Electronic supplementary information (ESI)

Experimental and theoretical insights into the photomagnetic effects in trinuclear and ionic Cu(II)-Mo(IV) systems

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Infrared (IR) spectroscopy

Infrared (IR) absorption spectra in KBr at room temperature for samples: {[Cu(tren)]$_2$(μ-tn)}·[Mo(CN)$_8$]·7.5H$_2$O (**1**), {[Cu(tren)]$_2$[Mo(CN)$_8$]}·{[Cu(tren)]$_2$(μ-tn)}·[Mo(CN)$_8$]·9H$_2$O (**2**), and reference compounds: [Cu(tn)$_2$]$_2$[Mo(CN)$_8$]·2H$_2$O (**3**)[S1] and [Cu(tren)]$_2$[Mo(CN)$_8$]·5.25H$_2$O (**4**)[S2] and K$_4$[Mo(CN)$_8$]·2H$_2$O (**K$_4$Mo**) salt[S3] are collected in **Figure S1**.

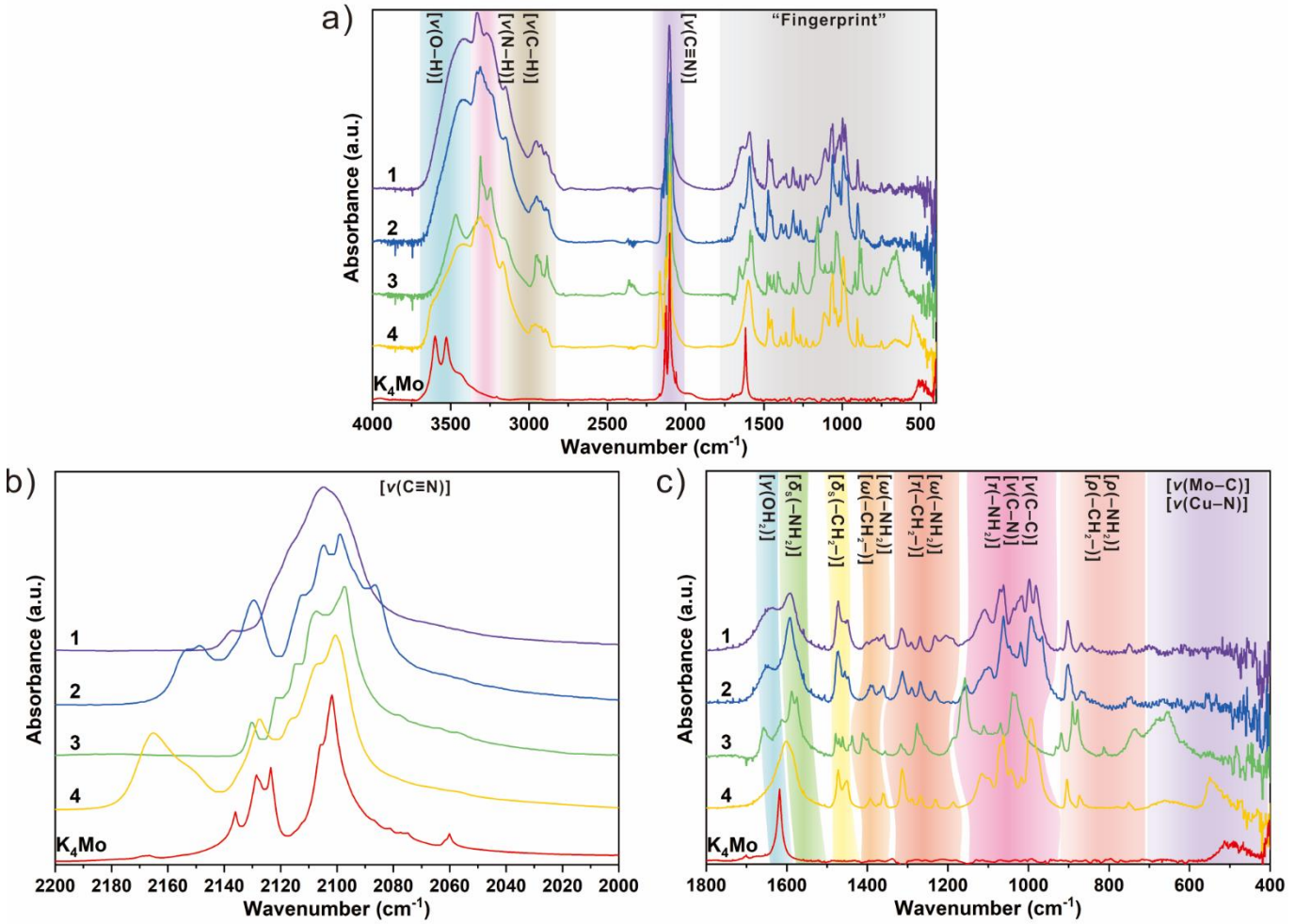


Figure S1. Infrared (IR) absorption spectra in KBr of **1** – **4** and **K$_4$Mo** in: the 4000 – 400 cm^{-1} range (**a**), the cyanide stretching bands (**b**), and the fingerprint region (**c**) with assignment.[S4]

Thermogravimetric analysis

Thermogravimetric studies in under air for powdered samples of **1** – **4** are shown in **Figure S2**. Most compounds show several step endothermic process of water evaporation in the 25 - 130°C temperature range. Compound **1** released in total about 7H_2O molecules in three steps at 49, 59, and 81°C. Complex **2** shows similar behavior with a three-step release of approx. 4.5H_2O at slightly higher temperatures 66, 88, and 108°C. While two reference compounds **3** and **4** exhibits single-step release of 2H_2O at 93°C and a three-step release of about 3H_2O at 84, 107 and 127°C, respectively. Comparing all the samples, it can be stated that introducing neutral cyanido-bridged V-shaped trinuclear molecules into the structure leads to an increase of crystallization water thermal stability. Simultaneously, attention should be paid to the considerable discrepancies between the amounts of water determined by the crystal structure analysis, TGA, and elemental analysis for **2** and **4**, which suggest that the crystals immediately lose some water after vacuum filtration and grinding. In the case of **1** and **2**, there is no such discrepancy. After losing the solvent, the samples are stable up to 144, 145, 157, and 164°C for **1**, **3**, **2,** and **4**, respectively, after which they decompose with the release of cyanides and other organic components. Two exothermic peak at about 270 and 370°C corresponding to the decomposition of organic components, and the oxidation of volatiles, char part and residues of metals.

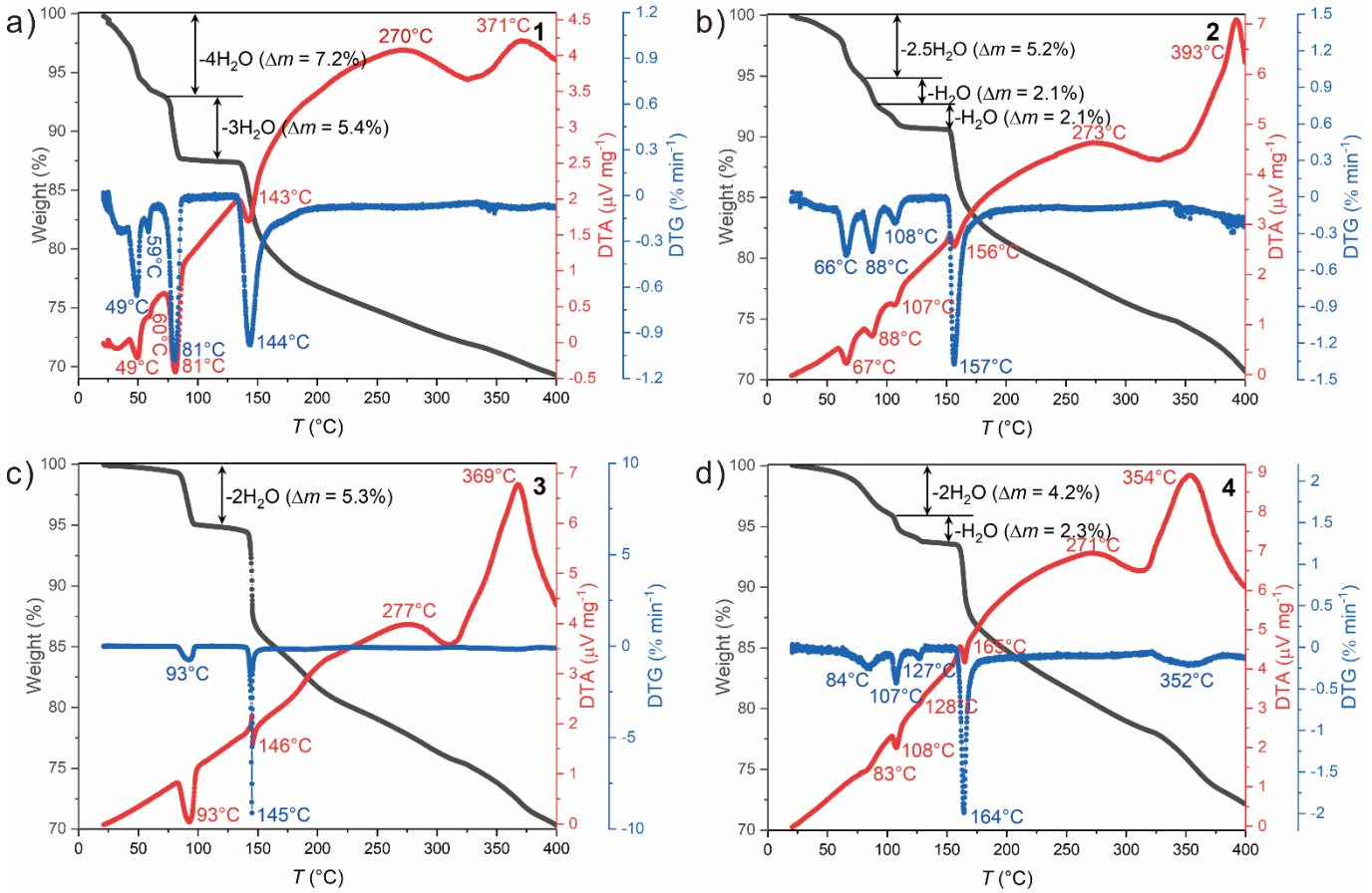


Figure S2. Thermogravimetric analyses (TGA – black, DTA – red and DTG - blue) of **1** – **4** (**a** – **d**).

Powder X-ray diffraction (PXRD) studies

The measured and calculated formulas for **1** - **4** (**Figure S3**) overlap almost perfectly, which confirms the high purity and homogeneity of the powder samples. The slight shift in the position of the experimental diffraction peaks of **1**, **2,** and **4** in relation to the calculated ones is due to the difference in the measurement temperature (PXRD - room temperature (293 K), SCXRD – 120, 90, and 123 K for **1**, **2** and **4**, respectively). Moreover, the differences in the intensity of the diffraction peaks are due to the texture effect, especially for compound **4** with an almost needle crystal morphology.

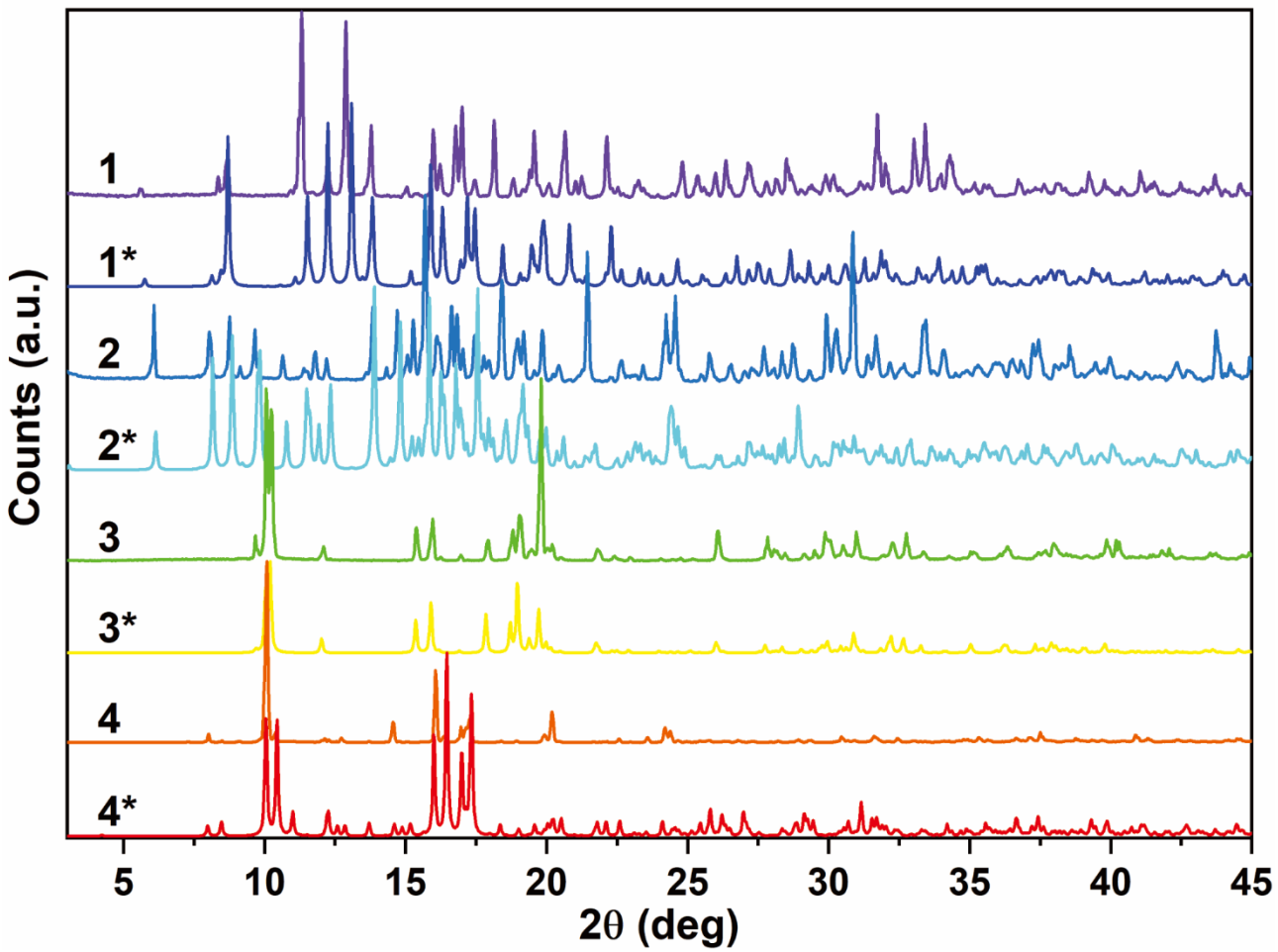


Figure S3. Experimental diffractograms of **1** – **4**, and calculated diffractograms **1*** – **4*** base on SCXRD data.

Single crystal X-ray diffraction (SCXRD) studies

Table S1. Selected crystallographic parameters for **1** and **2**.

	1	**2**
Formula	$C_{23}H_{61}Cu_2MoN_{18}O_{7.5}$	$C_{43}H_{100}Cu_4Mo_2N_{34}O_9$
M_W (g/mol)	932.91	1683.6
T (K)	120(2)	90(2)
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
a (Å)	16.6475(5)	10.2337(7)
b (Å)	14.2743(4)	11.6832(9)
c (Å)	18.1668(5)	57.516(4)
α (°)	90	90
β (°)	112.784(2)	90.691(6)
γ (°)	90	90
V (Å^3)	3980.2(2)	6876.3(8)
Z	4	4
ρ_{calc} (g/cm^3)	1.557	1.626
μ (mm-1)	1.433	1.642
F(000)	1940	3472
Crystal size (mm^3)	0.20 × 0.10 × 0.10	0.284 × 0.243 × 0.069
Radiation	MoK_α (λ = 0.71073)	MoK_α (λ = 0.71075)
2θ range (°)	9.476 to 54.818	6.026 to 54.97
Index ranges	-21 ≤ h ≤ 21, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -74 ≤ l ≤ 74
Reflections collected/unique	16972/8989 [R_{int} = 0.0324, R_Σ = 0.0484]	64860/15719 [R_{int} = 0.1716, R_Σ = 0.1535]
Refinement method	Full–matrix least–squares on F^2	Full–matrix least–squares on F^2
Data/restraints/parameters	8989/0/506	15719/24/882
GOF on F^2	1.058	1.046
R_1/wR_2 (I>2σ(I))	0.0364/0.0800	0.0816/0.1252
R_1/wR_2 (all data)	0.0605/0.0898	0.1596/0.1526
Largest diff. peak and hole (e/Å^3)	0.60/-0.56	3.34/-1.29
CCDC number	2123304	2123305

Table S2. CShM analysis for the five-coordinated Cu^{II} and eight-coordinated Mo^{IV} centers of **1** - **4**.

Geometry	S_{TBPY-5}	S_{SPY-5}	S_{vOC-5}	Geometry	S_{BTPR-8}	S_{SAPR-8}	S_{TDD-8}	Ref.
ideal TBPY-5	**0.000**	5.384	7.342	ideal BTP-8	**0.000**	2.262	2.709	**S5**, **S6**
ideal SPY-5	5.384	**0.000**	1.741	ideal SAPR-8	2.267	**0.000**	2.848	
ideal vOC-5	7.342	1.741	**0.000**	ideal TDD-8	2.717	2.848	**0.000**	
1_[Cu2(tren)(μ-tn)]	**0.771**	3.347	4.857	**1**_[Mo1(CN)$_8$]	2.035	**0.220**	2.160	This work
1_[Cu3(tren)(μ-tn)]	**0.326**	4.990	6.999					
2_[Cu2(tren)(μ-tn)]	**1.438**	2.408	3.573	**2**_[Mo1(CN)$_8$]	2.043	2.685	**0.305**	
2_[Cu3(tren)(μ-tn)]	**0.317**	4.644	6.476	**2**_[Mo4(CN)$_8$]	1.651	**0.633**	1.044	
2_[Cu5(tren)(μ-CN)]	**0.486**	4.050	5.761					
2_[Cu6(tren)(μ-CN)]	**0.666**	3.429	4.969					
3_[Cu1(tn)$_2$(μ-CN)]	2.455	**1.209**	2.279	**3**_[Mo1(CN)$_8$]	2.288	**0.154**	2.419	**S1**
4_[Cu1(tren)(μ-CN)]	2.530	**1.521**	2.694	**4**_[Mo1(CN)$_8$]	2.184	2.311	**0.227**	**S2**
4_[Cu2(tren)(μ-CN)]	**0.399**	4.190	6.176					

S_{TBPY-5}, S_{SPY-5}, S_{vOC-5} - the shape measure relative to trigonal bipyramid, square pyramid, and vacant octahedron, respectively; S_{BTPR-8}, S_{SAPR-8}, S_{TDD-8} - the shape measure relative to bicapped trigonal prism, square antiprism, and triangular dodecahedron, respectively; smaller S-value reflect a better match with the ideal geometry (S = 0).

Table S3. Selected distances and angles for **1** and **2**.

Distances [Å]										
1					**2**					
Cu2-N21	2.033(3)	C1-N1	1.163(4)		Cu2-N21	2.055(6)	Mo1-C1	2.155(9)	C1-N1	1.169(10)
Cu2-N22	2.074(3)	C2-N2	1.151(4)		Cu2-N22	2.072(6)	Mo1-C2	2.153(8)	C2-N2	1.165(9)
Cu2-N23	2.093(3)	C3-N3	1.159(4)		Cu2-N23	2.057(7)	Mo1-C3	2.159(8)	C3-N3	1.171(10)
Cu2-N24	2.131(3)	C4-N4	1.148(4)		Cu2-N24	2.170(6)	Mo1-C4	2.171(8)	C4-N4	1.146(9)
Cu2-N41	2.005(3)	C5-N5	1.151(4)		Cu2-N41	2.023(6)	Mo1-C5	2.188(8)	C5-N5	1.149(9)
Cu3-N31	2.038(3)	C6-N6	1.148(4)		Cu3-N31	2.048(6)	Mo1-C6	2.157(8)	C6-N6	1.166(10)
Cu3-N32	2.072(3)	C7-N7	1.154(4)		Cu3-N32	2.076(7)	Mo1-C7	2.130(8)	C7-N7	1.167(9)
Cu3-N33	2.097(2)	C8-N8	1.157(4)		Cu3-N33	2.097(6)	Mo1-C8	2.192(8)	C8-N8	1.137(9)
Cu3-N34	2.109(2)	<C-N>	1.154(4)		Cu3-N34	2.077(7)	Mo4-C11	2.182(8)	C11-N11	1.130(9)
Cu3-N42	1.989(2)				Cu3-N42	2.014(6)	Mo4-C12	2.165(8)	C12-N12	1.172(9)
$<Cu\text{-}N>_{ax}$	2.016(3)				Cu5-N51	2.036(6)	Mo4-C13	2.134(8)	C13-N13	1.145(9)
$<Cu\text{-}N>_{eq}$	2.096(3)				Cu5-N52	2.051(7)	Mo4-C14	2.162(7)	C14-N14	1.151(9)
Mo1-C1	2.157(3)				Cu5-N53	2.106(6)	Mo4-C15	2.164(8)	C15-N15	1.151(10)
Mo1-C2	2.149(3)				Cu5-N54	2.101(7)	Mo4-C16	2.166(7)	C16-N16	1.163(9)
Mo1-C3	2.156(3)				Cu5-N13	1.953(7)	Mo4-C17	2.169(7)	C17-N17	1.148(9)
Mo1-C4	2.158(3)				Cu6-N61	2.039(8)	Mo4-C18	2.167(8)	C18-N18	1.153(9)
Mo1-C5	2.168(3)				Cu6-N62	2.054(6)	<Mo-C>	2.163(8)	<C-N>	1.155(9)
Mo1-C6	2.176(3)				Cu6-N63	2.146(7)				
Mo1-C7	2.169(3)				Cu6-N64	2.063(6)				
Mo1-C8	2.169(3)				Cu6-N11	1.978(7)				
<Mo-C>	2.163(3)				$<Cu\text{-}N>_{ax}$	2.018(7)				
					$<Cu\text{-}N>_{eq}$	2.089(7)				

Angles [°]					
1		**2**			
Mo1-C1-N1	176.1(3)	Mo1-C1-N1	177.8(7)	Mo4-C15-N15	174.4(7)
Mo1-C2-N2	176.3(3)	Mo1-C2-N2	177.6(7)	Mo4-C16-N16	176.7(7)
Mo1-C3-N3	176.9(3)	Mo1-C3-N3	178.1(7)	Mo4-C17-N17	176.8(6)
Mo1-C4-N4	178.0(3)	Mo1-C4-N4	177.1(7)	Mo4-C18-N18	179.4(7)
Mo1-C5-N5	177.2(3)	Mo1-C5-N5	177.5(6)	<Mo-C-N>	177.1(7)
Mo1-C6-N6	177.9(3)	Mo1-C6-N6	178.9(7)	Cu5-N13-C13*	155.1(6)
Mo1-C7-N7	178.0(3)	Mo1-C7-N7	176.1(7)	Cu6-N11-C11*	149.4(6)
Mo1-C8-N8	178.4(3)	Mo1-C8-N8	178.6(7)	<Cu-N-C*>	152.3(6)
<Mo-C-N>	177.4(3)	Mo4-C11-N11*	176.4(6)	C11-Mo4-C13*	74.4(3)
		Mo4-C12-N12	177.6(6)		
		Mo4-C13-N13*	174.3(7)		
		Mo4-C14-N14	177.0(6)		

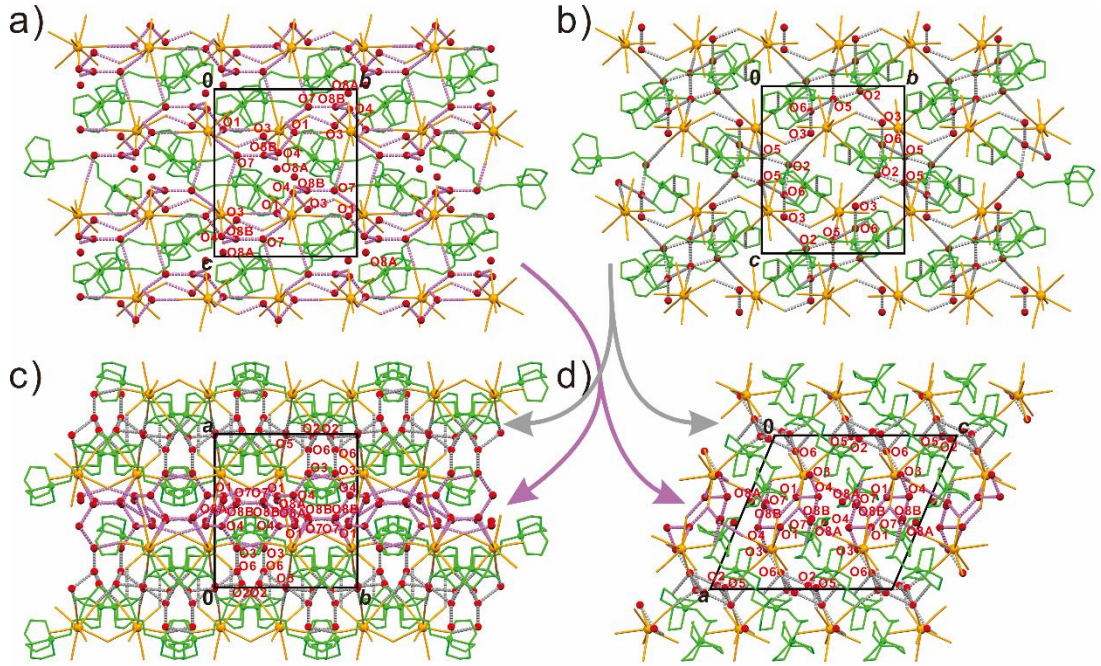


Figure S4. Packing of **1** and hydrogen bond networks (grey and pink dotted lines) along (100) (**a** – layer I and **b** – layer II), (010) (**c**) and (001) crystallographic directions (**d**). Legend: $\{[Cu(tren)]_2(\mu\text{-}tn)\}^{2+}$ ions – green sticks, isolated $[Mo(CN)_8]^{4-}$ anions – orange sticks, and crystallization water molecules – red balls. Hydrogen atoms have been omitted for clarity.

