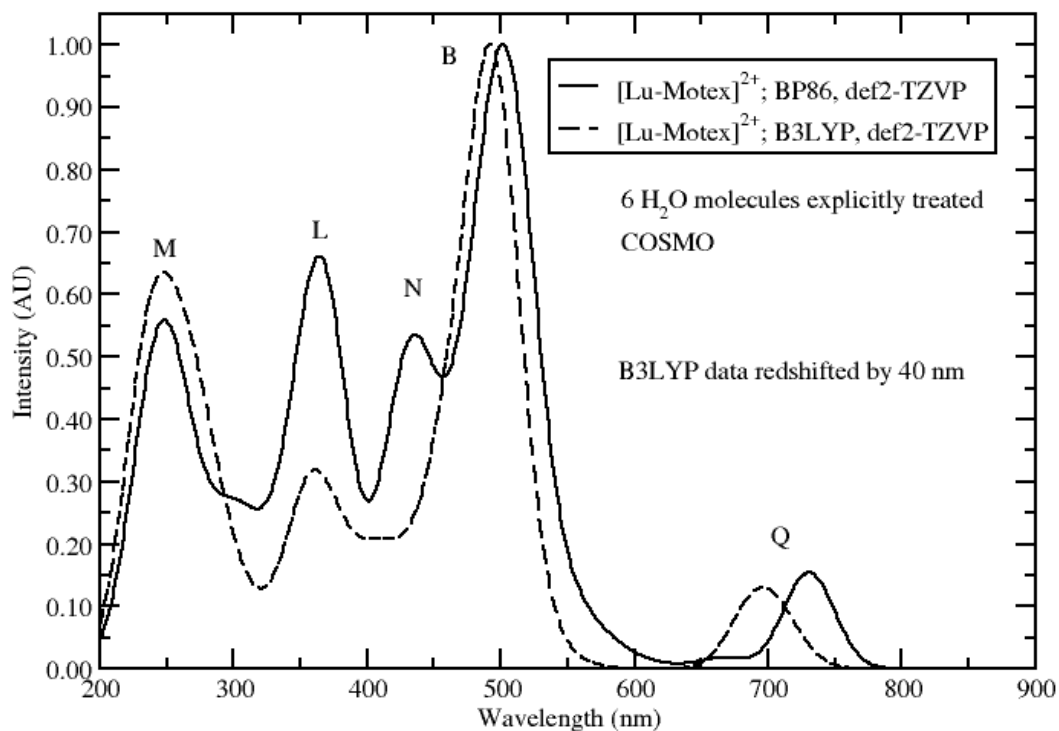


Fig. S8d:

Comparison of calculated BP86 and B3LYP UV-Vis absorption spectra for $[\text{Lu-Motex.6H}_2\text{O}]^{2+}$

The effect of bulk water was taken into account by COSMO. The B3LYP spectrum was shifted to larger wavelength by 40 nm for comparison.

II.c UV-Vis Absorption Spectra of Motexafin (Motex) Complexes of La, Gd and Lu from TD-DFT Calculations

Def2-TZVP basis sets and Ln large-core (4f-in-core) pseudopotentials (La: ECP46MWB; Gd: ECP53MWB; Lu: ECP60MWB) were used. Bulk water was simulated by COSMO.