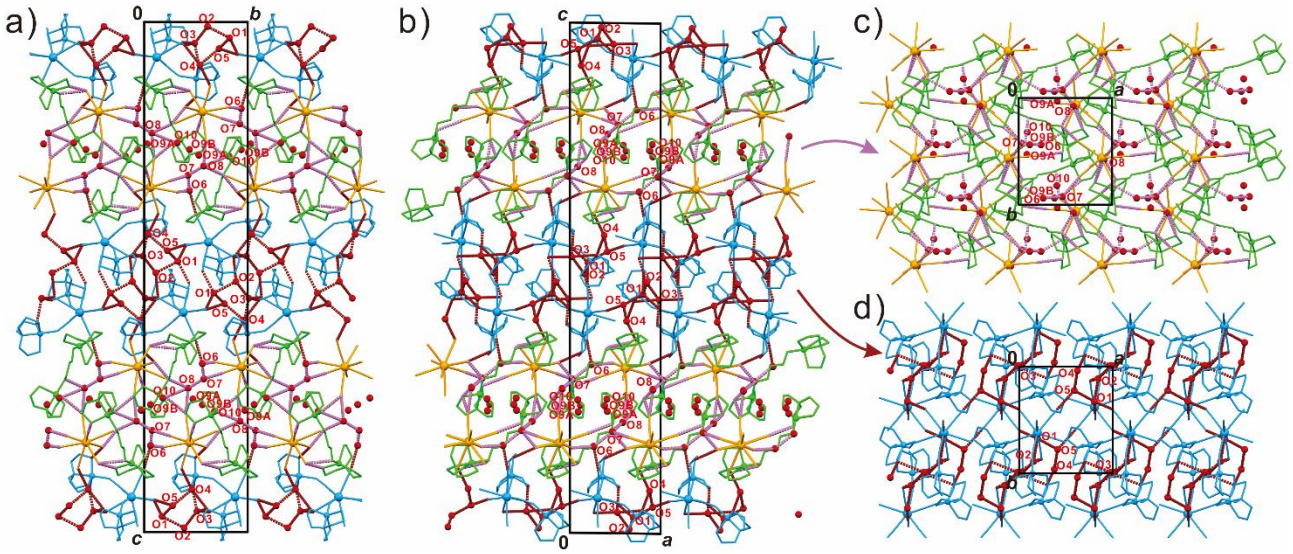


Figure S5. Packing of **2** and hydrogen bond networks (pink and dark red dotted lines) along (100) (**a**), (010) (**b**) and (001) crystallographic directions (**c** – layer I and **d** – layer II). Legend: $\{[Cu(tren)]_2(\mu\text{-}tn)\}^{2+}$ ions – green sticks, isolated $[Mo(CN)_8]^{4-}$ anions – orange sticks, neutral V-shaped trinuclear $\{[Cu^{II}(tren)]_2[Mo^{IV}(CN)_8]\}$ molecules – blue sticks, crystallization water molecules – red balls. Hydrogen atoms have been omitted for clarity.

Computational details

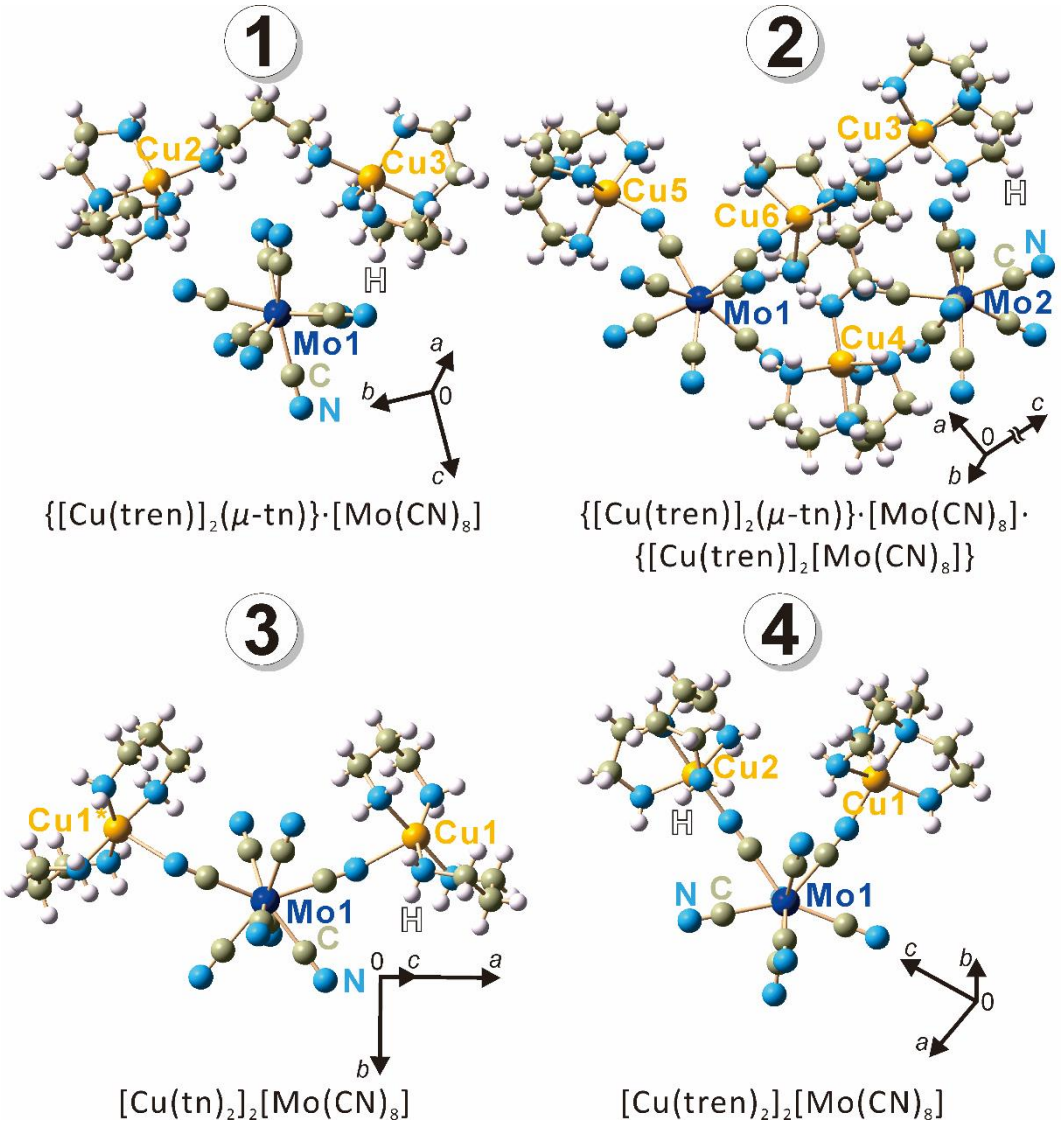
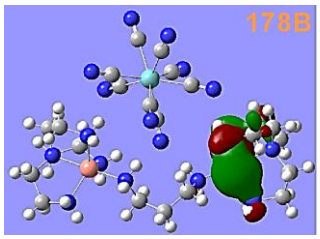
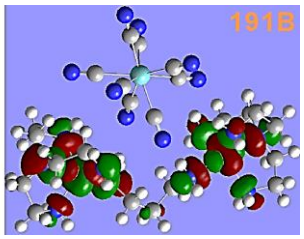


Figure S6. Models used for quantum chemical calculations. Water molecules are omitted.

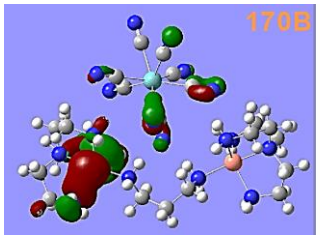
List of calculated excitation energies with non-zero oscillator strengths (*f*) for **1**.

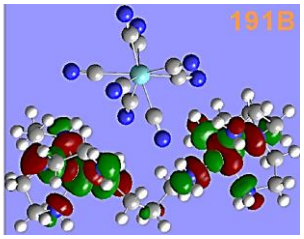
Excited State 3: 3.007-A 1.3640 eV 908.95 nm
f = 0.0005 <S^2> = 2.011
155B ->191B 0.15047
178B ->191B 0.98249



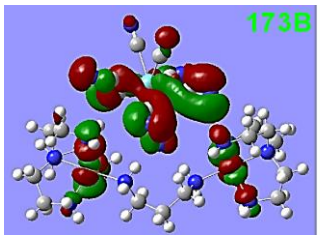


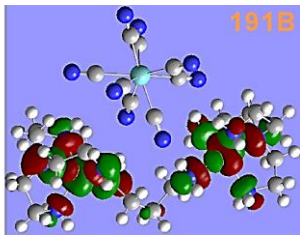
Excited State 5: 3.007-A 1.5325 eV 809.03 nm
f = 0.0010 <S^2> = 2.011
154B ->191B 0.11394
169B ->191B -0.20974
170B ->191B 0.40183



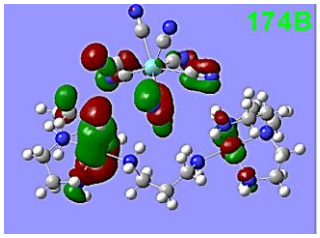


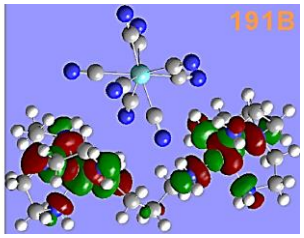
171B ->191B 0.21274
173B ->191B -0.40091



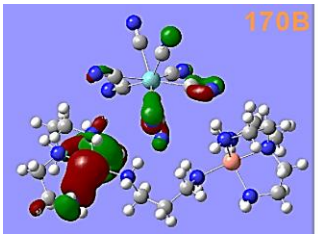


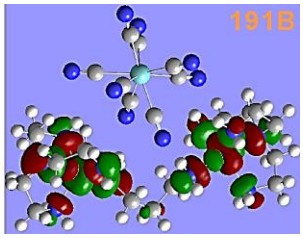
174B ->191B 0.71946



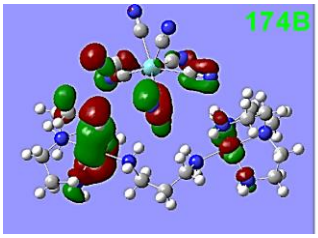


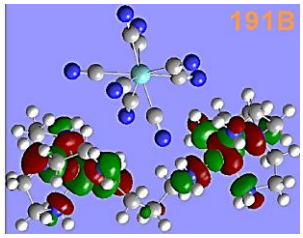
175B ->191B -0.11402
Excited State 7: 3.007-A 1.6067 eV 771.68 nm
f = 0.0009 <S^2> = 2.011
149B ->191B 0.10375
154B ->191B -0.11428
169B ->191B -0.13023
170B ->191B 0.83668



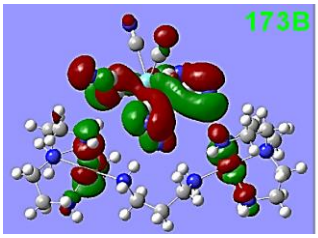


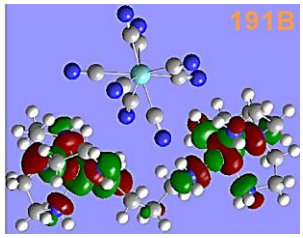
172B ->191B -0.10330
173B ->191B 0.20723
174B ->191B -0.34127



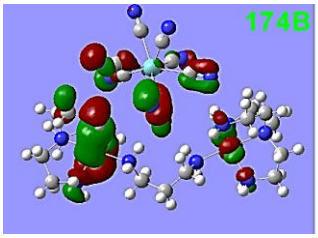


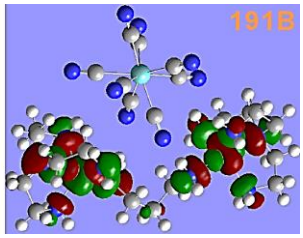
187B ->191B -0.23805
Excited State 8: 3.008-A 1.6547 eV 749.27 nm
f = 0.0006 <S^2> = 2.012
151B ->191B 0.10701
171B ->191B 0.13226
172B ->191B -0.11218
173B ->191B 0.44829



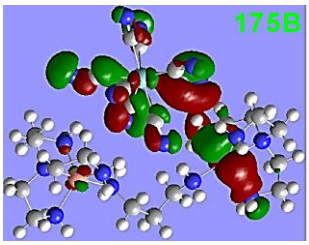


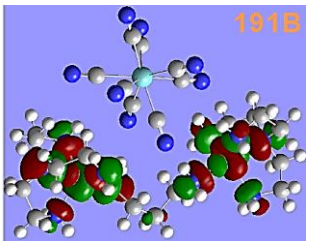
174B ->191B 0.33558





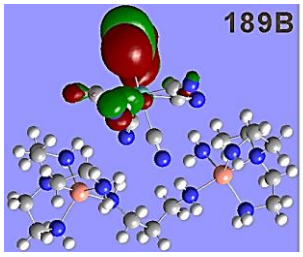
175B ->191B 0.77011

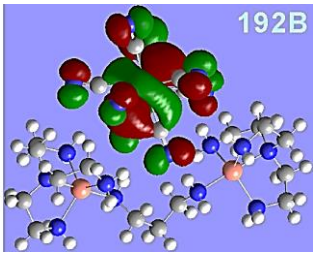




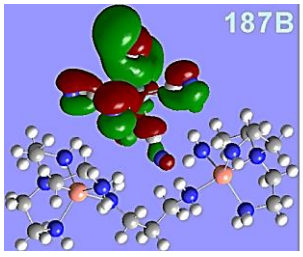
186B ->191B -0.12804

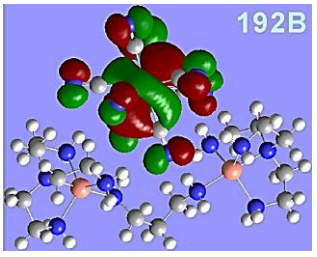
Excited State 22: 3.028-A 2.4191 eV 512.51 nm
f = 0.0010 <S^2> = 2.042
189B ->192B 0.98891



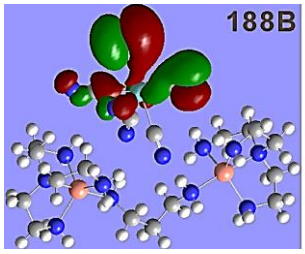


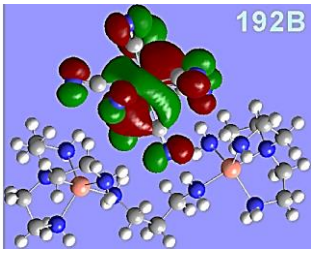
Excited State 25: 3.029-A 2.5492 eV 486.36 nm
f = 0.0028 <S^2> = 2.044
187B ->192B -0.23632



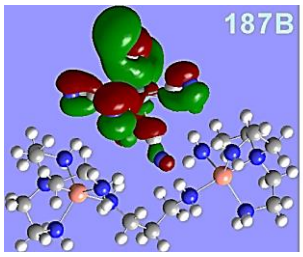


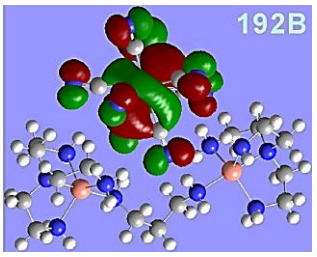
188B ->192B 0.95927



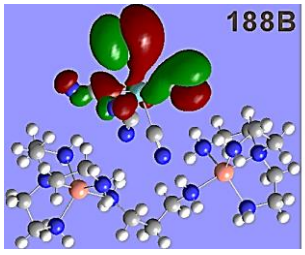


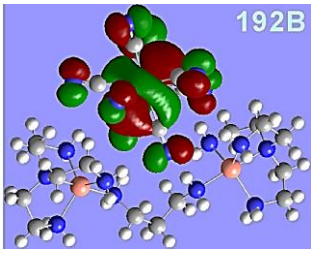
Excited State 27: 3.030-A 2.7411 eV 452.31 nm
f = 0.0095 <S^2> = 2.046
187B ->192B 0.95854



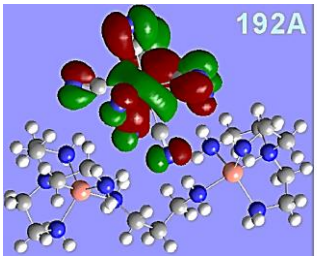


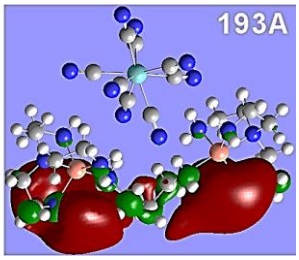
188B ->192B 0.23334





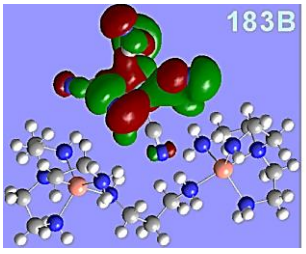
Excited State 28: 3.033-A 2.7754 eV 446.72 nm
f = 0.0007 <S^2> = 2.050
192A ->193A 0.99852

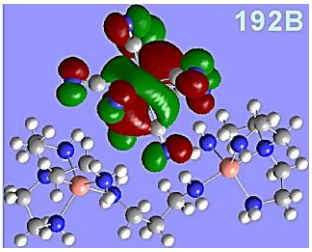




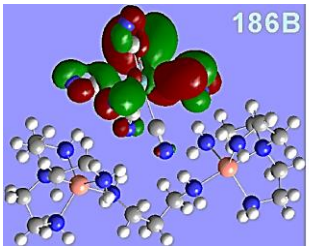
Excited State 29: 3.009-A 2.8837 eV 429.95 nm
f = 0.0002 <S^2> = 2.013
172B ->191B 0.21690
173B ->191B 0.38019
175B ->191B -0.33895
176B ->191B 0.81185

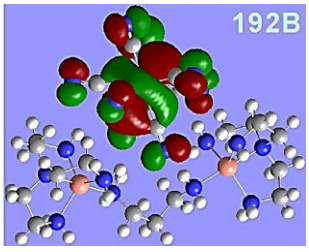
Excited State 30: 3.037-A 2.8954 eV 428.21 nm
f = 0.0095 <S^2> = 2.056
183B ->192B 0.10838



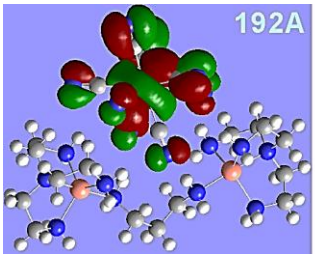


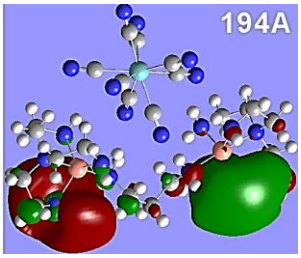
186B ->192B 0.97766



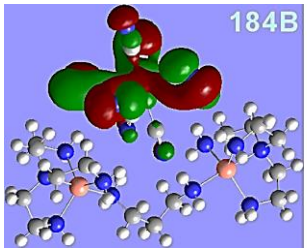


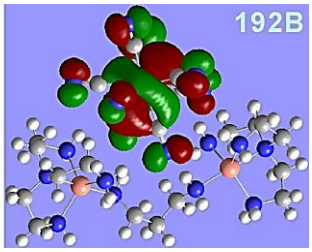
Excited State 33: 3.034-A 2.9932 eV 414.22 nm
f = 0.0012 <S^2> = 2.051
192A ->194A 0.99853



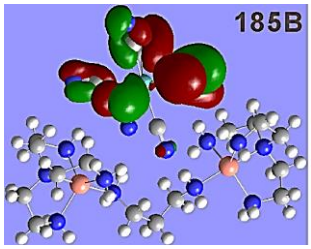


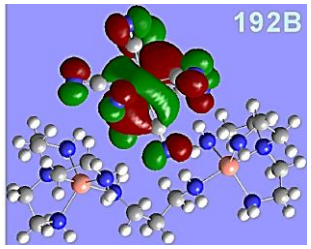
Excited State 35: 3.033-A 3.0399 eV 407.85 nm
f = 0.0024 <S^2> = 2.050
184B ->192B -0.38824



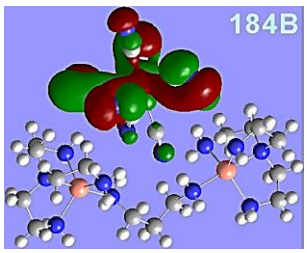


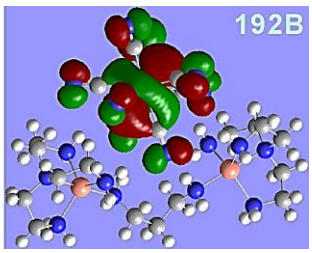
185B ->192B 0.90680



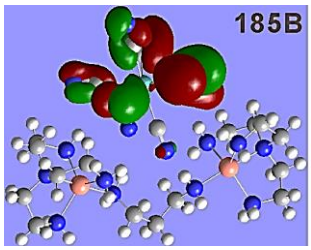


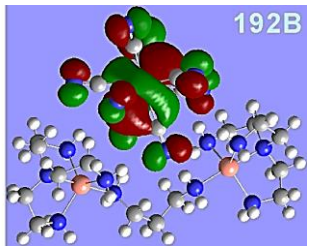
Excited State 37: 3.039-A 3.1871 eV 389.02 nm
f = 0.0029 <S^2> = 2.059
184B ->192B 0.90379



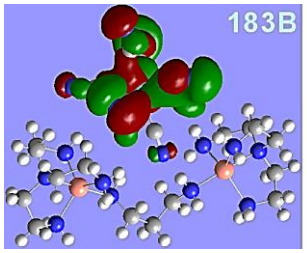


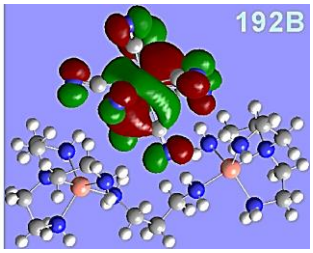
185B ->192B 0.39474



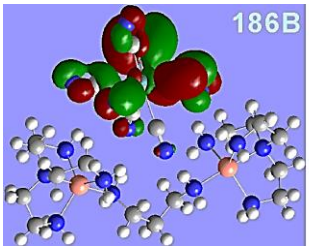


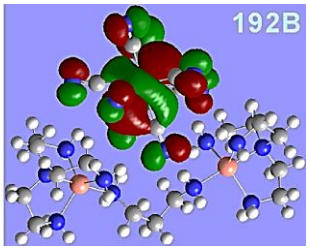
Excited State 38: 3.031-A 3.2696 eV 379.20 nm
f = 0.0029 <S^2> = 2.046
183B ->192B 0.96466



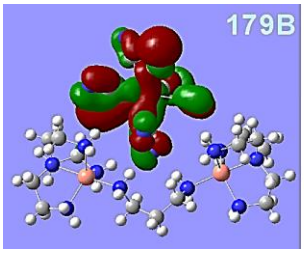


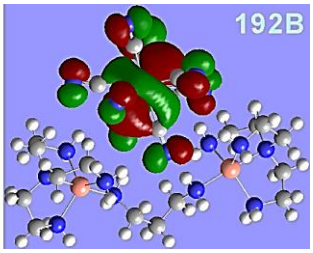
186B ->192B -0.11365



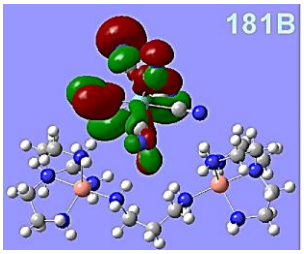


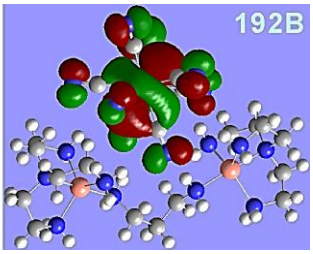
Excited State 40: 3.044-A 3.4807 eV 356.20 nm
f = 0.0050 <S^2> = 2.067
179B ->192B -0.30015