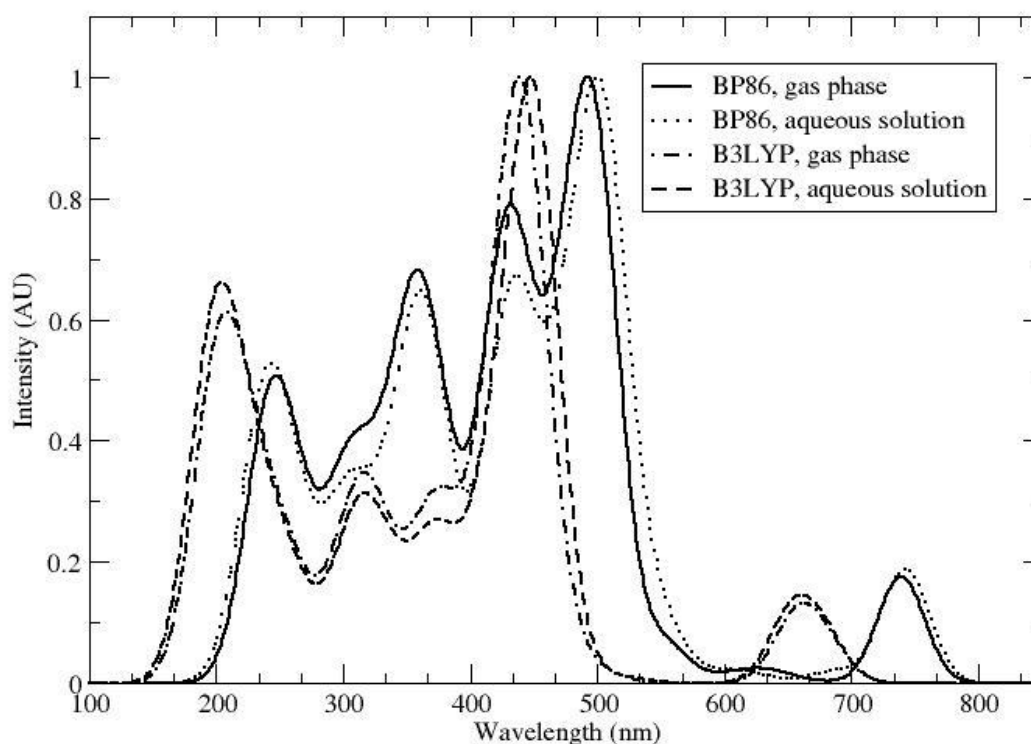


Fig. S9a:

TD-DFT/BP86 and B3LYP absorption spectra for $[\text{La-Motex.6H}_2\text{O}]^{2+}$.

In Figures 9a-9c the effect of bulk water was taken into account by COSMO. Relatively small changes in the positions of the band maxima and the relative intensities are observed when switching from a gas phase treatment to the one in solution.