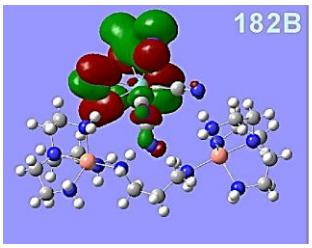


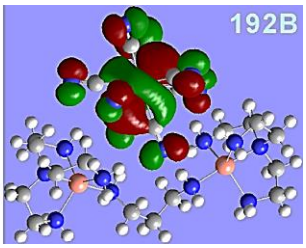
181B ->192B 0.27115



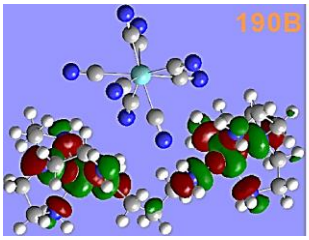


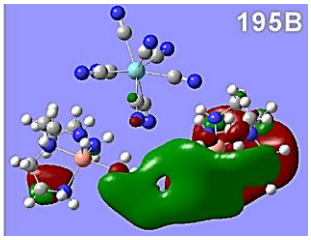
182B ->192B 0.87399



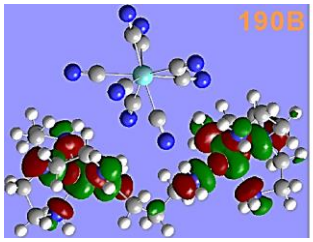


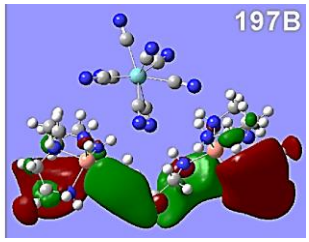
183B ->192B -0.10952
190B ->195B -0.12165
Excited State 41: 3.608-A 3.4842 eV 355.85 nm
f = 0.0014 <S^2> = 3.005
182B ->192B 0.11032
190B ->195B 0.96031





190B ->197B -0.21908



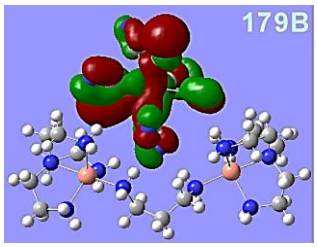


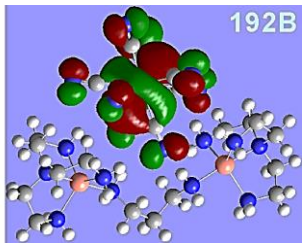
Excited State 42: 3.034-A 3.5700 eV 347.29 nm

f = 0.0007 <S^2> = 2.052

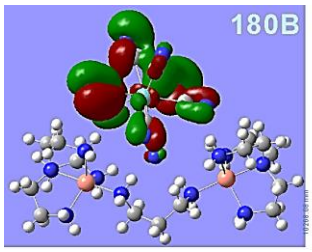
167B ->191B -0.11109

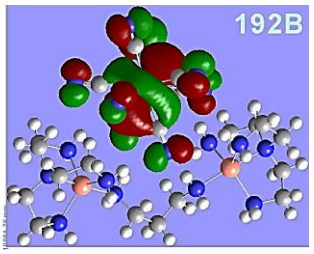
179B ->192B 0.24342



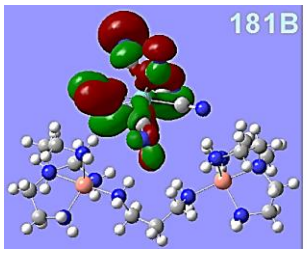


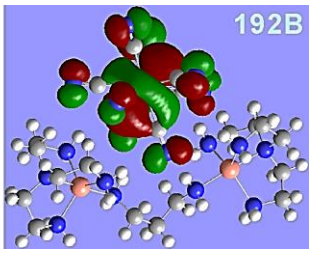
180B ->192B 0.41027





181B ->192B 0.83812



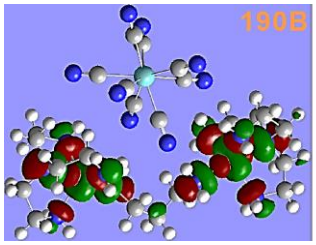


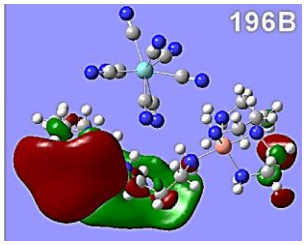
182B ->192B -0.18284

Excited State 44: 3.615-A 3.5794 eV 346.39 nm

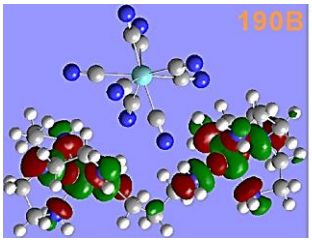
f = 0.0007 <S^2> = 3.017

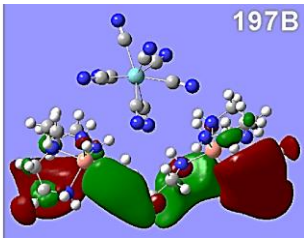
190B ->196B 0.96670





190B ->197B -0.24260





Excited State 46: 3.036-A 3.6203 eV 342.47 nm

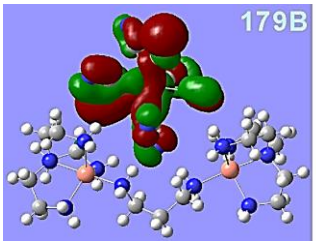
f = 0.0038 <S^2> = 2.055

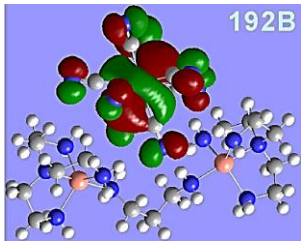
192A ->200A -0.24956

192A ->201A -0.13722

176B ->192B 0.11853

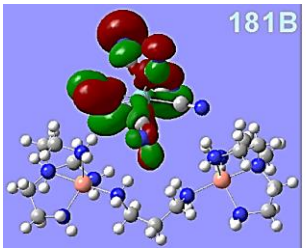
179B ->192B 0.77013

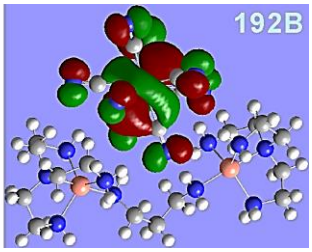




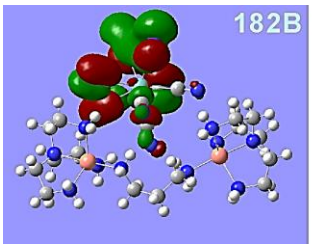
180B ->192B 0.19188

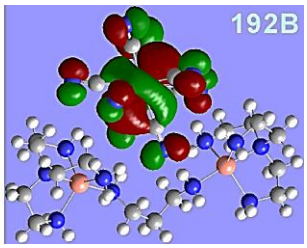
181B ->192B -0.22858





182B ->192B 0.40124

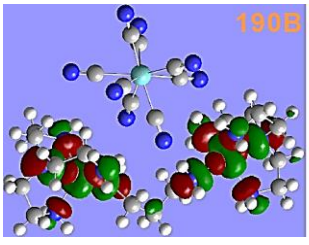


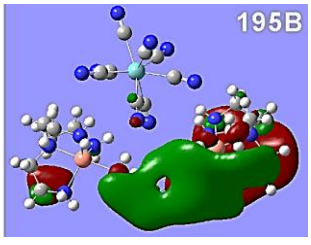


Excited State 48: 3.617-A 3.6471 eV 339.95 nm

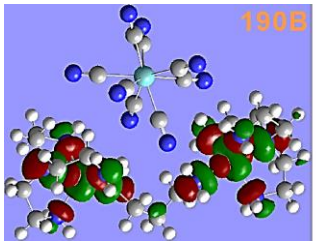
f = 0.0028 <S^2> = 3.021

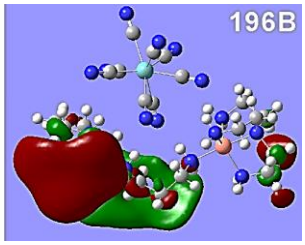
190B ->195B 0.23700



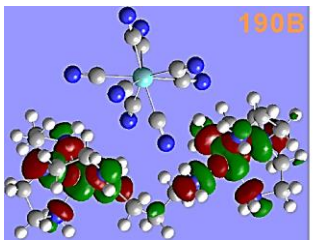


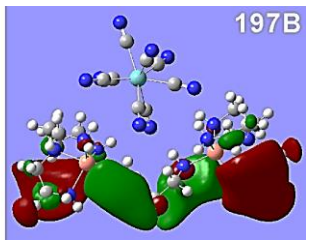
190B ->196B 0.22598





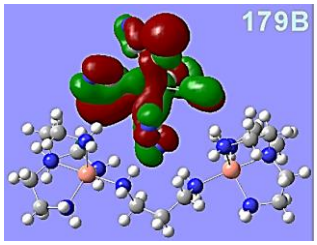
190B ->197B 0.94072

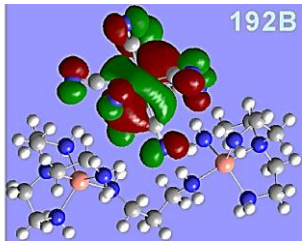




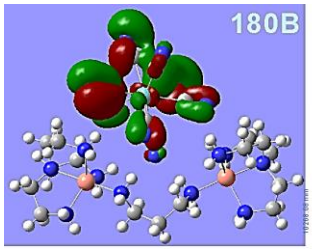
Excited State 49: 3.039-A 3.6846 eV 336.49 nm
f = 0.0084 $\langle S^2 \rangle$ = 2.059

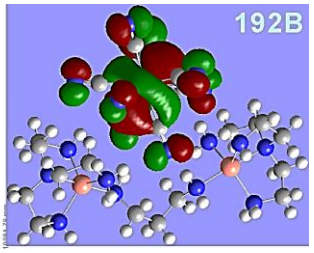
179B ->192B -0.27012



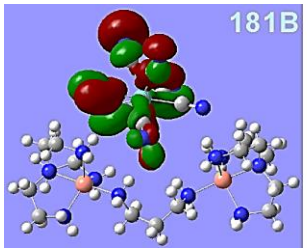


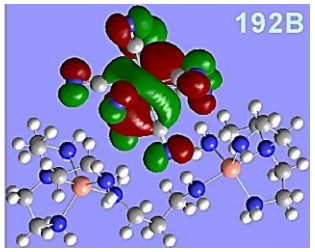
180B ->192B 0.87009





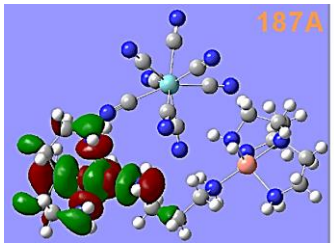
181B ->192B -0.35394

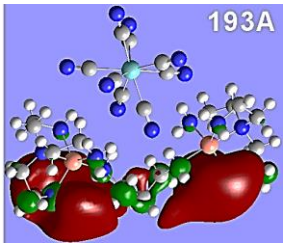




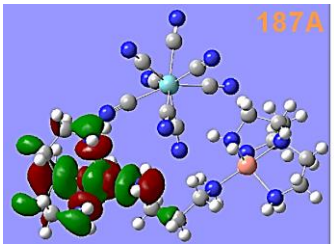
Excited State 52: 3.352-A 3.7338 eV 332.06 nm
f = 0.0019 $\langle S^2 \rangle$ = 2.560

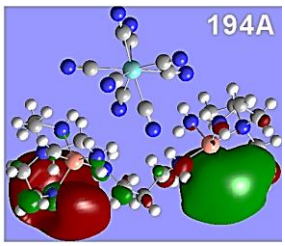
187A ->193A 0.79957





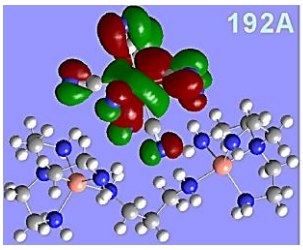
187A ->194A -0.58655

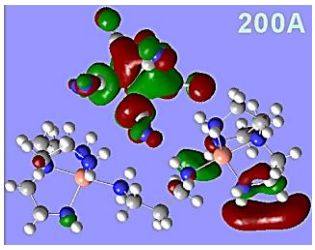




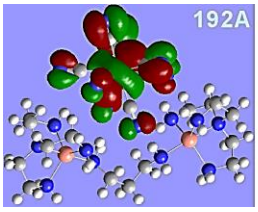
Excited State 54: 3.026-A 3.8245 eV 324.18 nm
f = 0.0022 $\langle S^2 \rangle$ = 2.039

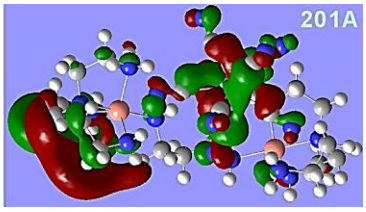
192A ->195A 0.12439
192A ->199A 0.11740
192A ->200A 0.52364



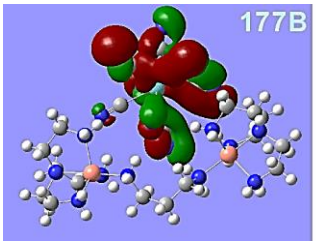


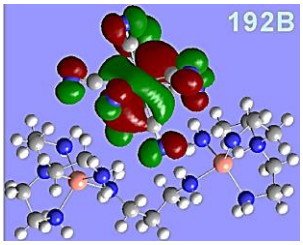
192A ->201A 0.30289



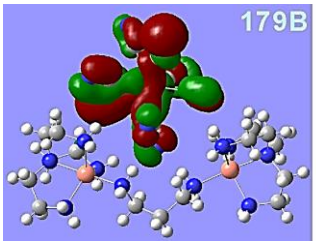


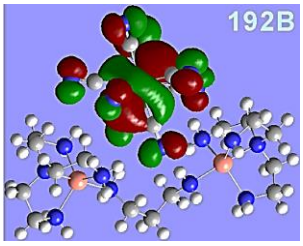
177B ->192B 0.65646





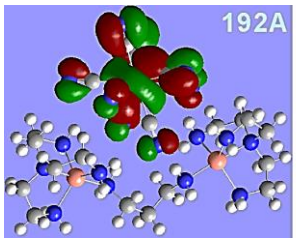
179B ->192B 0.31028

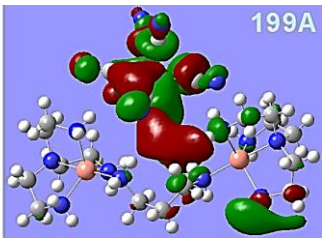




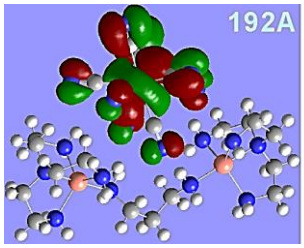
181B ->192B -0.11243

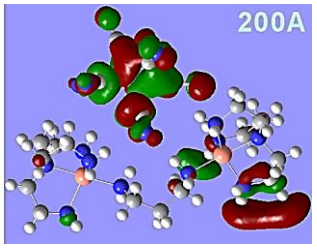
Excited State 56: 3.027-A 3.8458 eV 322.39 nm
f = 0.0013 <S^2> = 2.041
192A ->197A 0.11423
192A ->199A -0.56770



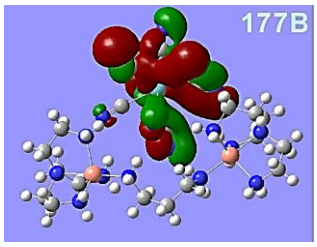


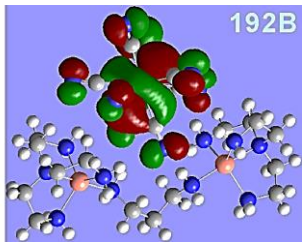
192A ->200A -0.45500





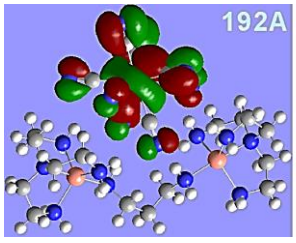
177B ->192B 0.57904

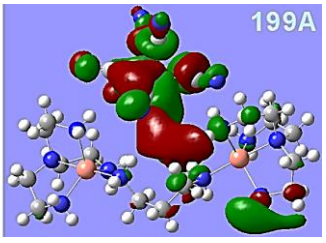




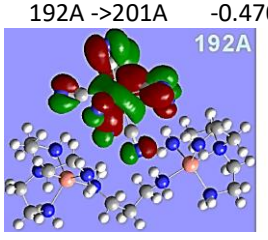
179B ->192B -0.17328
180B ->192B 0.10412

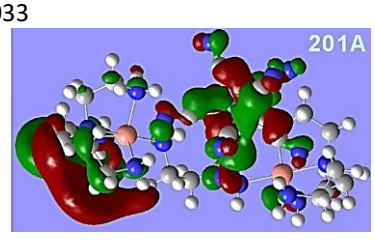
Excited State 59: 3.024-A 3.9181 eV 316.44 nm
f = 0.0011 <S^2> = 2.036
192A ->195A -0.26186
192A ->199A 0.59800





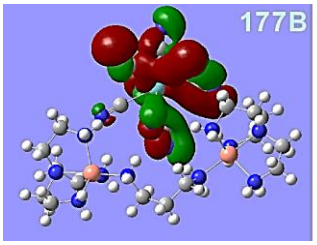
192A ->200A -0.25946
192A ->201A -0.47033

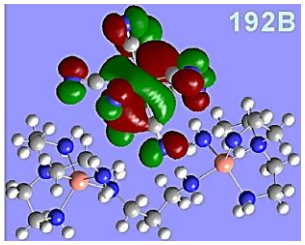




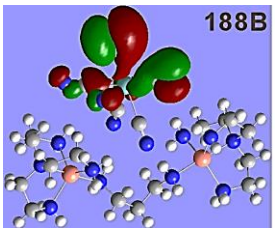
192A ->204A -0.13880
192A ->208A -0.12278

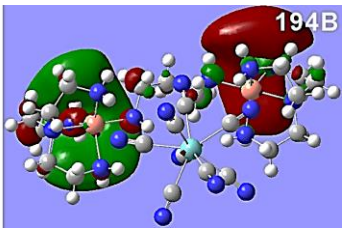
177B ->192B 0.41727



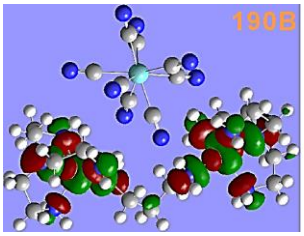


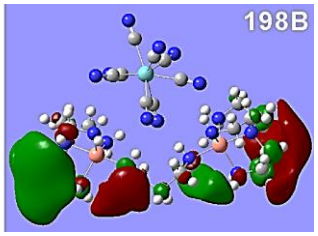
Excited State 61: 3.614-A 3.9510 eV 313.80 nm
f = 0.0014 <S^2> = 3.016
188B ->194B -0.18011



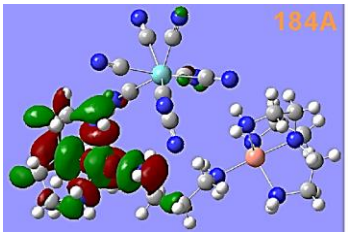


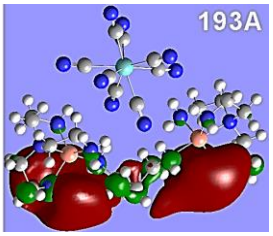
190B ->198B 0.97703



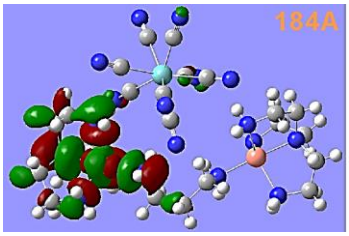


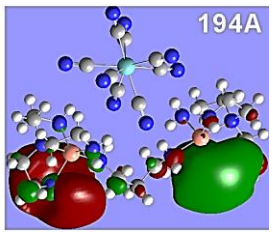
Excited State 65: 3.304-A 4.0420 eV 306.74 nm
f = 0.0021 <S^2> = 2.480
184A ->193A 0.82696



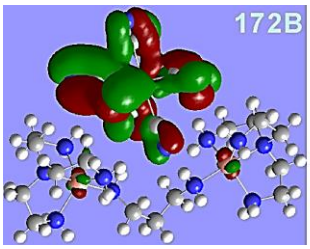


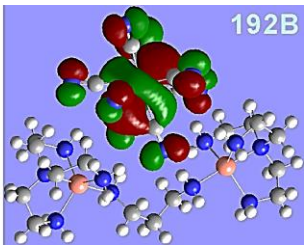
184A ->194A 0.51341



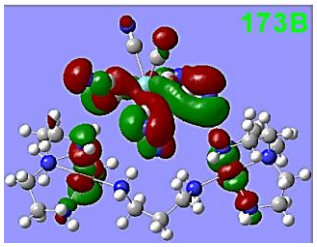


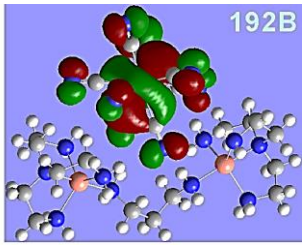
Excited State 67: 3.053-A 4.1368 eV 299.71 nm
f = 0.0010 <S^2> = 2.080
172B ->192B 0.24177



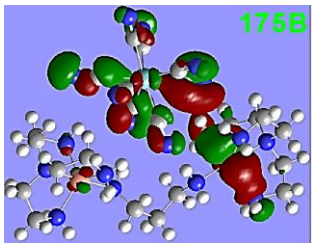


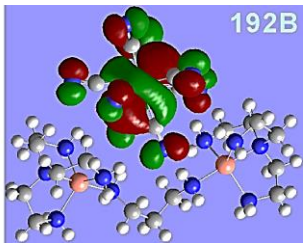
173B ->192B 0.28030



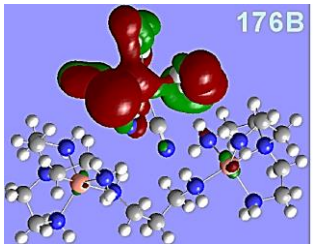


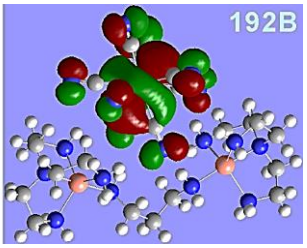
175B ->192B -0.27850





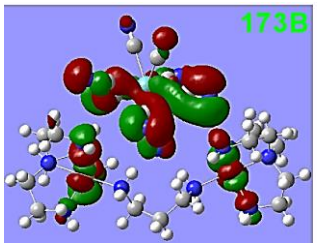
176B ->192B 0.84658

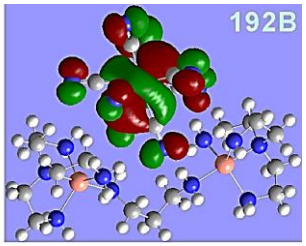




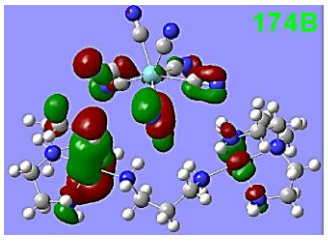
Excited State 70: 3.602-A 4.1606 eV 297.99 nm
f = 0.0002 $\langle S^2 \rangle$ = 2.994
188A ->193A 0.97947
189A ->194A 0.15664

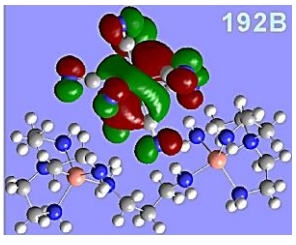
Excited State 71: 3.048-A 4.1710 eV 297.25 nm
f = 0.0029 $\langle S^2 \rangle$ = 2.073
169B ->192B 0.16958
172B ->192B 0.12950
173B ->192B 0.60193



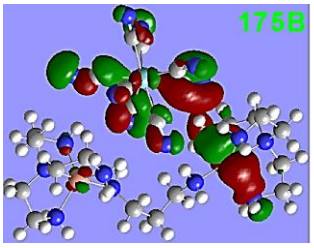


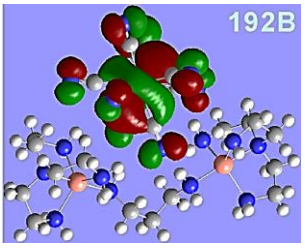
174B ->192B 0.32812



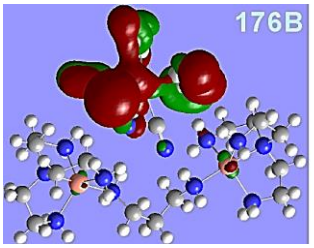


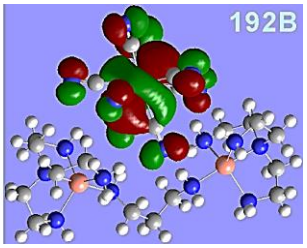
175B ->192B -0.49042





176B ->192B -0.42230



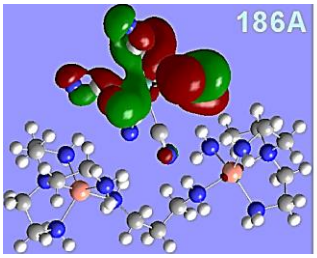


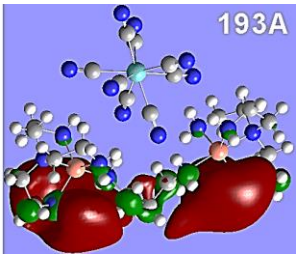
179B ->192B 0.10272

Excited State 72: 3.010-A 4.1845 eV 296.30 nm
f = 0.0003 $\langle S^2 \rangle$ = 2.015
160B ->191B 0.85026
161B ->191B -0.41279
162B ->191B -0.28881