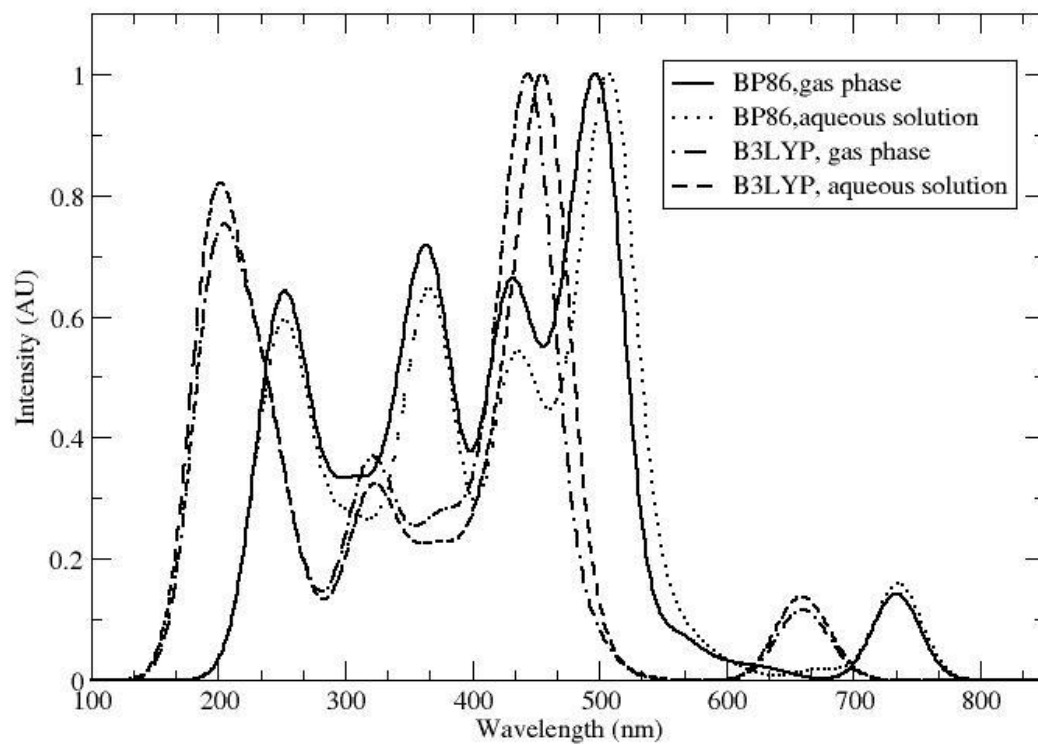


Fig. S9b:
TD-DFT/BP86 and B3LYP absorption spectra for [Gd-Motex.6H₂O]²⁺.

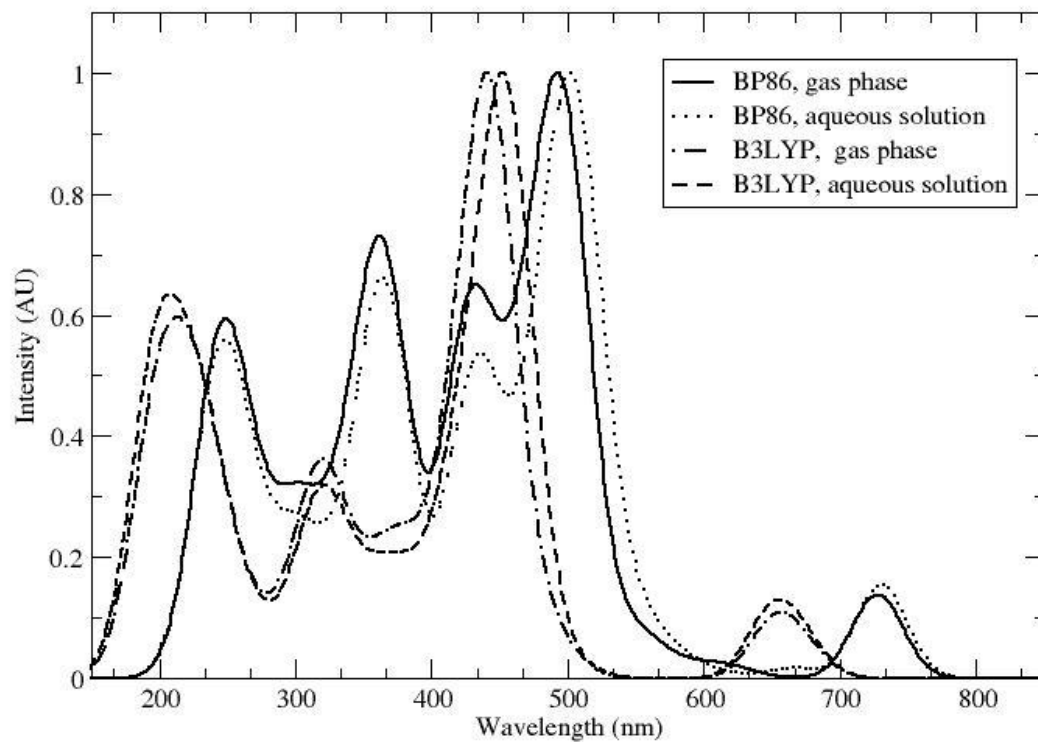


Fig. S9c:
TD-DFT/BP86 and B3LYP absorption spectra for [Lu-Motex.6H₂O]²⁺.

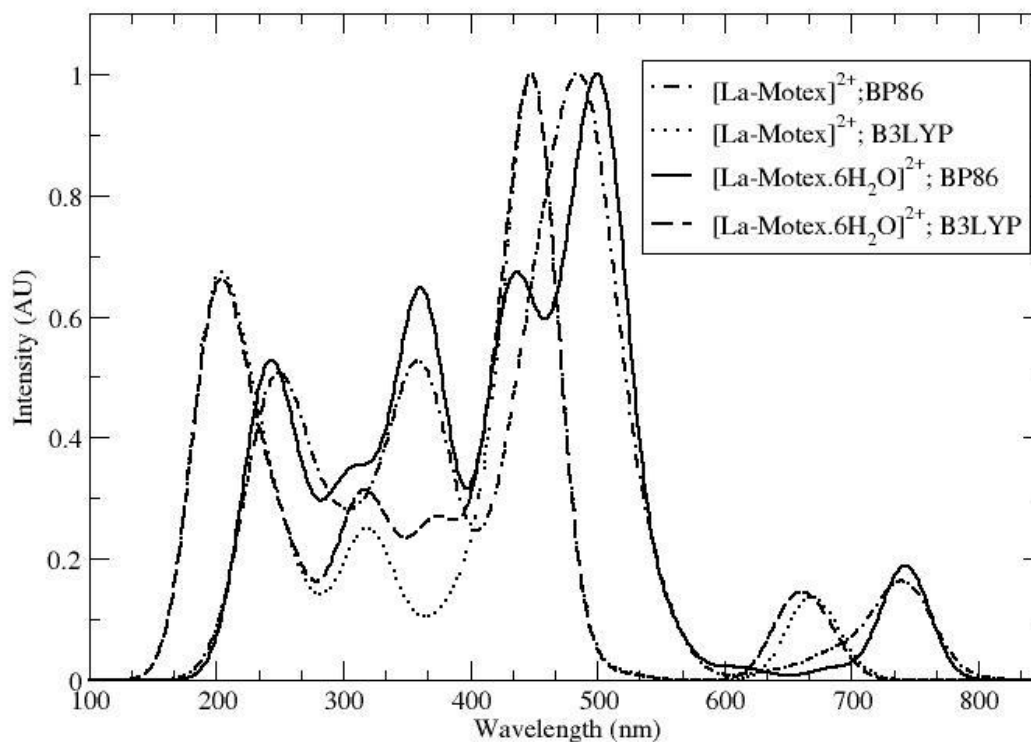


Fig. S10a:
TD-DFT/BP86 and B3LYP absorption spectra in aqueous solution for [La-Motex]²⁺ and [La-Motex.6H₂O]²⁺.

In Figures 10a-10c bulk water was taken into account by COSMO. The lowest 200 singlet-singlet excitations were calculated, i.e., the drop of the intensities to zero below 200 nm is due to the limited number of excitations calculated. When taking the six most strongly bound water molecules explicitly into account, the Soret-band undergoes a slight red shift (10-15 nm) and an additional band appears near 441 nm at the BP86 level. At the B3LYP level the Soret-band maximum is not changed by explicitly treating these strongly bound water molecules, whereas slightly higher intensities arise between 300 nm and 400 nm.