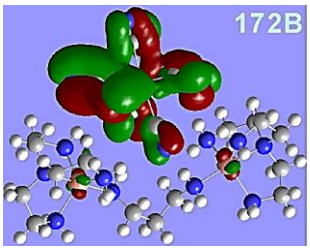
Excited State 75: 3.235-A 4.2474 eV 291.90 nm
f = 0.0122 $\langle S^2 \rangle$ = 2.366

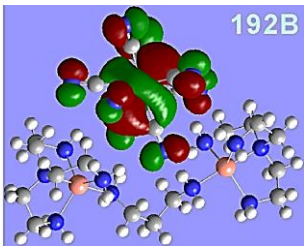
186A ->193A 0.53570



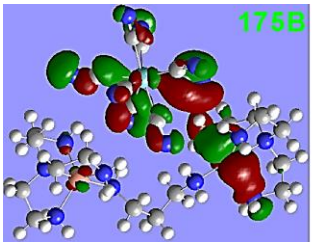


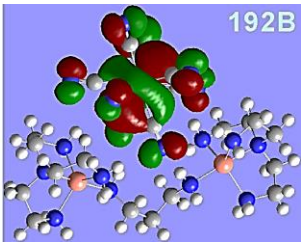
172B ->192B 0.75623



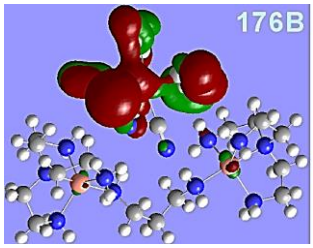


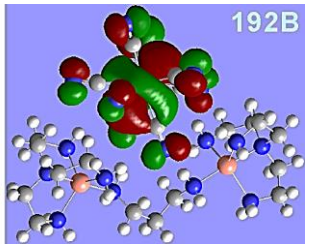
175B ->192B 0.21232





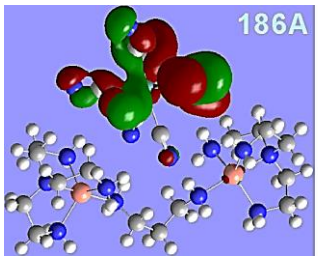
176B ->192B -0.13828

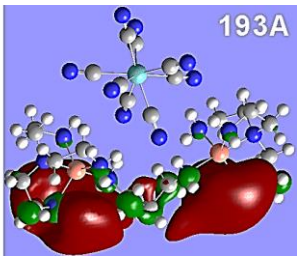




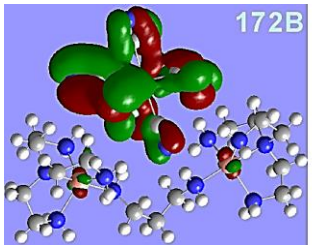
Excited State 76: 3.448-A 4.2492 eV 291.78 nm *f* = 0.0052 $<S^2>$ = 2.721

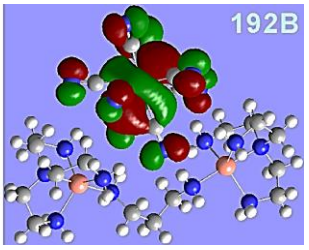
186A ->193A 0.82142



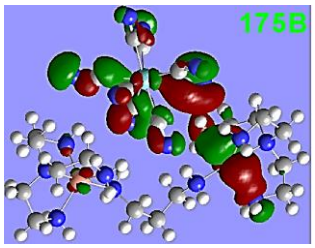


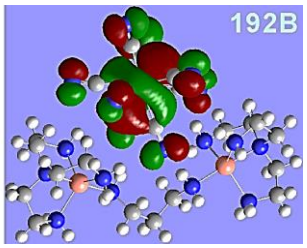
172B ->192B -0.49940





175B ->192B -0.14010



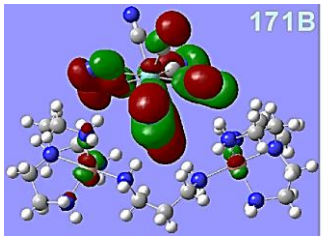


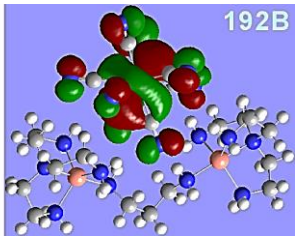
Excited State 77: 3.051-A 4.2521 eV 291.58 nm *f* = 0.0016 $<S^2>$ = 2.077

192A ->195A -0.14709

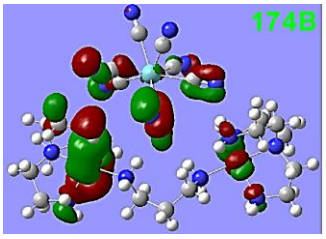
169B ->192B -0.20084

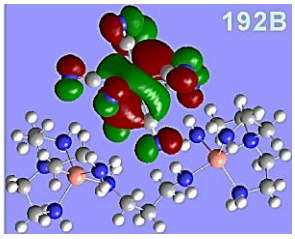
171B ->192B 0.87500





174B ->192B -0.28759





175B ->192B -0.11541

178B ->192B -0.13883

Excited State 79: 3.037-A 4.2773 eV 289.87 nm *f* = 0.0004 $<S^2>$ = 2.055

192A ->195A 0.76335

192A ->196A -0.55857

192A ->197A 0.13026

192A ->200A -0.14772

192A ->201A -0.14005

171B ->192B 0.10771

Excited State 80: 3.053-A 4.2898 eV 289.02 nm *f* = 0.0003 $<S^2>$ = 2.080

171B ->192B 0.10578

178B ->192B 0.96920

178B ->193B 0.11032

Excited State 81: 3.367-A 4.2922 eV 288.86 nm *f* = 0.0005 $<S^2>$ = 2.584

187A ->193A 0.58403

187A ->194A 0.79696

Excited State 82: 3.034-A 4.3082 eV 287.79 nm *f* = 0.0004 $<S^2>$ = 2.052

192A ->195A 0.53308

192A ->196A 0.76817

192A ->197A -0.25033

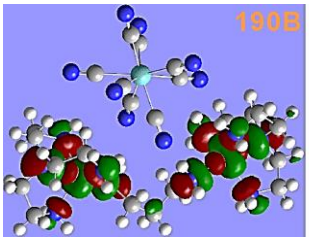
192A ->199A 0.14675

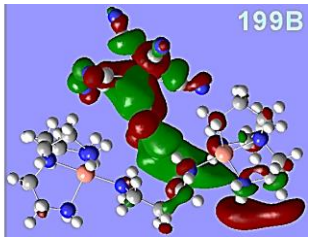
192A ->201A -0.11139

Excited State 83: 3.614-A 4.3259 eV 286.61 nm *f* = 0.0029 $<S^2>$ = 3.015

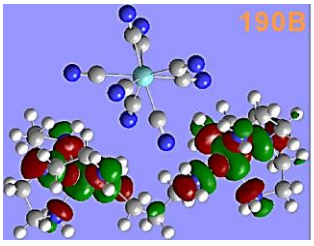
184B ->193B 0.12924

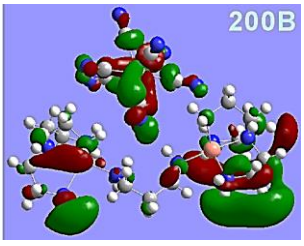
190B ->199B 0.21241





190B ->200B 0.96045

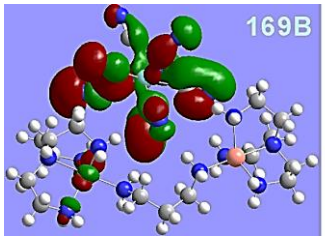


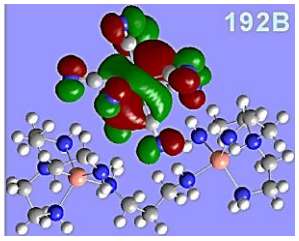


Excited State 84: 3.615-A 4.3282 eV 286.46 nm
f = 0.0002 <S^2> = 3.017
184B ->193B 0.97316
185B ->194B 0.15207
190B ->200B -0.12897

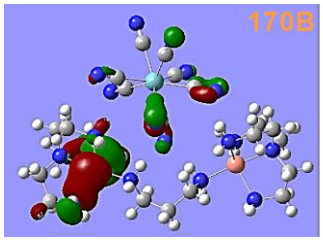
Excited State 85: 3.009-A 4.3337 eV 286.09 nm
f = 0.0002 <S^2> = 2.014
159B ->191B 0.98905

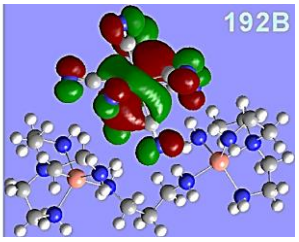
Excited State 86: 3.055-A 4.3592 eV 284.42 nm
f = 0.0080 <S^2> = 2.084
169B ->192B 0.87883



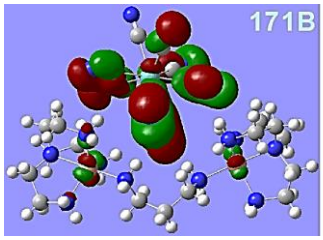


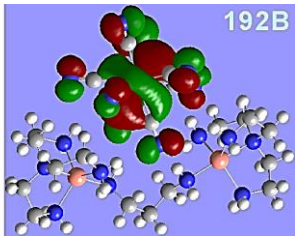
170B ->192B 0.20118



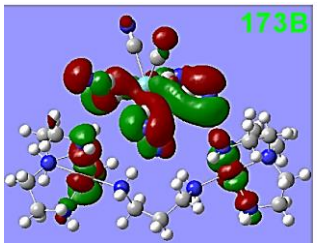


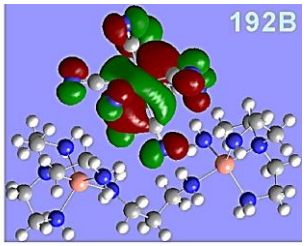
171B ->192B 0.26810





172B ->192B 0.11111
173B ->192B -0.17999

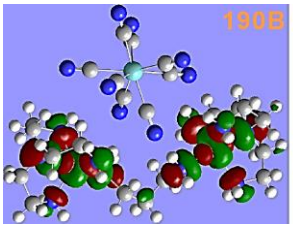


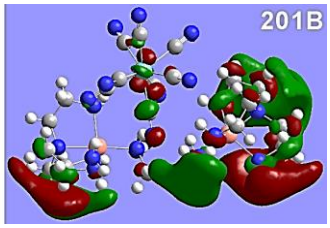


177B ->192B -0.10170

Excited State 87: 3.583-A 4.3731 eV 283.52 nm
f = 0.0002 <S^2> = 2.960
185A ->193A 0.19076
188A ->194A 0.95196
192A ->197A -0.18323

Excited State 88: 3.615-A 4.3767 eV 283.28 nm
f = 0.0006 <S^2> = 3.017
190B ->201B 0.98012

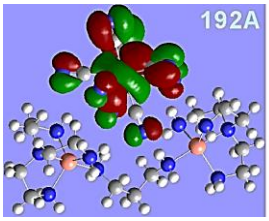


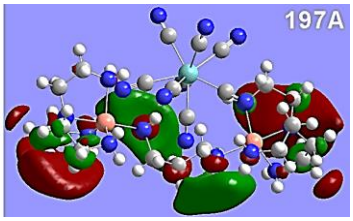


190B ->202B 0.11997

Excited State 89: 3.537-A 4.3834 eV 282.85 nm
f = 0.0003 <S^2> = 2.877
185A ->193A 0.88749
188A ->194A -0.25666
192A ->196A -0.10422
192A ->197A -0.32508

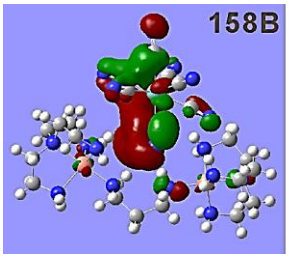
Excited State 90: 3.135-A 4.3855 eV 282.71 nm
f = 0.0005 <S^2> = 2.207
185A ->193A 0.38471
192A ->196A 0.23109
192A ->197A 0.85175

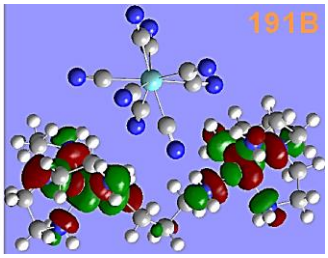




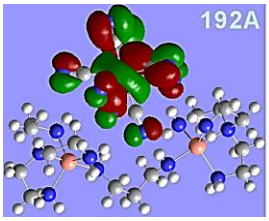
192A ->199A 0.12894
157B ->191B 0.12572

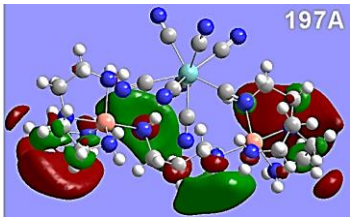
Excited State 91: 3.009-A 4.3918 eV 282.31 nm
f = 0.0047 <S^2> = 2.014
154B ->191B -0.12597
156B ->191B -0.14165
158B ->191B 0.96936



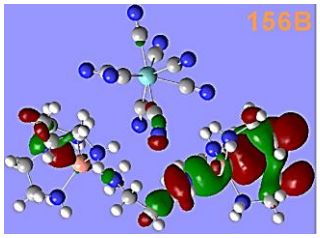


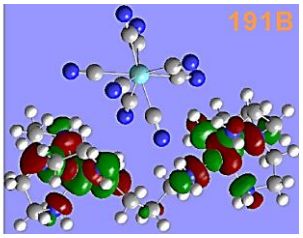
Excited State 92: 3.013-A 4.4036 eV 281.55 nm
f = 0.0545 <S^2> = 2.019
192A ->197A -0.13772



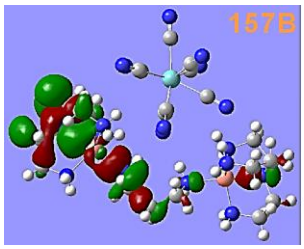


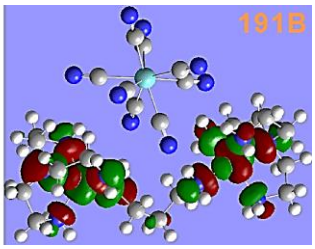
156B ->191B -0.20801



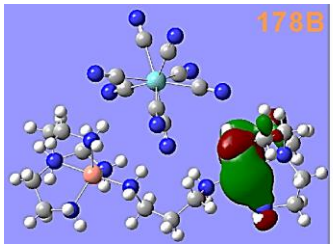


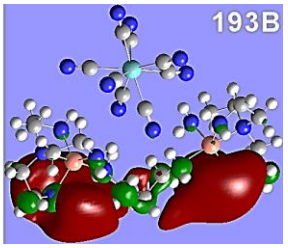
157B ->191B 0.94389



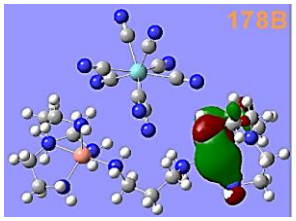


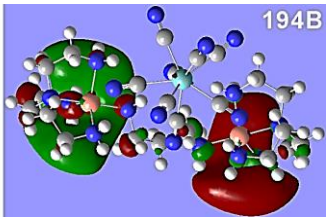
Excited State 94: 3.710-A 4.4393 eV 279.28 nm
f = 0.0005 $\langle S^2 \rangle$ = 3.192
155B ->191B -0.10228
178B ->192B -0.14038
178B ->193B 0.77406



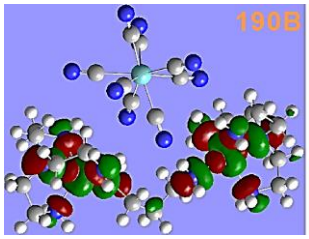


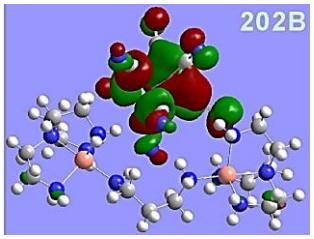
178B ->194B -0.57236



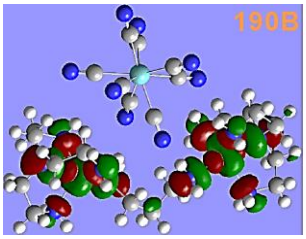


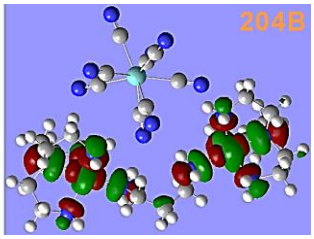
Excited State 96: 3.612-A 4.4907 eV 276.09 nm
f = 0.0006 $\langle S^2 \rangle$ = 3.012
190B ->201B -0.12652
190B ->202B 0.91307



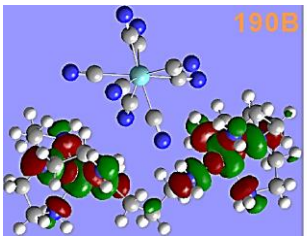


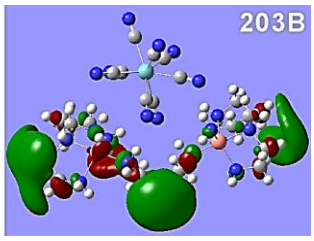
190B ->204B 0.36604



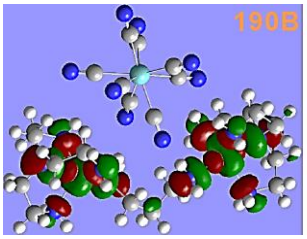


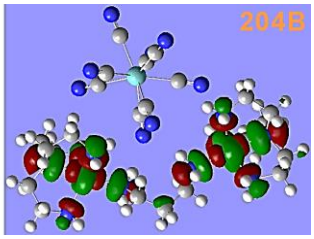
Excited State 98: 3.618-A 4.5389 eV 273.16 nm
f = 0.0026 $\langle S^2 \rangle$ = 3.023
190B ->203B 0.97309



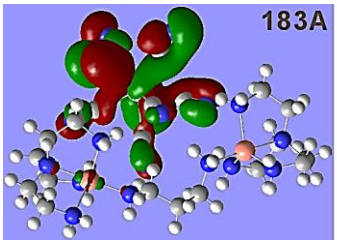


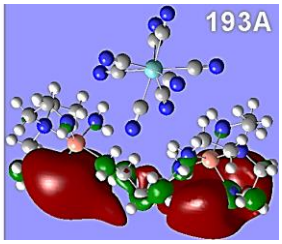
190B ->204B 0.15313





Excited State 100: 3.592-A 4.5541 eV 272.25 nm
f = 0.0005 $\langle S^2 \rangle$ = 2.976
183A ->193A 0.96831

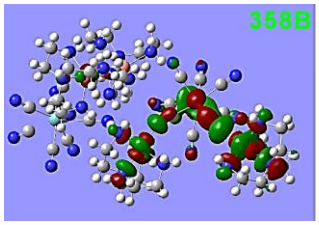


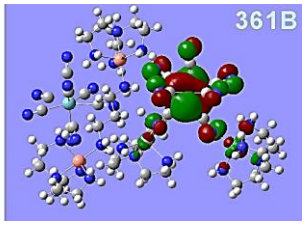


184A ->193A 0.13731
186A ->194A 0.10417
156B ->191B -0.10139

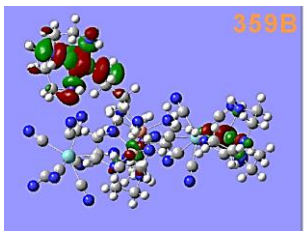
List of calculated excitation energies with non-zero oscillator strengths (*f*) for **2**.

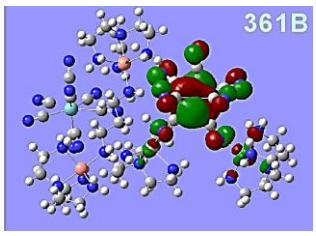
Excited State 4: 5.018-A 0.5893 eV 2103.94 nm
f = 0.0018 <S^2> = 6.046
358B -> 361B 0.38427



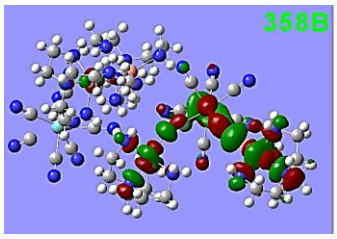


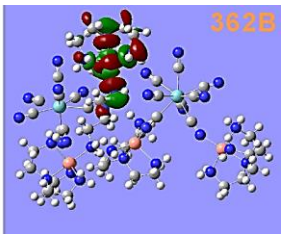
359B -> 361B 0.92465



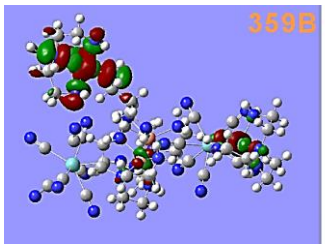


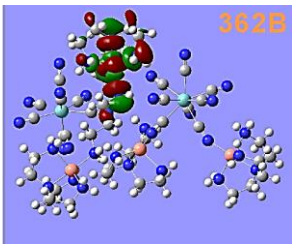
Excited State 5: 5.012-A 0.6706 eV 1848.72 nm
f = 0.0080 <S^2> = 6.031
358B -> 362B 0.20019



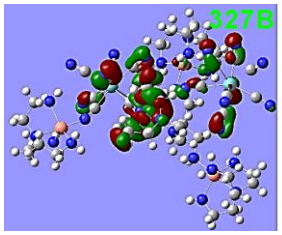


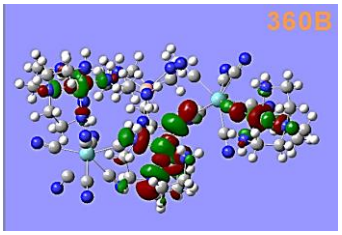
359B -> 362B 0.97896





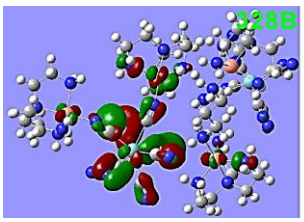
Excited State 7: 5.011-A 1.3584 eV 912.69 nm
f = 0.0007 <S^2> = 6.028
271B -> 360B 0.12097
278B -> 360B 0.11103
321B -> 360B -0.21068
323B -> 360B 0.13896
325B -> 360B 0.19206
327B -> 360B 0.74113

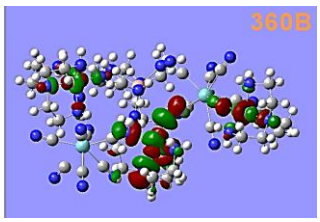




327B -> 361B 0.11805

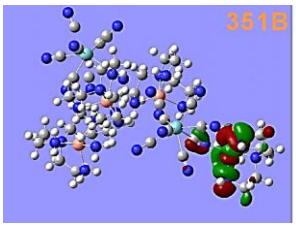
328B -> 360B -0.32492

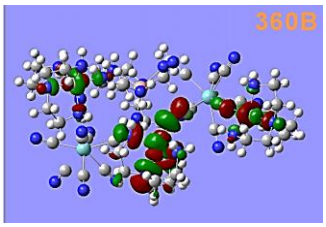




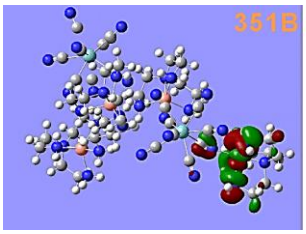
329B -> 360B -0.13616
330B -> 360B -0.24638

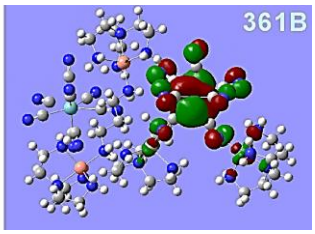
Excited State 8: 5.016-A 1.3727 eV 903.20 nm
f = 0.0019 <S^2> = 6.041
351B -> 360B 0.88722