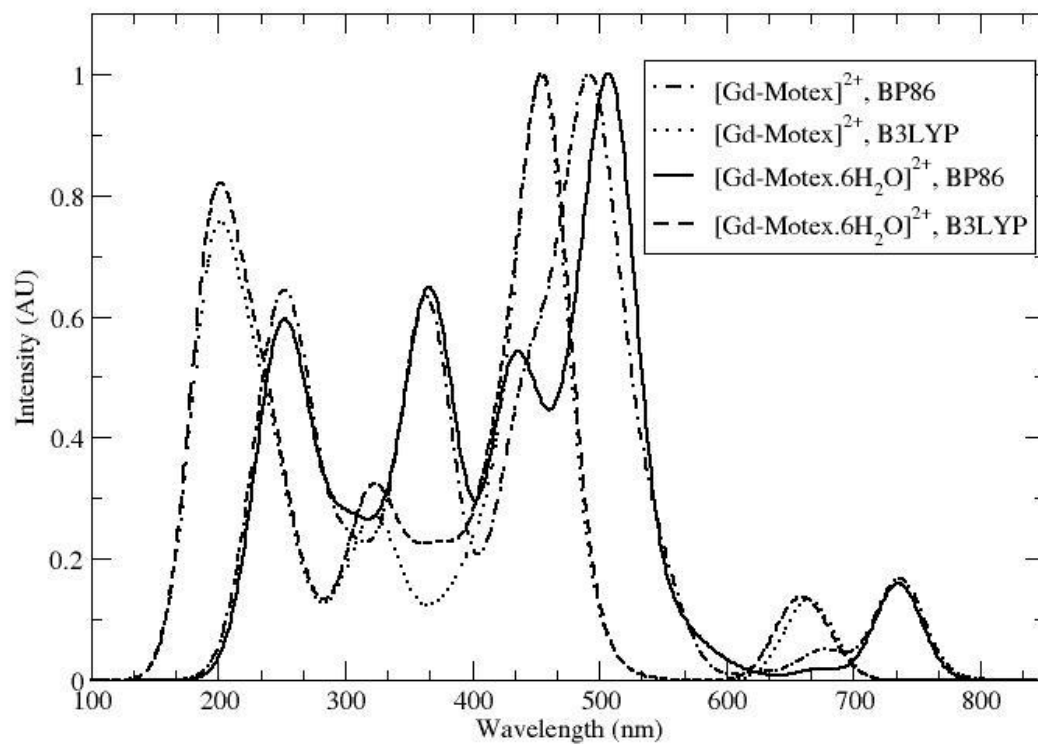


Fig. S10b:
TD-DFT/BP86 and B3LYP absorption spectra in aqueous solution for $[Gd-Motex]^{2+}$ and $[Gd-Motex.6H_2O]^{2+}$.

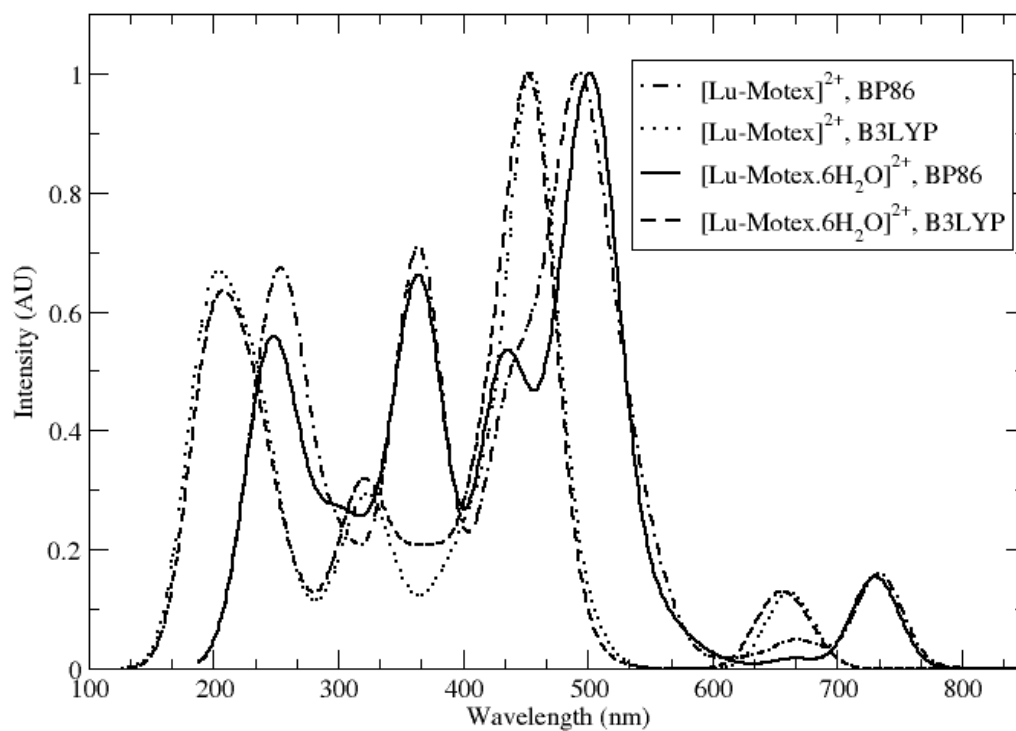


Fig. S10c:
TD-DFT/BP86 and B3LYP absorption spectra in aqueous solution for [Lu-Motex]²⁺ and [Lu-Motex.6H₂O]²⁺.