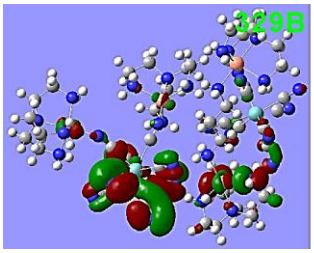


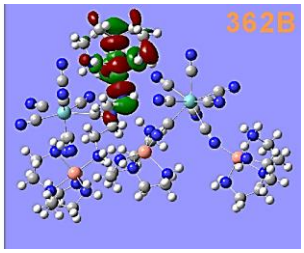
351B -> 361B -0.42760



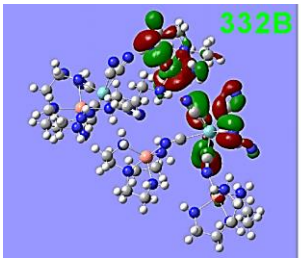


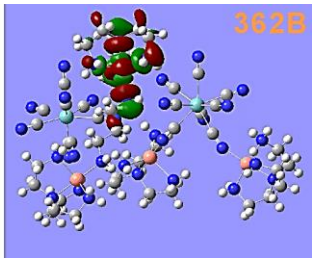
Excited State 9: 5.011-A 1.3994 eV 886.00 nm
f = 0.0011 <S^2> = 6.027
279B -> 362B -0.15136
282B -> 362B 0.23881
284B -> 362B -0.12854
327B -> 362B 0.10398
328B -> 362B 0.17175
329B -> 362B 0.39192





332B -> 362B 0.77636



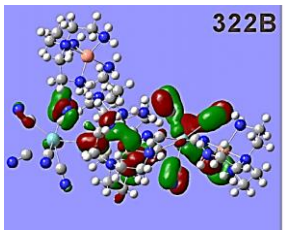


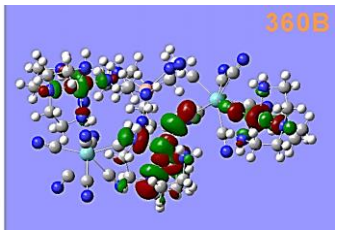
Excited State 10: 5.013-A 1.4098 eV 879.44 nm
f = 0.0001 <S^2> = 6.034
354B -> 360B 0.98853
355B -> 360B 0.12344

Excited State 12: 5.013-A 1.5049 eV 823.86 nm
f = 0.0001 <S^2> = 6.034
353B -> 360B 0.99600

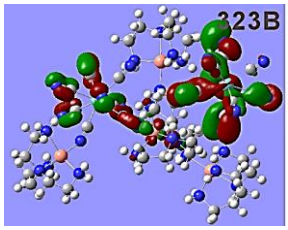
Excited State 14: 5.017-A 1.5705 eV 789.44 nm
f = 0.0005 <S^2> = 6.042
347B -> 360B 0.88109
347B -> 361B -0.43867

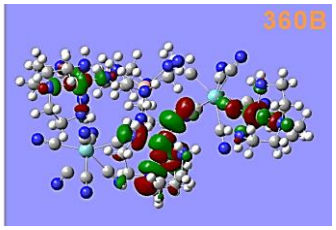
Excited State 15: 5.011-A 1.5924 eV 778.58 nm
f = 0.0016 <S^2> = 6.028
278B -> 360B -0.11446
285B -> 360B 0.11630
287B -> 360B -0.14348
288B -> 360B -0.10744
289B -> 360B 0.18713
315B -> 360B 0.10666
316B -> 360B 0.17459
321B -> 360B 0.22761
322B -> 360B 0.43846



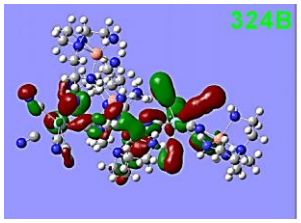


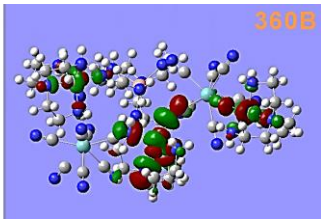
323B -> 360B -0.25205



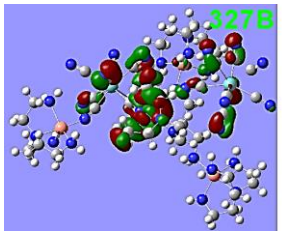


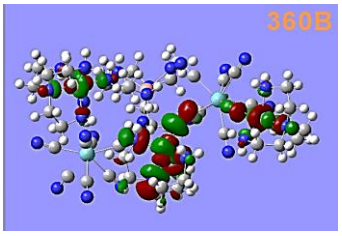
324B -> 360B 0.55818





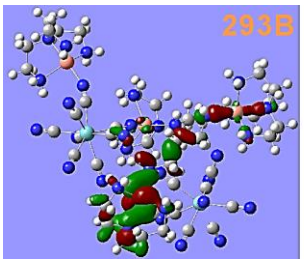
325B -> 360B -0.24476
327B -> 360B 0.30365

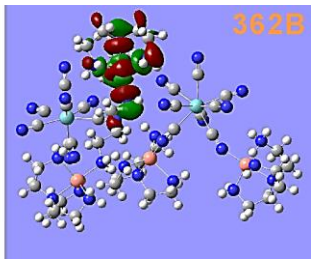




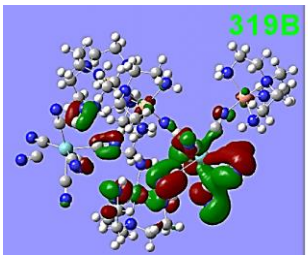
Excited State 17: 5.441-A 1.7207 eV 720.54 nm
f = 0.0003 <S^2> = 7.152
358B -> 364B 0.20223
359B -> 364B 0.95278
359B -> 365B -0.20004

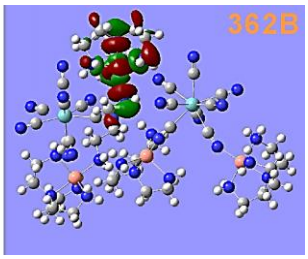
Excited State 20: 5.011-A 1.9054 eV 650.70 nm
f = 0.0031 <S^2> = 6.027
280B -> 362B -0.15505
283B -> 362B -0.17072
284B -> 362B -0.12276
291B -> 362B 0.25418
293B -> 362B 0.31458



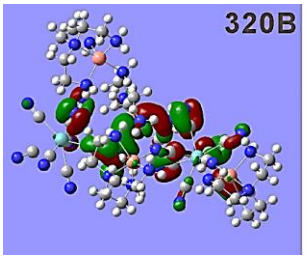


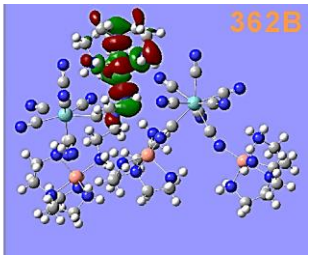
319B -> 362B -0.35839



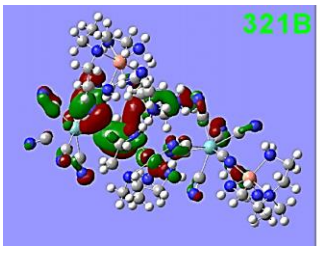


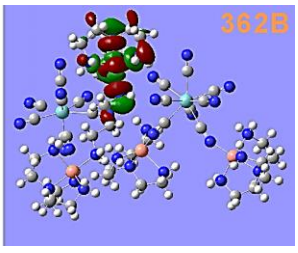
320B -> 362B 0.62989





321B -> 362B -0.38311

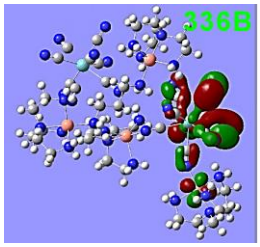


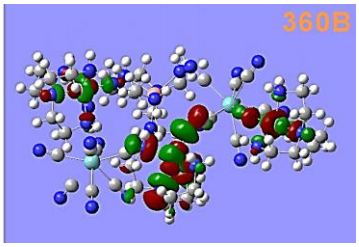


Excited State 23: 5.017-A 1.9423 eV 638.33 nm
f = 0.0004 <S^2> = 6.044
329B -> 360B 0.11205
334B -> 360B -0.22680
334B -> 361B 0.11830
336B -> 360B -0.23845
336B -> 361B 0.12572
338B -> 360B 0.62006
338B -> 361B -0.32422

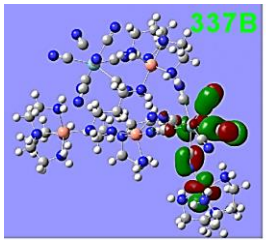
339B -> 360B 0.36947
339B -> 361B -0.19280
341B -> 360B -0.32473
341B -> 361B 0.17141

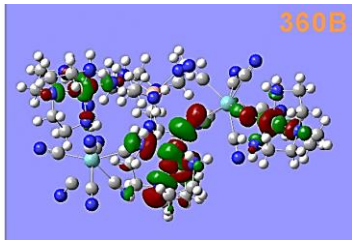
Excited State 24: 5.020-A 1.9824 eV 625.42 nm
f = 0.0033 $\langle S^2 \rangle$ = 6.050
334B -> 360B 0.21599
334B -> 361B -0.11165
336B -> 360B 0.39110



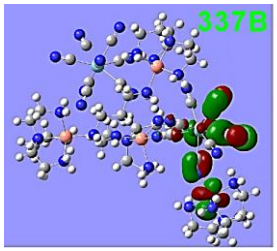


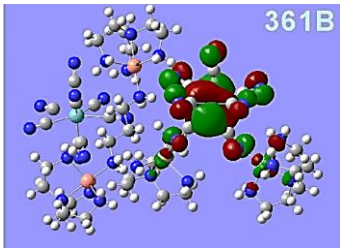
336B -> 361B -0.20472
337B -> 360B 0.70807





337B -> 361B -0.37611

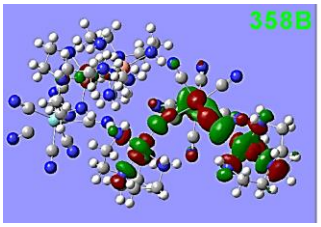


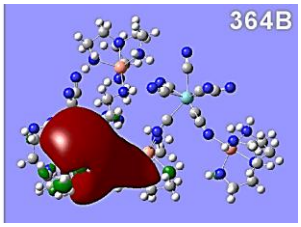


338B -> 360B 0.13274

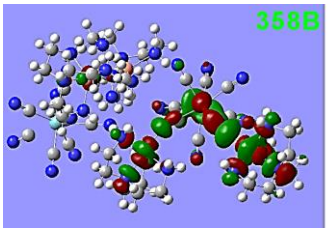
Excited State 28: 5.011-A 2.1038 eV 589.33 nm
f = 0.0002 $\langle S^2 \rangle$ = 6.029
283B -> 360B -0.13222
289B -> 360B 0.12440
292B -> 360B 0.22723
298B -> 360B -0.27308
299B -> 360B 0.19520
300B -> 360B 0.16163
301B -> 360B 0.22689
302B -> 360B -0.16892
304B -> 360B 0.34619
306B -> 360B 0.41720
308B -> 360B 0.43938
309B -> 360B -0.15658
312B -> 360B -0.11753
313B -> 360B 0.15999
337B -> 360B -0.11955

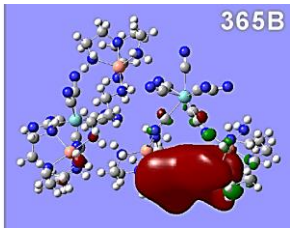
Excited State 31: 5.408-A 2.1567 eV 574.89 nm
f = 0.0047 $\langle S^2 \rangle$ = 7.061
358B -> 364B 0.58532





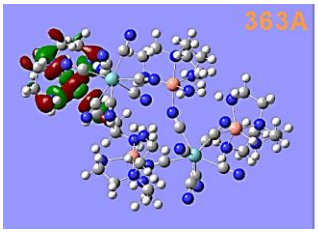
358B -> 365B 0.74070

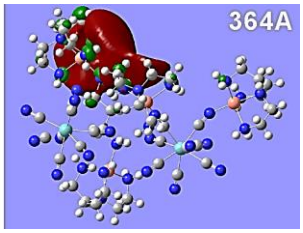




359B -> 364B -0.14310
359B -> 365B -0.24265

Excited State 33: 5.303-A 2.2271 eV 556.70 nm
f = 0.0015 $\langle S^2 \rangle$ = 6.781
363A -> 364A 0.96451

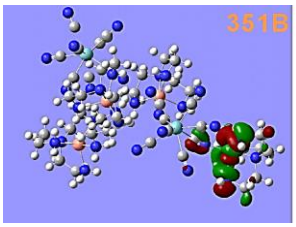


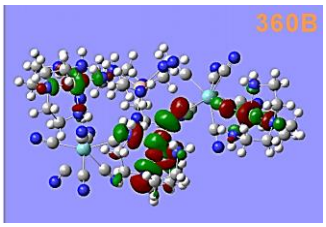


363A -> 365A -0.23977

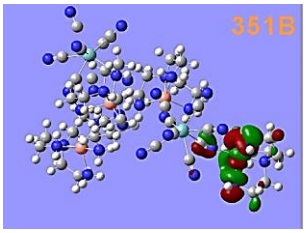
Excited State 37: 5.021-A 2.3079 eV 537.22 nm
f = 0.0002 $\langle S^2 \rangle$ = 6.054
355B -> 363B 0.12830
357B -> 363B 0.98569

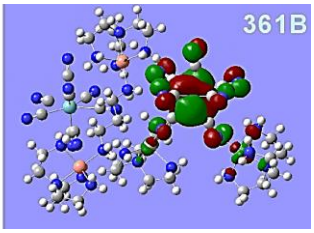
Excited State 38: 5.028-A 2.3409 eV 529.65 nm
f = 0.0032 $\langle S^2 \rangle$ = 6.070
351B -> 360B 0.43280





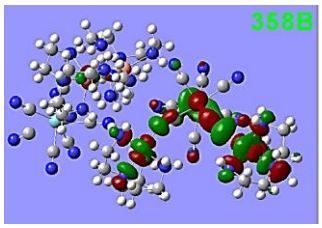
351B -> 361B 0.88510

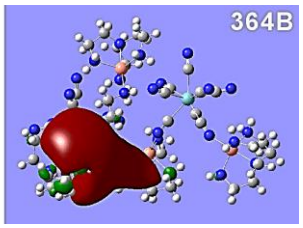




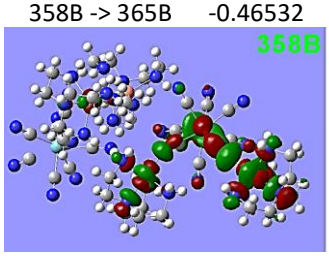
358B -> 364B 0.12946

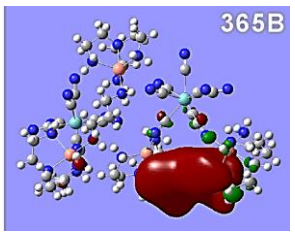
Excited State 40: 5.391-A 2.3733 eV 522.41 nm
f = 0.0007 <S^2> = 7.016
351B -> 361B -0.11947
358B -> 364B 0.75022



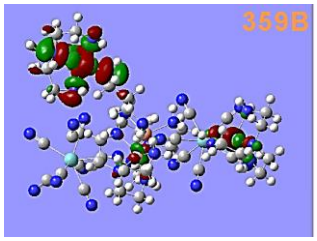


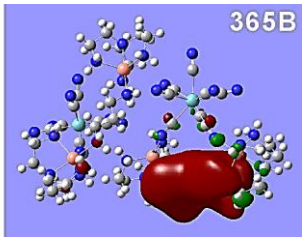
358B -> 365B -0.46532





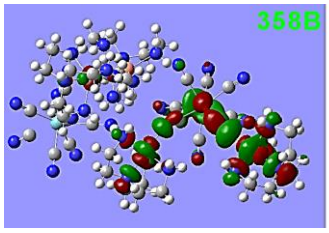
358B -> 366B 0.13424
359B -> 365B 0.41393

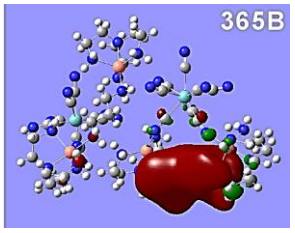




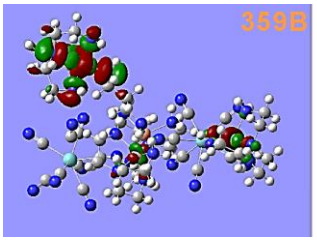
Excited State 41: 5.011-A 2.3836 eV 520.16 nm
f = 0.0002 <S^2> = 6.027
282B -> 362B -0.14071
284B -> 362B 0.13885
291B -> 362B -0.27560
293B -> 362B 0.40868
294B -> 362B -0.51470
295B -> 362B -0.61968

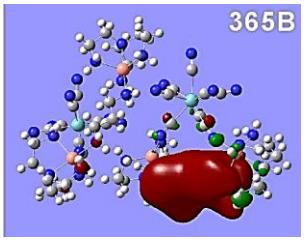
Excited State 45: 5.395-A 2.4406 eV 508.01 nm
f = 0.0009 <S^2> = 7.027
358B -> 364B -0.16851
358B -> 365B 0.44209





359B -> 364B 0.23111
359B -> 365B 0.82955

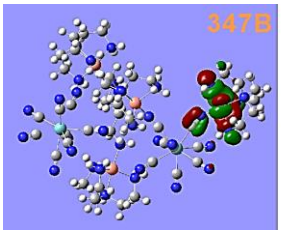


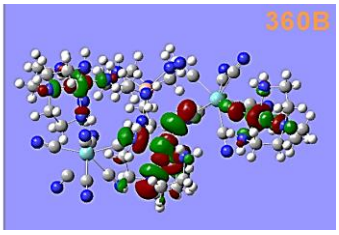


359B -> 366B 0.15879

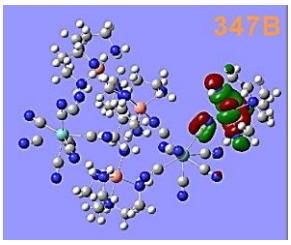
Excited State 46: 5.014-A 2.4474 eV 506.60 nm
f = 0.0004 <S^2> = 6.034
354B -> 362B 0.98570

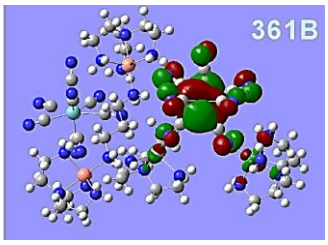
Excited State 52: 5.021-A 2.5731 eV 481.85 nm
f = 0.0017 <S^2> = 6.051
347B -> 360B 0.44265



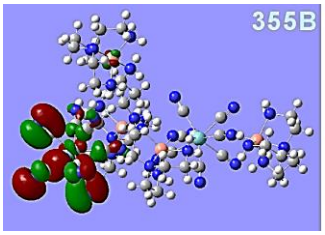


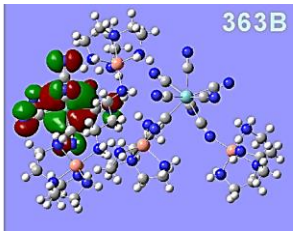
347B -> 361B 0.88130



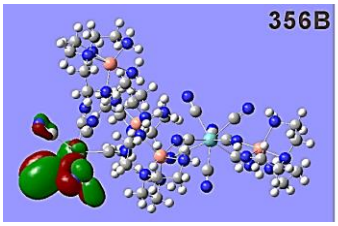


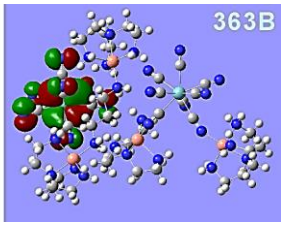
Excited State 53: 5.024-A 2.5974 eV 477.35 nm
f = 0.0058 <S^2> = 6.060
355B -> 363B -0.18970



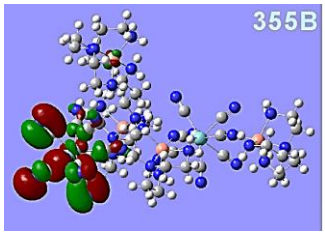


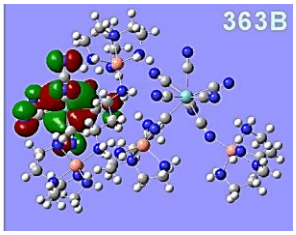
356B -> 363B 0.96827





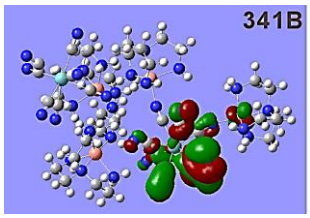
Excited State 55: 5.022-A 2.6453 eV 468.70 nm
f = 0.0026 <S^2> = 6.055
354B -> 363B -0.11214
355B -> 363B 0.95854

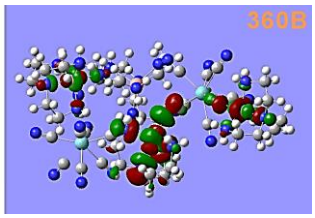




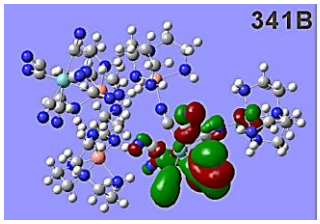
356B -> 363B 0.19515
357B -> 363B -0.12187

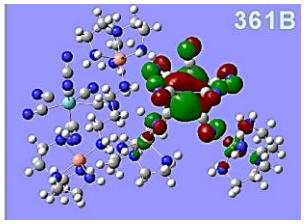
Excited State 57: 5.017-A 2.6815 eV 462.37 nm
f = 0.0012 <S^2> = 6.042
337B -> 360B 0.12482
338B -> 360B 0.21279
338B -> 361B -0.18721
339B -> 360B 0.19561
341B -> 360B 0.70078



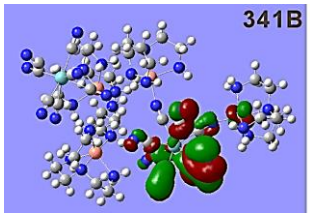


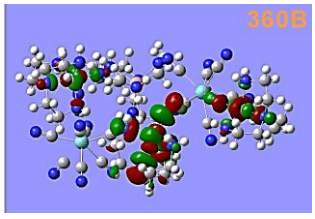
341B -> 361B -0.58217



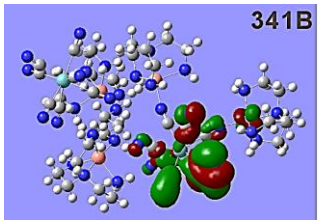


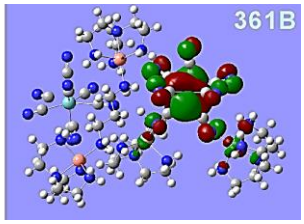
Excited State 58: 5.019-A 2.7172 eV 456.30 nm
f = 0.0028 <S^2> = 6.047
338B -> 361B 0.19120
339B -> 360B 0.23994
339B -> 361B -0.11152
341B -> 360B 0.57093



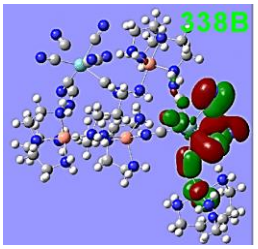


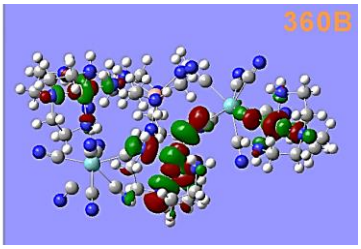
341B -> 361B 0.71934



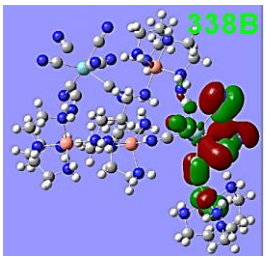


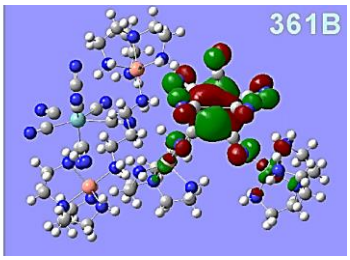
Excited State 61: 5.019-A 2.7495 eV 450.93 nm
f = 0.0026 <S^2> = 6.047
338B -> 360B 0.27462



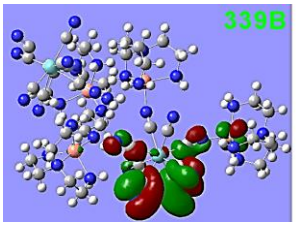


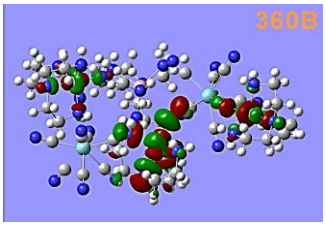
338B -> 361B -0.39402



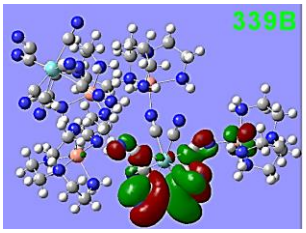


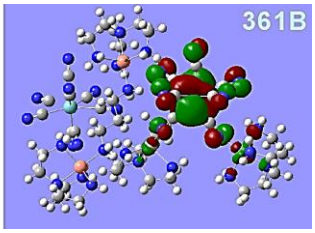
339B -> 360B -0.42963





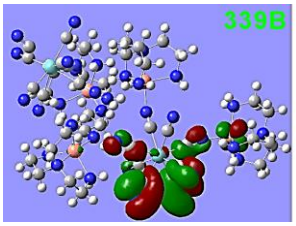
339B -> 361B 0.68972

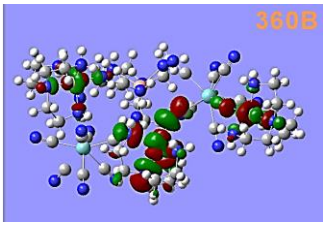




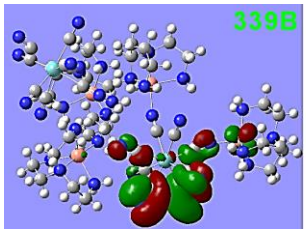
341B -> 360B 0.15578
341B -> 361B 0.22411

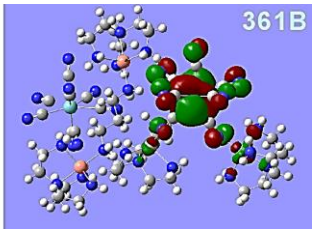
Excited State 64: 5.016-A 2.7866 eV 444.93 nm
f = 0.0008 <S^2> = 6.041
338B -> 360B -0.39682
338B -> 361B -0.21873
339B -> 360B 0.69134





339B -> 361B 0.47538





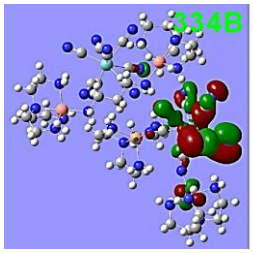
341B -> 360B -0.10675
349B -> 361B 0.21865
350B -> 361B -0.11114

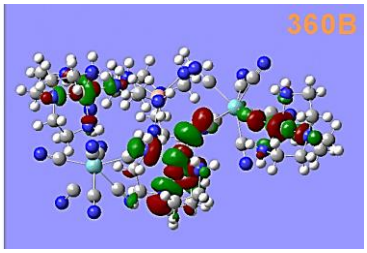
Excited State 65: 5.019-A 2.7874 eV 444.80 nm
f = 0.0001 $\langle S^2 \rangle$ = 6.047

339B -> 360B -0.17500
339B -> 361B -0.12110
349B -> 361B 0.82364
350B -> 361B -0.48413

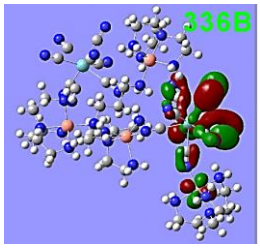
Excited State 68: 5.016-A 2.8485 eV 435.26 nm
f = 0.0009 $\langle S^2 \rangle$ = 6.040

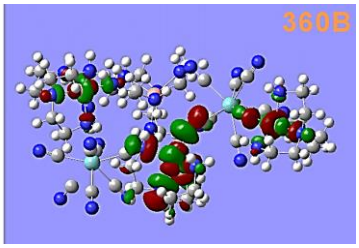
334B -> 360B 0.32562



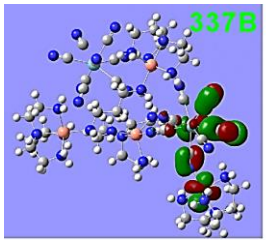


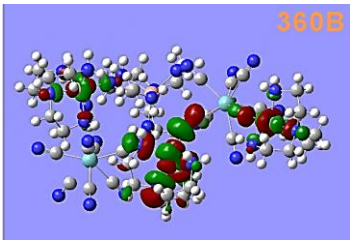
334B -> 361B -0.18068
336B -> 360B 0.58969





336B -> 361B -0.26524
337B -> 360B -0.48574



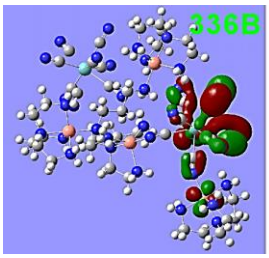


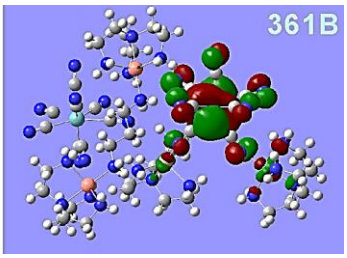
337B -> 361B 0.22744
338B -> 360B 0.26603
338B -> 361B -0.10927
339B -> 360B 0.15865
339B -> 361B -0.12803

Excited State 69: 5.021-A 2.8699 eV 432.02 nm
f = 0.0016 $\langle S^2 \rangle$ = 6.052

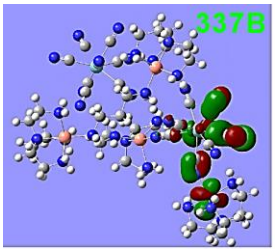
334B -> 360B -0.11833
334B -> 361B -0.24050

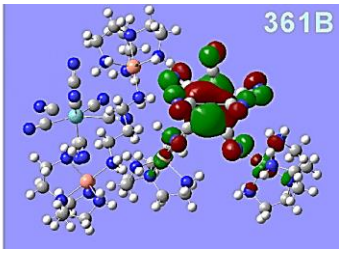
336B -> 360B -0.21190
336B -> 361B -0.45831



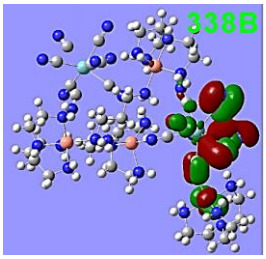


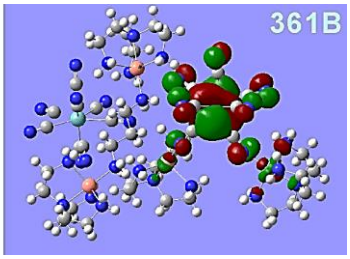
337B -> 360B 0.24610
337B -> 361B 0.50584



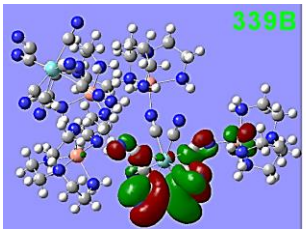


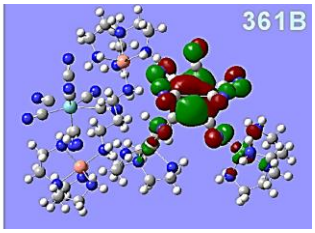
338B -> 360B -0.24710
338B -> 361B -0.37882





339B -> 360B -0.10924
339B -> 361B -0.31465



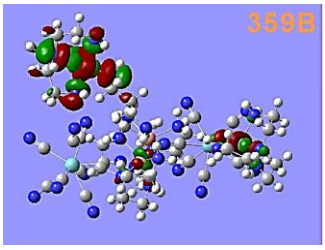


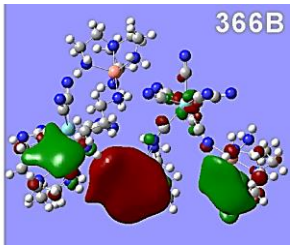
Excited State 70: 5.025-A 2.8802 eV 430.47 nm
f = 0.0001 $\langle S^2 \rangle$ = 6.063

362A -> 364A 0.99774

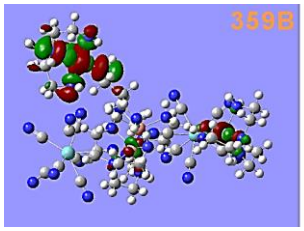
Excited State 71: 5.410-A 2.9000 eV 427.53 nm
f = 0.0035 $\langle S^2 \rangle$ = 7.067

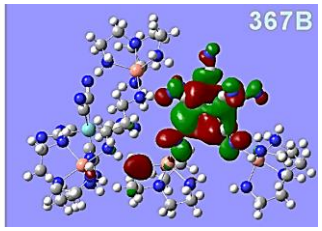
358B -> 367B 0.21466
359B -> 365B -0.15250
359B -> 366B 0.81537





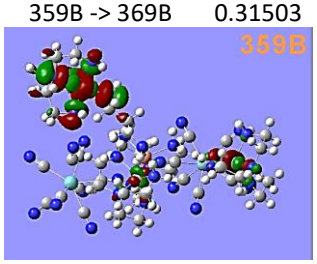
359B -> 367B 0.31793

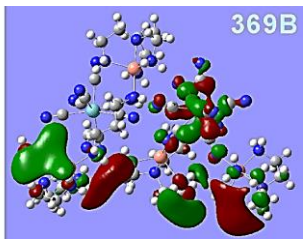




359B -> 368B 0.12418

359B -> 369B 0.31503



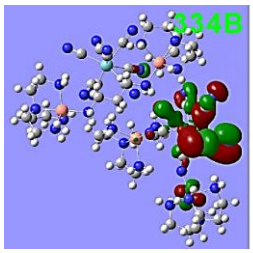


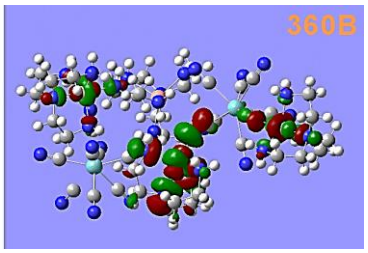
Excited State 73: 5.098-A 2.9388 eV 421.89 nm

f = 0.0019 $\langle S^2 \rangle$ = 6.247

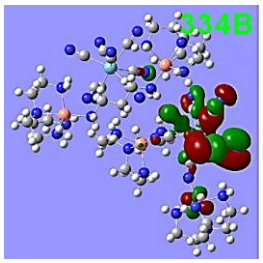
329B -> 361B 0.16626

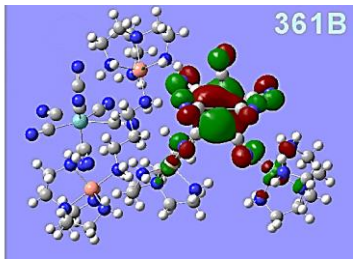
334B -> 360B 0.47077





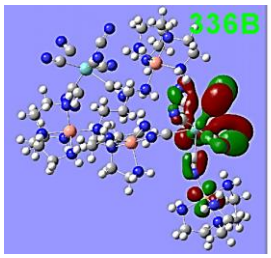
334B -> 361B -0.46116

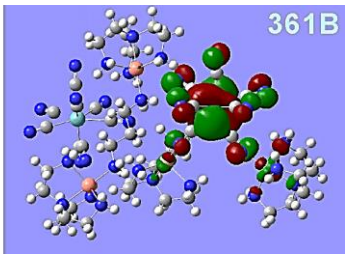




336B -> 360B -0.26355

336B -> 361B 0.39452



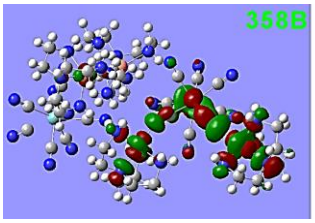


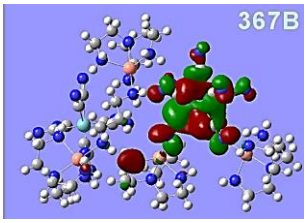
338B -> 361B -0.23995

339B -> 361B -0.10097

358B -> 366B -0.23351

358B -> 367B 0.32276





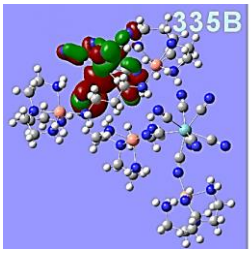
359B -> 367B -0.13532

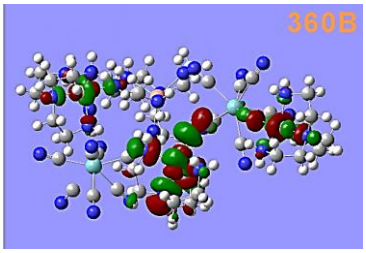
Excited State 74: 5.055-A 2.9446 eV 421.05 nm

f = 0.0015 $\langle S^2 \rangle$ = 6.139

334B -> 360B -0.10814

335B -> 360B 0.91997





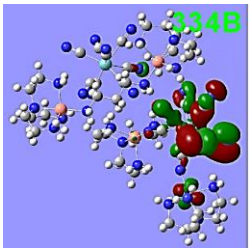
358B -> 366B -0.17724

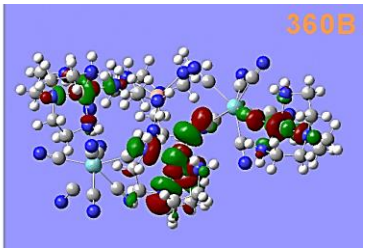
358B -> 367B 0.23845

Excited State 75: 5.281-A 2.9468 eV 420.74 nm

f = 0.0095 $\langle S^2 \rangle$ = 6.722

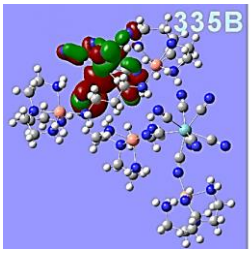
334B -> 360B -0.32261

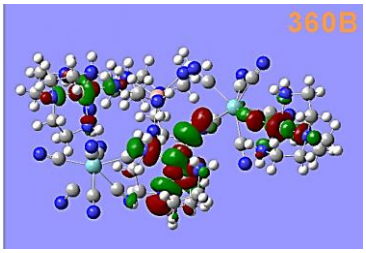




334B -> 361B 0.21747

335B -> 360B -0.32783

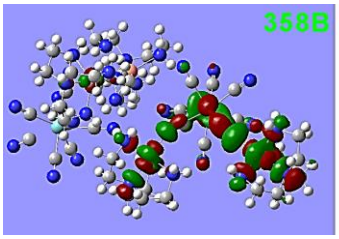


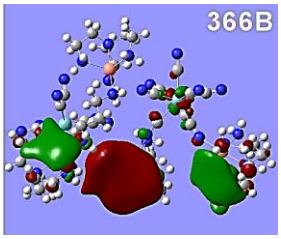


336B -> 360B 0.19448

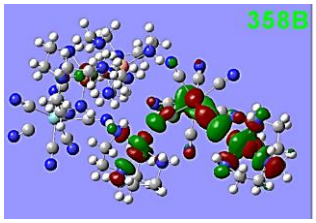
336B -> 361B -0.13326

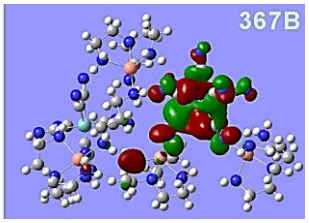
358B -> 366B -0.45963





358B -> 367B 0.60849





359B -> 367B -0.24717

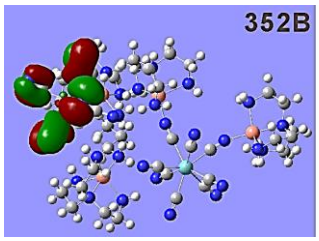
Excited State 76: 5.029-A 2.9573 eV 419.24 nm

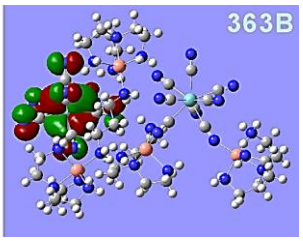
f = 0.0055 $<S^2>$ = 6.072

348B -> 363B 0.26317

350B -> 363B 0.24336

352B -> 363B 0.91546



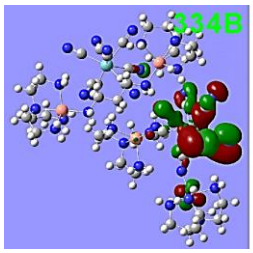


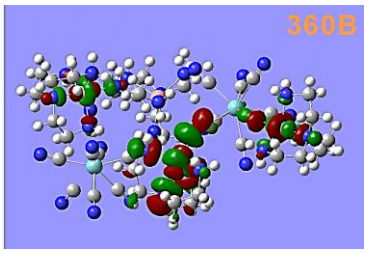
Excited State 77: 5.036-A 2.9611 eV 418.71 nm

f = 0.0012 $<S^2>$ = 6.090

329B -> 361B -0.17535

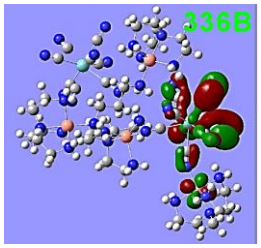
334B -> 360B 0.46962

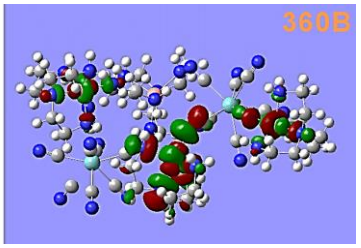




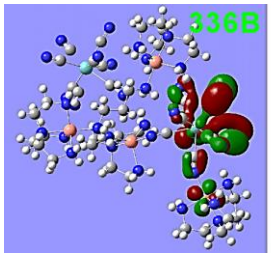
334B -> 361B 0.16275

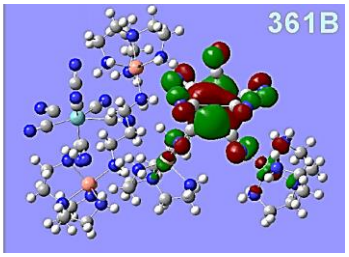
336B -> 360B -0.40763





336B -> 361B -0.37168

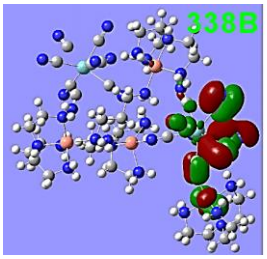


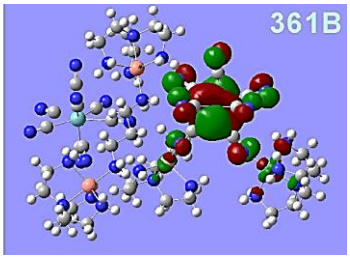


337B -> 361B 0.17858

338B -> 360B 0.23798

338B -> 361B 0.40386





339B -> 360B 0.12119

339B -> 361B 0.20625

358B -> 366B -0.13336

358B -> 367B 0.15530

Excited State 80: 5.013-A 3.0184 eV 410.76 nm

f = 0.0001 $<S^2>$ = 6.033

343B -> 362B -0.19631

344B -> 361B -0.22193

344B -> 362B 0.92684

349B -> 362B -0.14423

Excited State 81: 5.345-A 3.0186 eV 410.74 nm

f = 0.0003 $<S^2>$ = 6.893

363A -> 364A 0.24367

363A -> 365A 0.94369

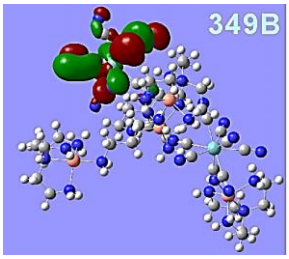
363A -> 367A 0.18943

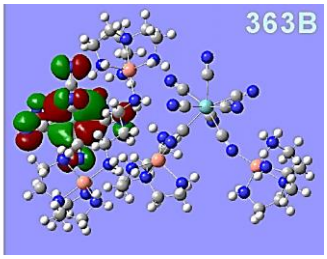
Excited State 82: 5.026-A 3.0262 eV 409.71 nm

f = 0.0021 $<S^2>$ = 6.064

348B -> 363B -0.23499

349B -> 363B 0.93471





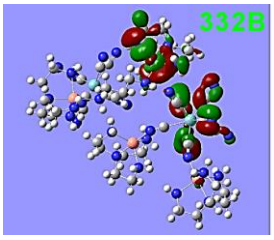
350B -> 363B 0.18230

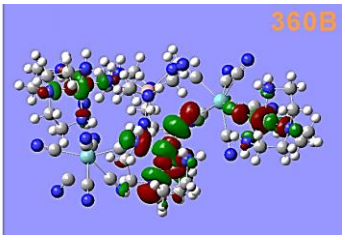
Excited State 83: 5.021-A 3.0293 eV 409.28 nm

f = 0.0022 $<S^2>$ = 6.052

329B -> 360B 0.14671

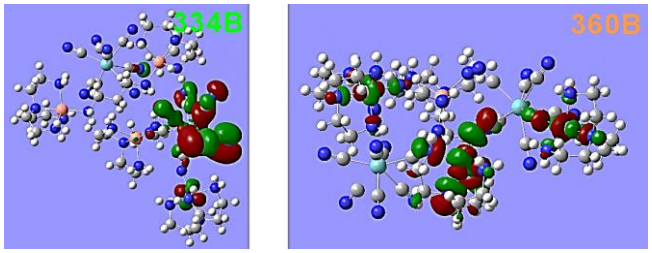
332B -> 360B -0.43539



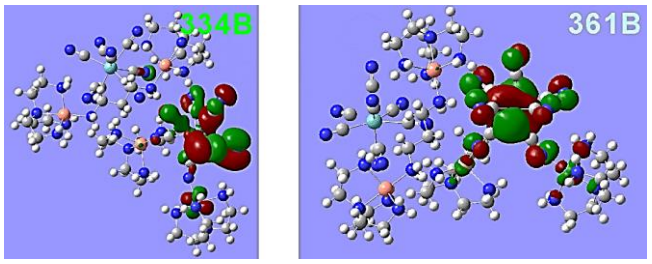


333B -> 360B -0.12778

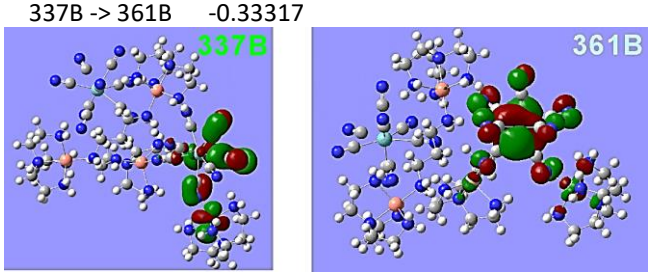
334B -> 360B 0.28517



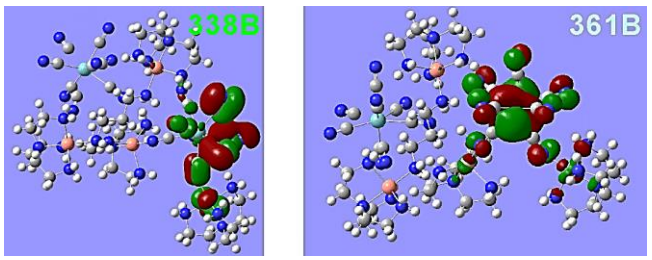
334B -> 361B 0.45635



336B -> 360B -0.14073
336B -> 361B -0.20313
337B -> 360B -0.18220
337B -> 361B -0.33317



338B -> 360B -0.26184
338B -> 361B -0.34411



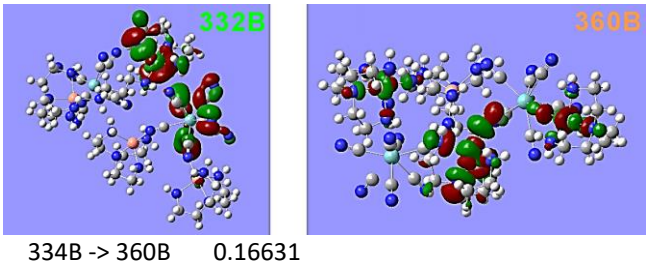
339B -> 361B -0.15080
341B -> 361B 0.11605

Excited State 84: 5.014-A 3.0365 eV 408.31 nm
f = 0.0001 <S^2> = 6.034
333B -> 360B 0.97098

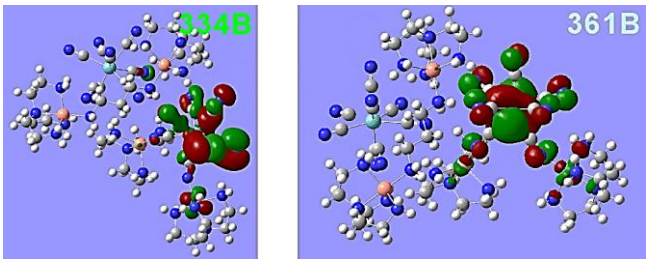
Excited State 85: 5.013-A 3.0428 eV 407.46 nm
f = 0.0001 <S^2> = 6.032
343B -> 362B 0.15422
346B -> 362B 0.97852

Excited State 86: 5.017-A 3.0469 eV 406.92 nm
f = 0.0011 <S^2> = 6.041
328B -> 360B -0.20477
329B -> 360B -0.19160
329B -> 361B 0.13015
330B -> 360B 0.10558

332B -> 360B 0.79412

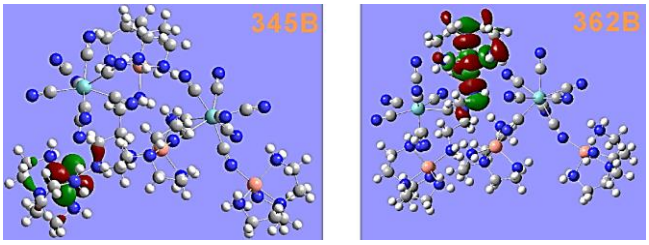


334B -> 360B 0.16631
334B -> 361B 0.26640

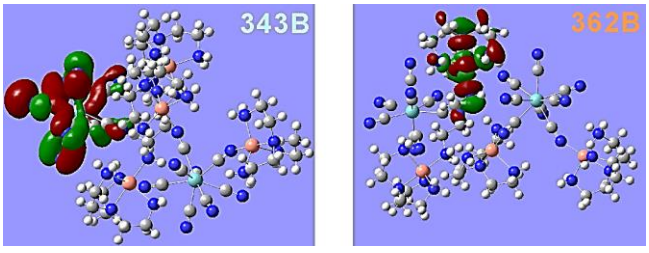


336B -> 361B -0.12893
337B -> 361B -0.19497
338B -> 361B -0.22447

Excited State 88: 5.013-A 3.0528 eV 406.13 nm
f = 0.0007 <S^2> = 6.032
343B -> 362B 0.30271
344B -> 361B 0.10465
345B -> 362B 0.92980