II.d. Spin-orbit Effects on the TD-DFT/BP86 Absorption Spectrum of a $C_{30}H_{30}N_5Lu$ Model System

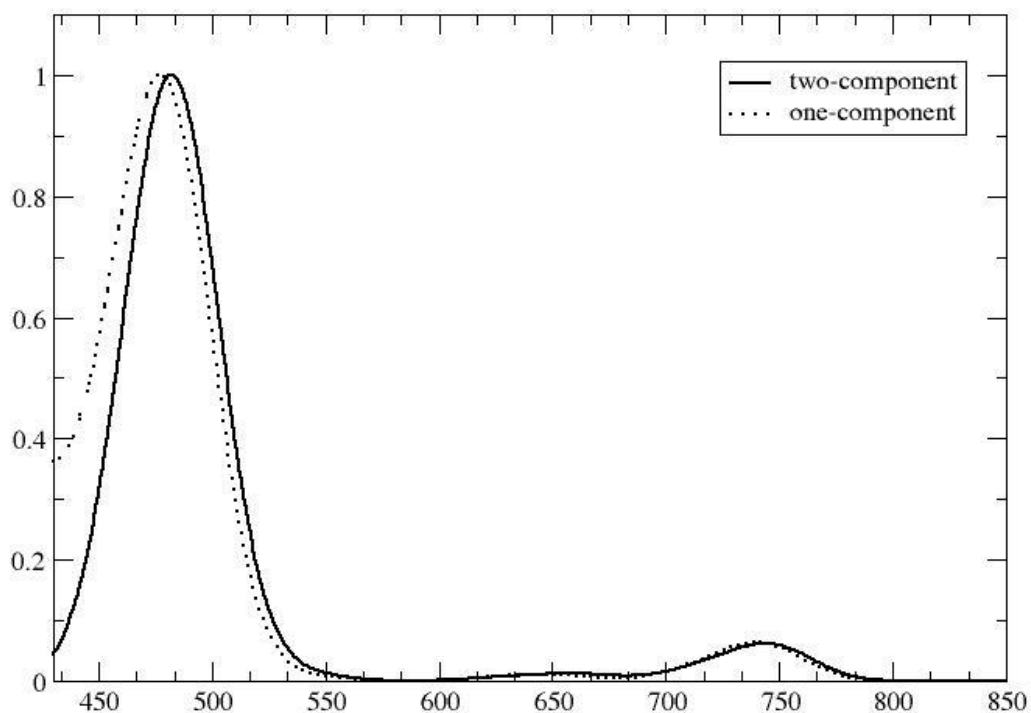
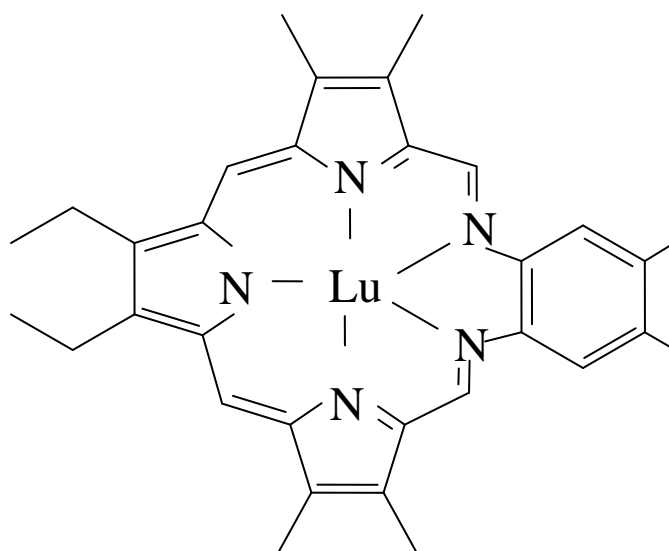


Fig. S11:
Calculated TD-DFT/BP86 absorption spectra in aqueous solution for the model system $C_{30}H_{30}N_5Lu$ (see scheme S3) using a one- and a two-component formalism.

Obviously spin-orbit effects (originating mainly from the Lu center) have only small effects on the position and the relative intensity of the B- and Q-bands.

2+



Scheme S3:
Model system $C_{30}H_{30}N_5Lu$ used in Fig. S11.