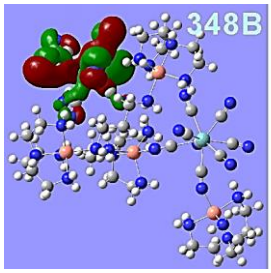


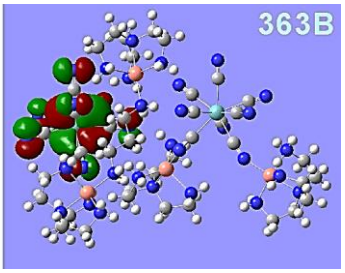
Excited State 89: 5.013-A 3.0582 eV 405.41 nm
f = 0.0005 <S^2> = 6.032
342B -> 362B -0.21625
343B -> 361B -0.11675
343B -> 362B 0.81585



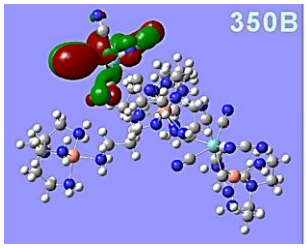
344B -> 361B 0.14987
344B -> 362B 0.24332
345B -> 362B -0.35221
346B -> 362B -0.14101
348B -> 362B -0.15016

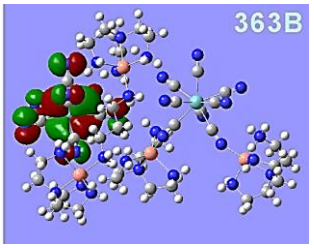
Excited State 91: 5.030-A 3.0959 eV 400.47 nm
f = 0.0054 <S^2> = 6.076
348B -> 363B 0.41461



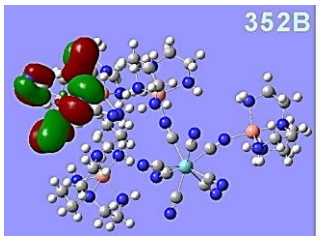


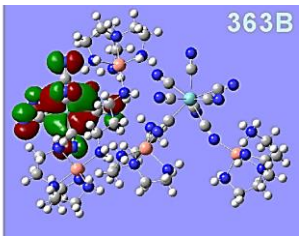
350B -> 363B 0.81802



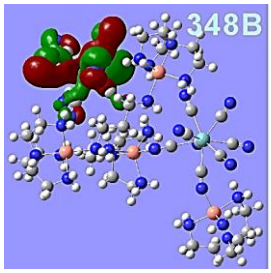


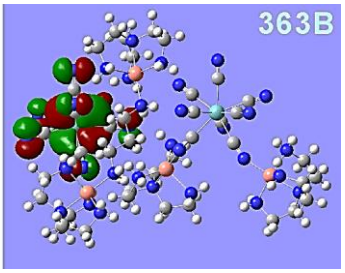
352B -> 363B -0.34941



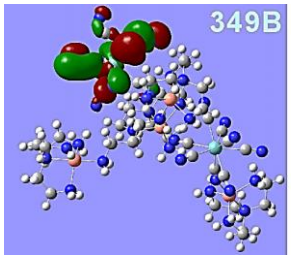


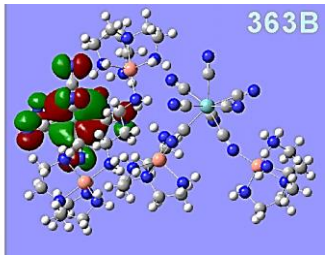
Excited State 96: 5.028-A 3.1370 eV 395.23 nm
f = 0.0111 <S^2> = 6.070
344B -> 363B 0.10079
348B -> 363B 0.79921



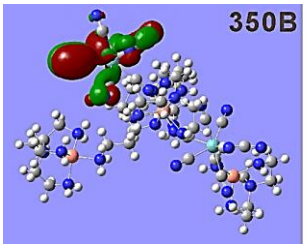


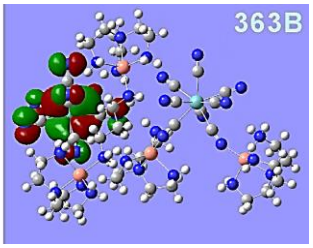
349B -> 363B 0.30187



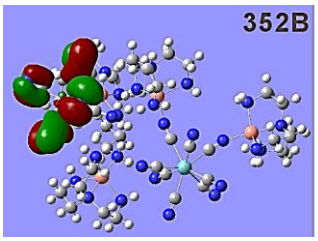


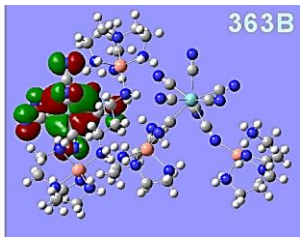
350B -> 363B -0.45507



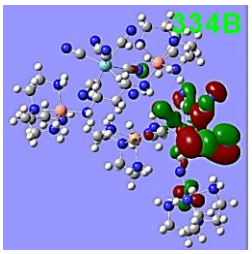


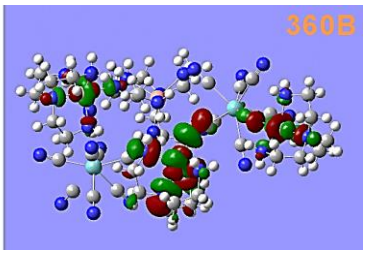
352B -> 363B -0.12017



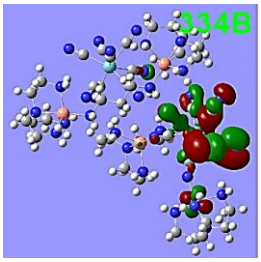


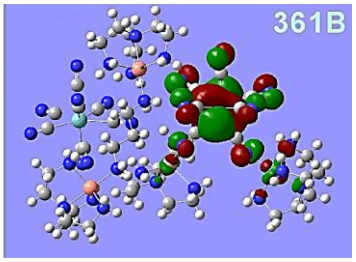
Excited State 97: 5.035-A 3.1544 eV 393.05 nm
f = 0.0050 <S^2> = 6.088
361A -> 365A 0.11517
329B -> 360B -0.11671
330B -> 360B 0.12759
334B -> 360B 0.24110



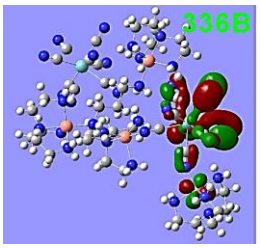


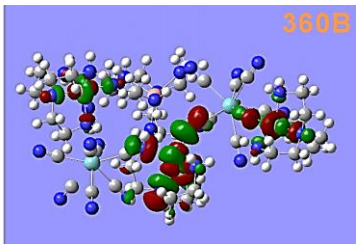
334B -> 361B 0.48342



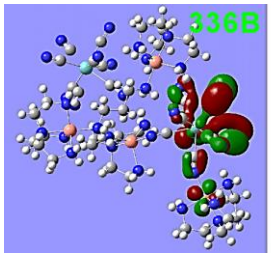


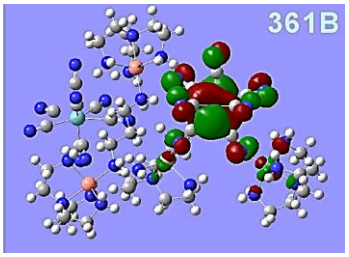
336B -> 360B 0.23356



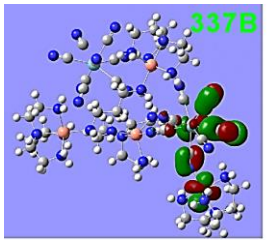


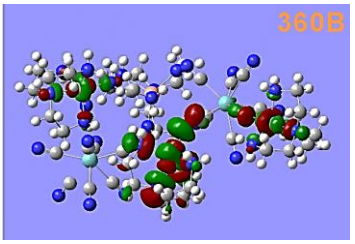
336B -> 361B 0.42571



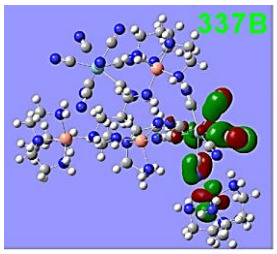


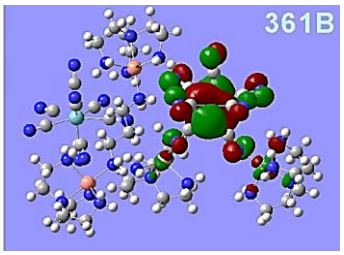
337B -> 360B 0.28871





337B -> 361B 0.51570





Excited State 98: 5.015-A 3.1681 eV 391.36 nm

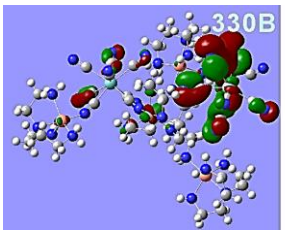
f = 0.0006 $\langle S^2 \rangle$ = 6.036

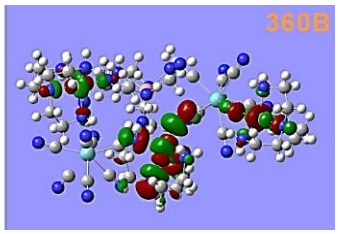
321B -> 360B -0.11547

328B -> 360B -0.27392

329B -> 361B -0.19365

330B -> 360B 0.84336





330B -> 361B 0.10116

331B -> 360B 0.22475

332B -> 360B -0.15078

332B -> 361B 0.15557

Excited State 99: 5.017-A 3.1910 eV 388.55 nm

f = 0.0003 $\langle S^2 \rangle$ = 6.043

327B -> 360B 0.15746

328B -> 361B 0.10075

329B -> 360B 0.77542

329B -> 361B 0.35263

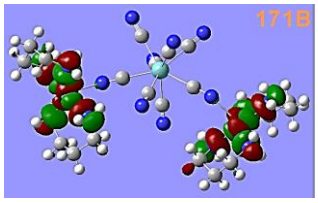
330B -> 360B 0.23310

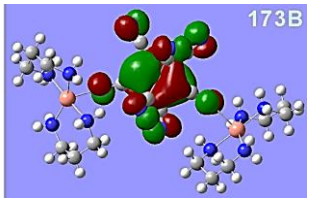
332B -> 360B 0.12538

332B -> 361B -0.31231

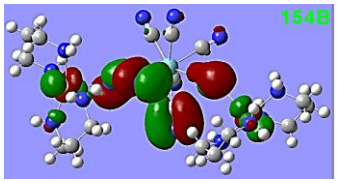
List of calculated excitation energies with non-zero oscillator strengths (*f*) for **3**.

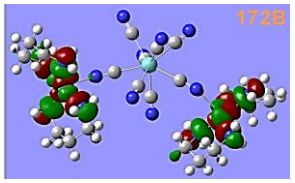
Excited State 2: 3.026-A 1.1261 eV 1100.98 nm
f = 0.0003 <S^2> = 2.039
171B ->173B 1.00015



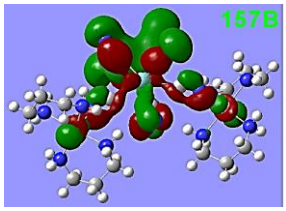


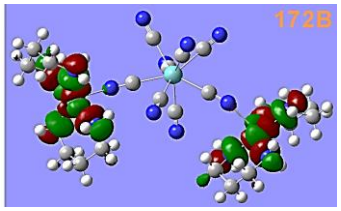
Excited State 4: 3.005-A 1.8138 eV 683.57 nm
f = 0.0013 <S^2> = 2.007
140B ->172B 0.11727
153B ->172B -0.25674
154B ->172B -0.39083



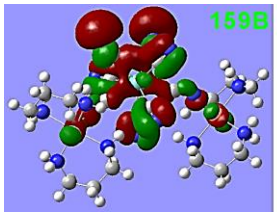


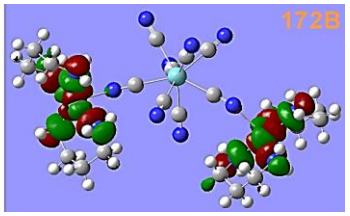
157B ->172B -0.48280



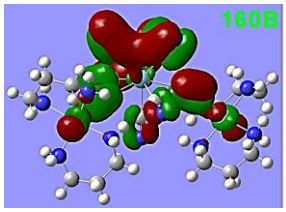


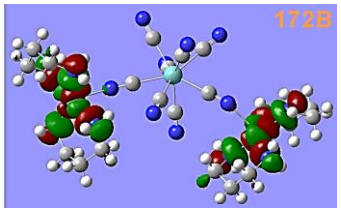
159B ->172B -0.34885





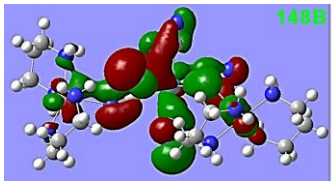
160B ->172B 0.53686

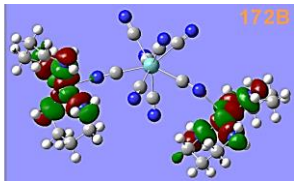




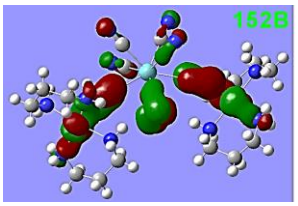
163B ->172B -0.24716
165B ->172B -0.19773

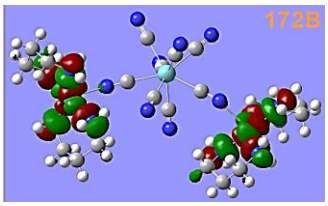
Excited State 9: 3.008-A 2.1392 eV 579.58 nm
f = 0.0006 <S^2> = 2.012
143B ->172B -0.12645
148B ->172B -0.36663



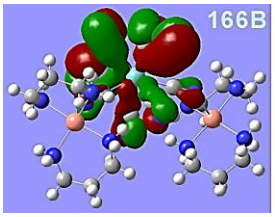


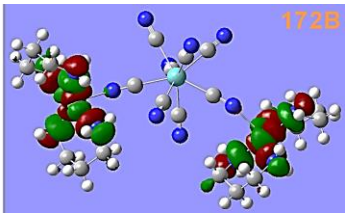
150B ->172B -0.15433
152B ->172B 0.72837





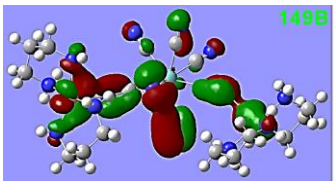
156B ->172B 0.13355
162B ->172B 0.15446
164B ->172B 0.22107
166B ->172B 0.38593

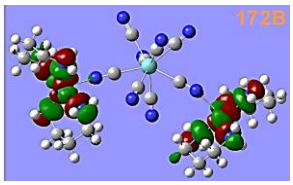




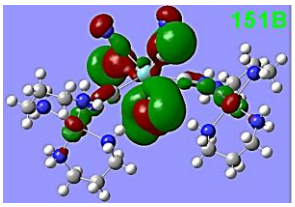
169B ->172B 0.13228

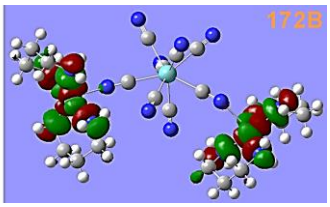
Excited State 11: 3.112-A 2.1671 eV 572.12 nm
f = 0.0008 <S^2> = 2.172
149B ->172B 0.57447



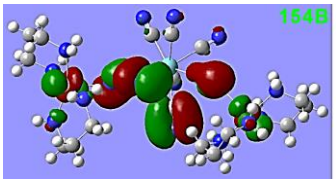


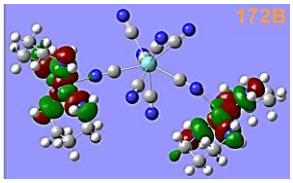
151B ->172B -0.32478



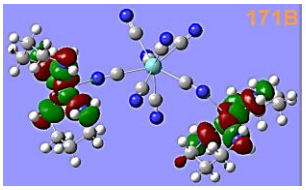


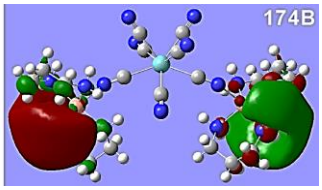
153B ->172B -0.27404
154B ->172B 0.39618



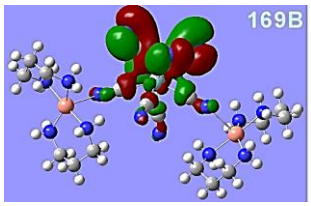


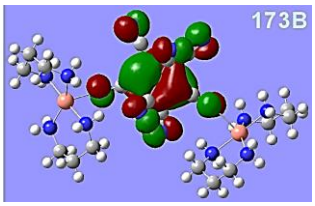
157B ->172B 0.12799
160B ->172B 0.15182
165B ->172B -0.18397
167B ->172B -0.27800
171B ->174B 0.39150



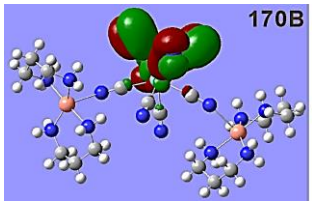


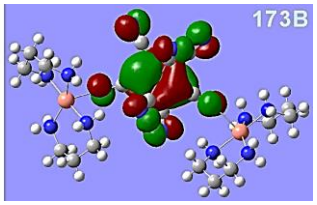
Excited State 12: 3.621-A 2.1791 eV 568.96 nm
f = 0.0002 <S^2> = 3.028
171B ->175B 0.99685
Excited State 14: 3.007-A 2.3037 eV 538.19 nm
f = 0.0002 <S^2> = 2.010
142B ->172B 0.13100
147B ->172B 0.76502
149B ->172B 0.20809
153B ->172B 0.27491
154B ->172B 0.18154
160B ->172B 0.14468
163B ->172B -0.14147
165B ->172B 0.40646
167B ->172B 0.14254
Excited State 18: 3.007-A 2.4471 eV 506.66 nm
f = 0.0002 <S^2> = 2.011
146B ->172B 0.15585
148B ->172B 0.16988
152B ->172B -0.25237
162B ->172B 0.14646
164B ->172B 0.90494
Excited State 20: 3.027-A 2.6028 eV 476.35 nm
f = 0.0014 <S^2> = 2.041
169B ->173B -0.11658



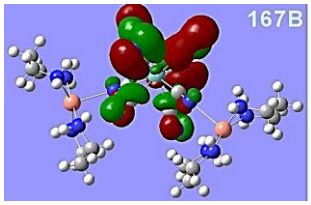


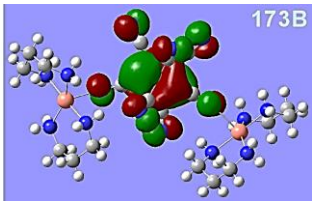
170B ->173B 0.98486



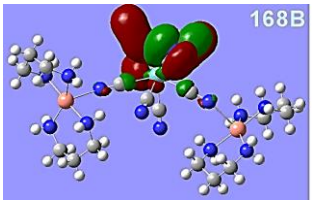


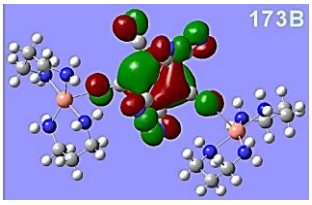
Excited State 21: 3.007-A 2.7862 eV 445.00 nm
f = 0.0002 <S^2> = 2.011
147B ->172B 0.12484
159B ->172B -0.12725
160B ->172B 0.20669
163B ->172B 0.95019
Excited State 22: 3.028-A 2.8013 eV 442.60 nm
f = 0.0009 <S^2> = 2.043
167B ->173B 0.43823



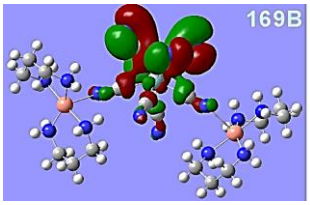


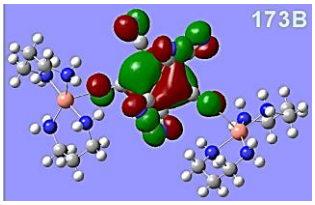
168B ->173B 0.88756



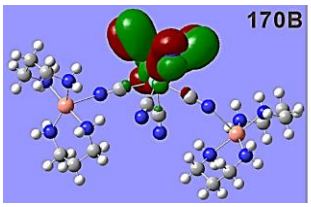


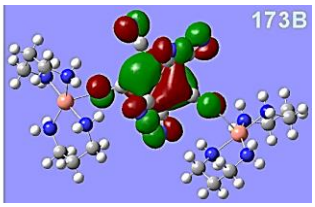
Excited State 23: 3.034-A 2.8126 eV 440.82 nm
f = 0.0147 <S^2> = 2.051
169B ->173B 0.97903



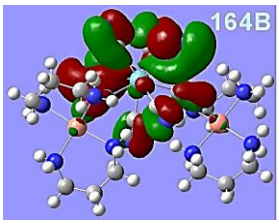


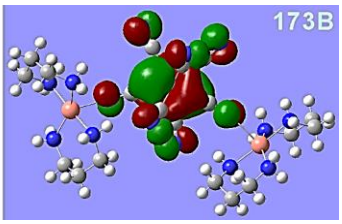
170B ->173B 0.11706



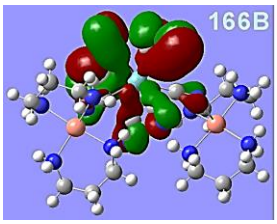


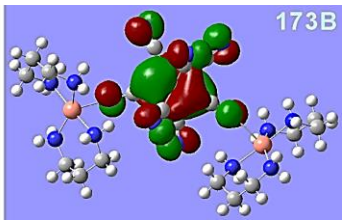
Excited State 27: 3.031-A 3.0616 eV 404.97 nm
f = 0.0023 <S^2> = 2.046
164B ->173B -0.31400



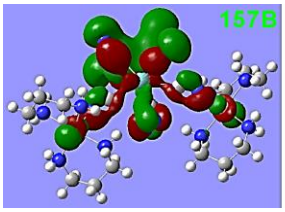


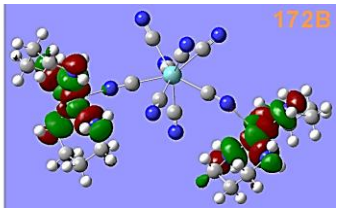
166B ->173B 0.92381



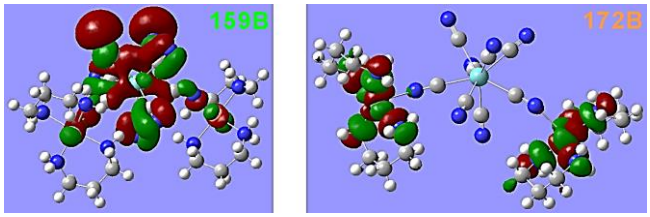


Excited State 30: 3.007-A 3.1436 eV 394.40 nm
f = 0.0009 <S^2> = 2.011
149B ->172B 0.16607
153B ->172B -0.15330
154B ->172B -0.16495
157B ->172B -0.58826

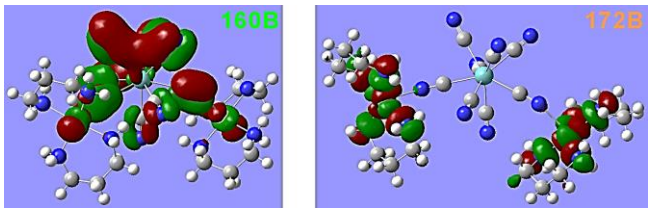




159B ->172B 0.68616



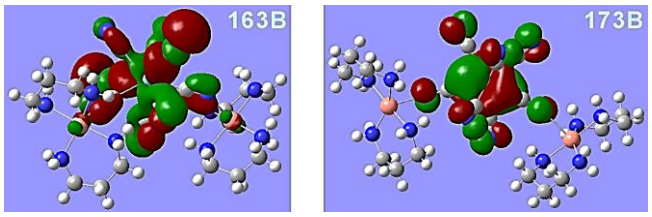
160B ->172B -0.27885



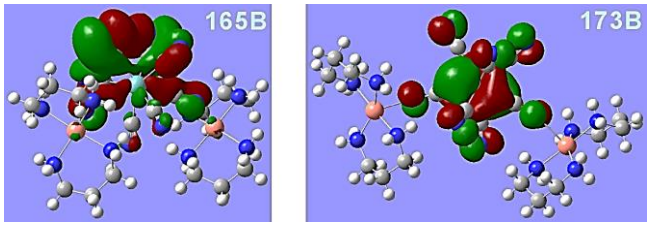
Excited State 31: 3.030-A 3.1939 eV 388.19 nm

f = 0.0007 <S^2> = 2.046

163B ->173B 0.14035



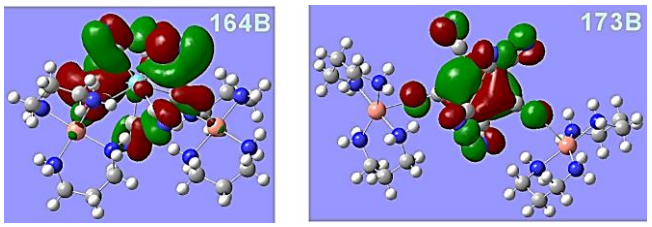
165B ->173B 0.97134



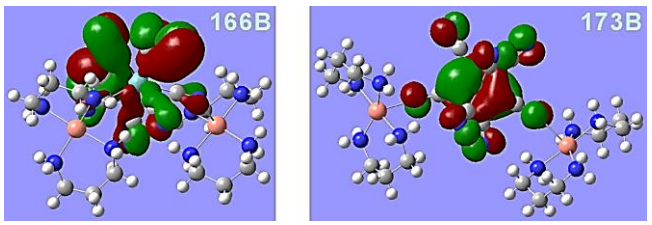
Excited State 32: 3.037-A 3.2436 eV 382.24 nm

f = 0.0045 <S^2> = 2.056

164B ->173B 0.93658



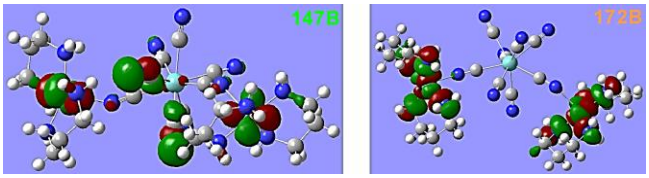
166B ->173B 0.31311



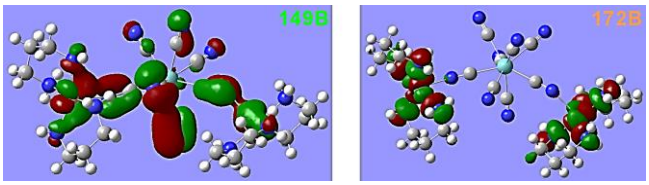
Excited State 34: 3.007-A 3.2954 eV 376.23 nm

f = 0.0040 <S^2> = 2.011

147B ->172B -0.25405

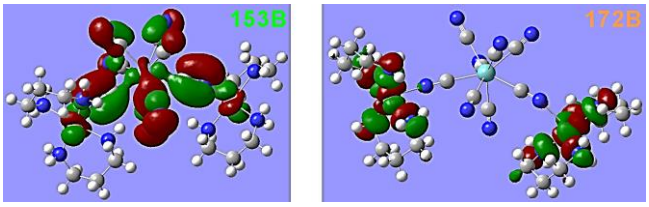


149B ->172B -0.22877

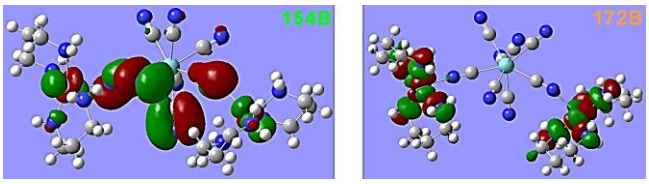


151B ->172B 0.10865

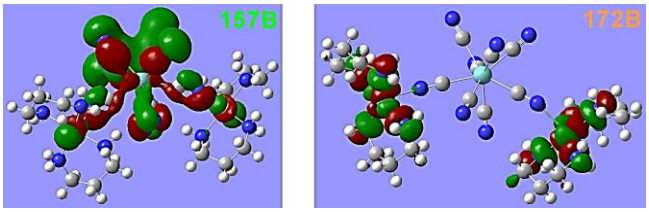
153B ->172B 0.24217



154B ->172B 0.69593



157B ->172B -0.53601



160B ->172B 0.15501

Excited State 35: 3.030-A 3.4470 eV 359.68 nm

f = 0.0003 <S^2> = 2.045

173A ->174A 0.99778

Excited State 36: 3.029-A 3.4564 eV 358.70 nm

f = 0.0004 <S^2> = 2.044

173A ->175A 0.96860

163B ->173B 0.19846

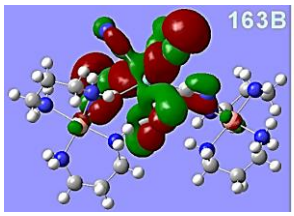
Excited State 37: 3.619-A 3.4710 eV 357.20 nm

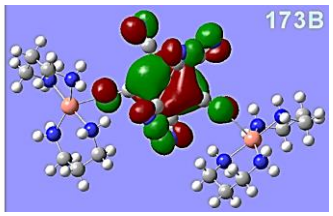
f = 0.0003 <S^2> = 3.024

171B ->176B 0.98428

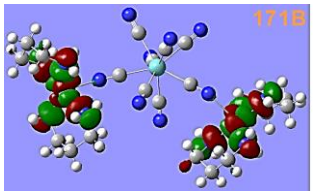
171B ->178B -0.15879

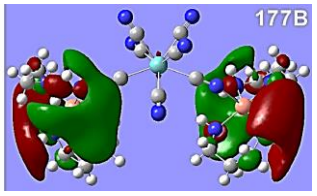
Excited State 38: 3.030-A 3.4776 eV 356.53 nm
f = 0.0013 <S^2> = 2.046
173A ->175A -0.22610
163B ->173B 0.92538



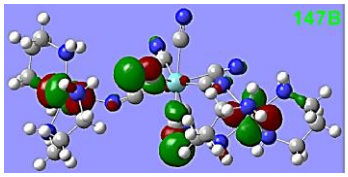


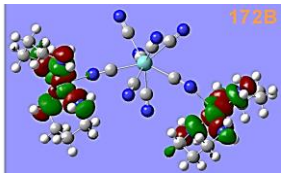
165B ->173B -0.15360
Excited State 39: 3.617-A 3.4805 eV 356.23 nm
f = 0.0010 <S^2> = 3.021
171B ->177B 0.98543



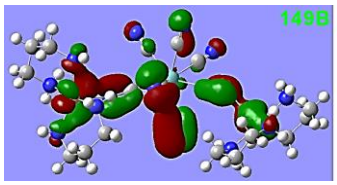


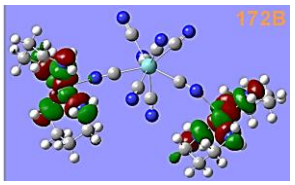
171B ->179B 0.13925
Excited State 40: 3.007-A 3.5352 eV 350.71 nm
f = 0.0013 <S^2> = 2.011
147B ->172B -0.30324



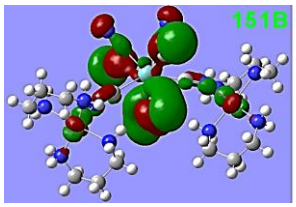


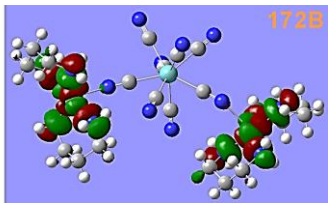
149B ->172B 0.35190



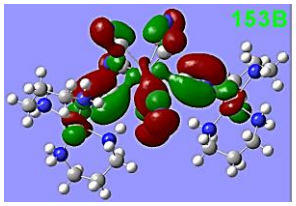


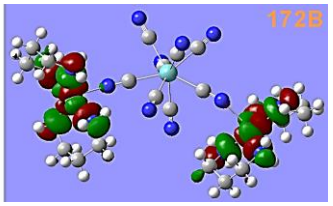
151B ->172B -0.32599



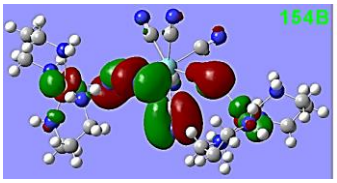


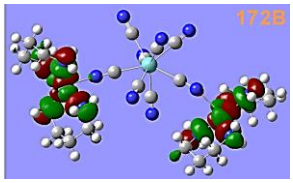
153B ->172B 0.75278



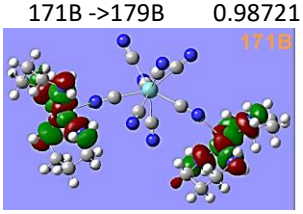


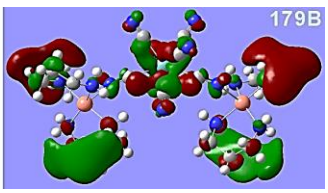
154B ->172B -0.29452



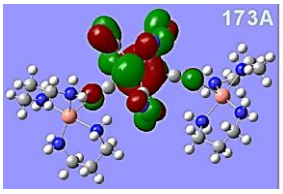


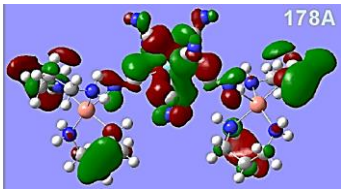
Excited State 42: 3.615-A 3.6772 eV 337.17 nm
f = 0.0003 <S^2> = 3.016
171B ->176B 0.15618
171B ->178B 0.98448
Excited State 43: 3.615-A 3.7037 eV 334.76 nm
f = 0.0005 <S^2> = 3.017
171B ->177B -0.13769
171B ->179B 0.98721



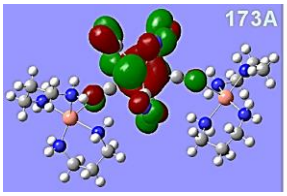


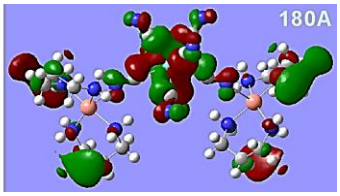
Excited State 44: 3.031-A 3.7147 eV 333.77 nm
f = 0.0052 <S^2> = 2.047
173A ->178A -0.25072



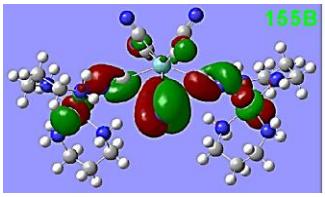


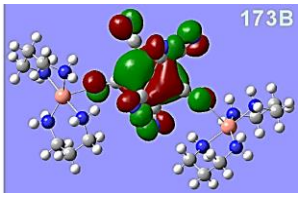
173A ->180A 0.23433



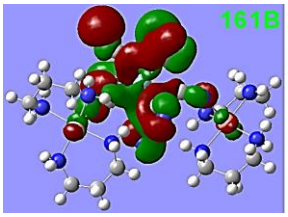


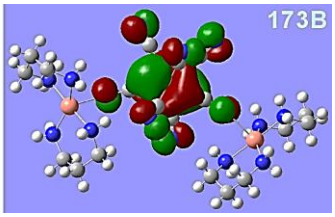
155B ->173B -0.16483



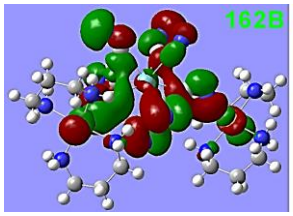


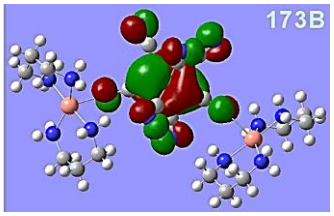
158B ->173B -0.10504
161B ->173B 0.87135





162B ->173B 0.14441





166B ->173B 0.12911

Excited State 46: 3.038-A 3.7943 eV 326.76 nm

f = 0.0004 $\langle S^2 \rangle$ = 2.057

155B ->173B -0.19602

158B ->173B 0.20041

161B ->173B -0.15957

162B ->173B 0.93440

Excited State 47: 3.008-A 3.8408 eV 322.81 nm

f = 0.0005 $\langle S^2 \rangle$ = 2.012

146B ->172B 0.62615

148B ->172B -0.14935

150B ->172B 0.75720

Excited State 48: 3.016-A 3.8571 eV 321.45 nm

f = 0.0004 $\langle S^2 \rangle$ = 2.024

173A ->177A 0.18755

173A ->179A 0.67672

173A ->181A 0.60704

157B ->173B 0.13071

159B ->173B 0.12837

163B ->173B -0.17025

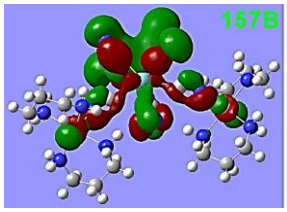
Excited State 49: 3.040-A 3.8676 eV 320.57 nm

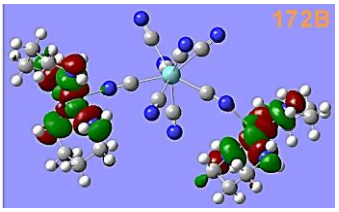
f = 0.0125 $\langle S^2 \rangle$ = 2.060

173A ->179A -0.11843

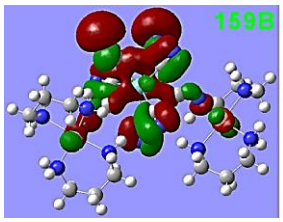
173A ->181A -0.10723

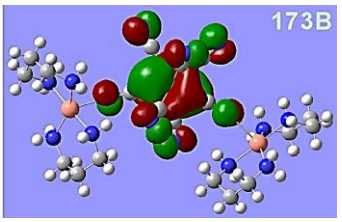
157B ->173B 0.24479



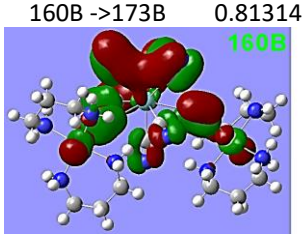


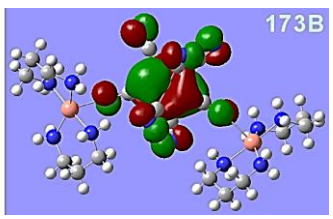
159B ->173B 0.47227





160B ->173B 0.81314





Excited State 50: 3.028-A 3.8776 eV 319.74 nm

f = 0.0004 $\langle S^2 \rangle$ = 2.042

173A ->178A 0.53479

173A ->180A -0.47477

156B ->173B -0.12330

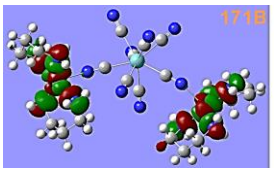
158B ->173B 0.52837

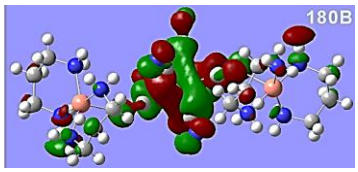
161B ->173B 0.38439

Excited State 51: 3.607-A 3.9263 eV 315.78 nm

f = 0.0008 $\langle S^2 \rangle$ = 3.002

171B ->180B 0.96705



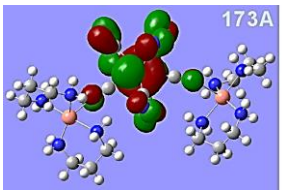


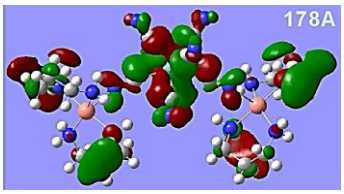
171B ->183B -0.21509

Excited State 52: 3.038-A 3.9414 eV 314.57 nm

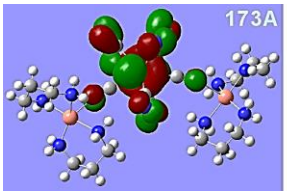
f = 0.0015 $\langle S^2 \rangle$ = 2.057

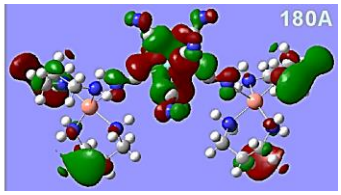
173A ->178A -0.40556





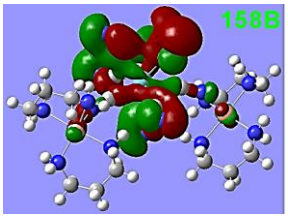
173A ->180A 0.36441

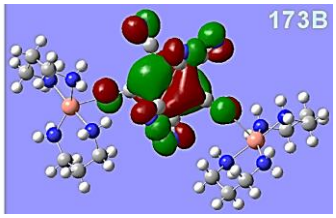




156B ->173B -0.22323

158B ->173B 0.75056





162B ->173B -0.15457

Excited State 53: 3.608-A 3.9455 eV 314.24 nm

f = 0.0003 $\langle S^2 \rangle$ = 3.004

171B ->181B 0.97967

171B ->182B -0.13876

Excited State 54: 3.057-A 3.9678 eV 312.48 nm

f = 0.0058 $\langle S^2 \rangle$ = 2.086

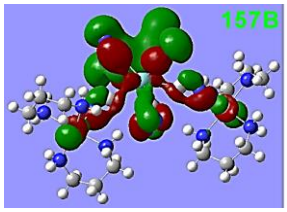
170A ->175A -0.15837

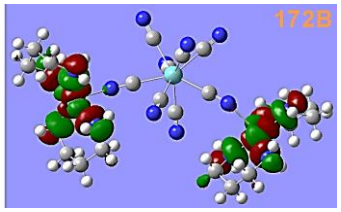
171A ->174A -0.16121

153B ->173B -0.14066

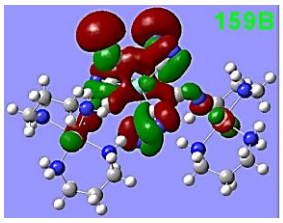
154B ->173B -0.13809

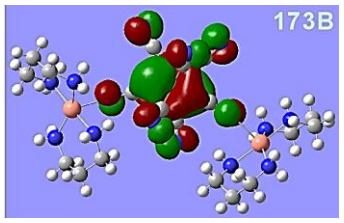
157B ->173B -0.20550



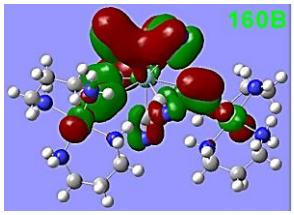


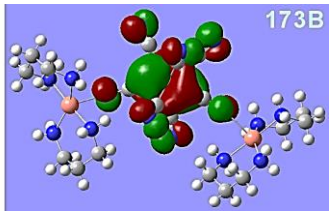
159B ->173B 0.81603





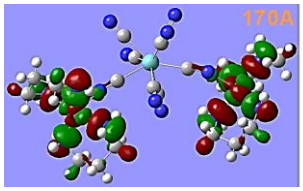
160B ->173B -0.41612

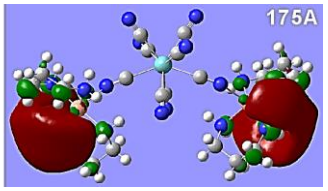




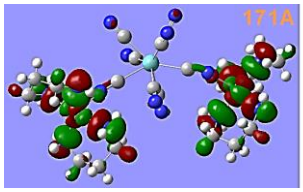
Excited State 55: 3.329-A 3.9715 eV 312.18 nm
f = 0.0004 <S^2> = 2.520
170A ->174A 0.70645
171A ->175A 0.68816

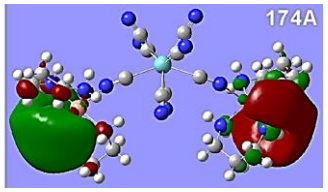
Excited State 56: 3.305-A 3.9720 eV 312.14 nm
f = 0.0016 <S^2> = 2.482
170A ->175A 0.66918





171A ->174A 0.68142

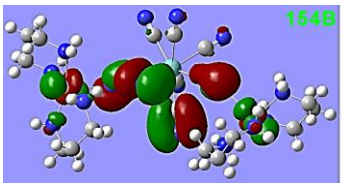


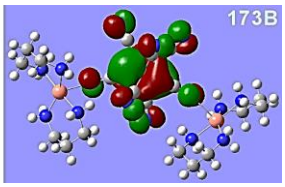


159B ->173B 0.18720
171B ->181B -0.12016

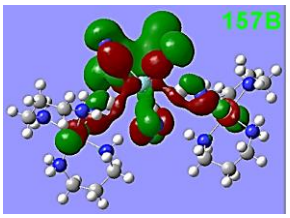
Excited State 58: 3.615-A 4.0505 eV 306.10 nm
f = 0.0003 <S^2> = 3.018
171B ->180B 0.21804
171B ->183B 0.97165

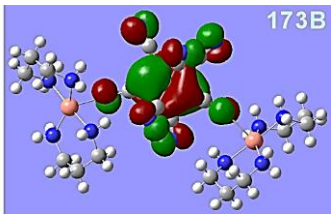
Excited State 59: 3.044-A 4.1093 eV 301.72 nm
f = 0.0064 <S^2> = 2.066
153B ->173B -0.16911
154B ->173B -0.30277



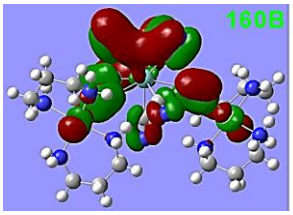


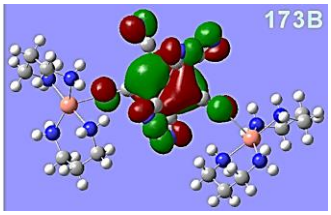
157B ->173B 0.87498



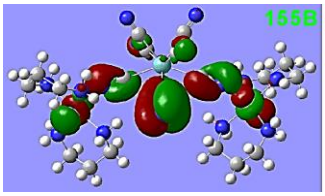


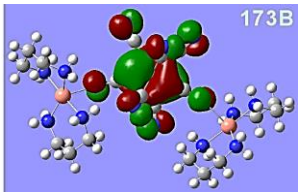
160B ->173B -0.28094



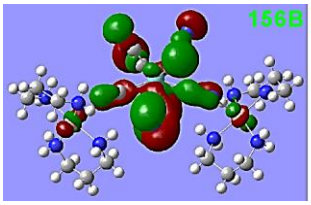


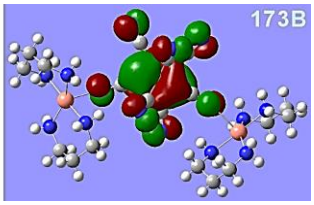
Excited State 60: 3.048-A 4.1430 eV 299.26 nm
f = 0.0123 <S^2> = 2.073
155B ->173B 0.31060



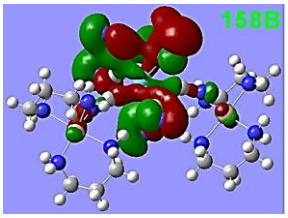


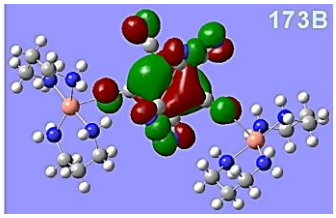
156B ->173B 0.90422



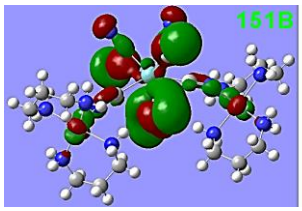


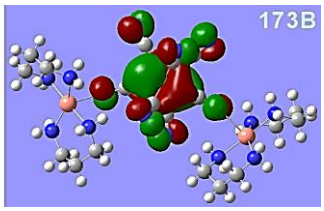
158B ->173B 0.23176



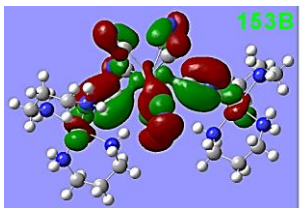


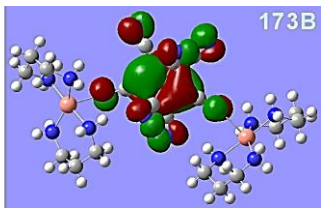
Excited State 63: 3.054-A 4.3628 eV 284.19 nm
f = 0.0054 $\langle S^2 \rangle$ = 2.082
149B ->173B -0.17095
151B ->173B 0.29882



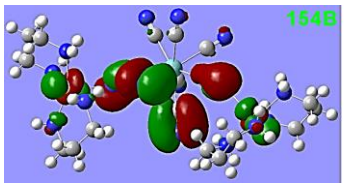


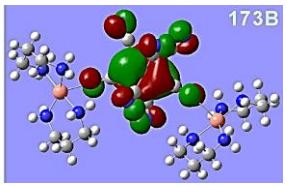
153B ->173B -0.58201





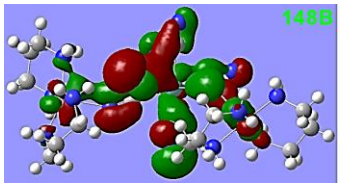
154B ->173B 0.69507

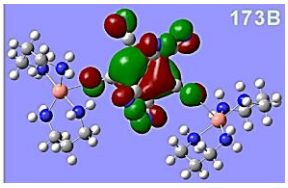




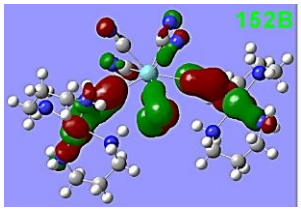
157B ->173B 0.10274

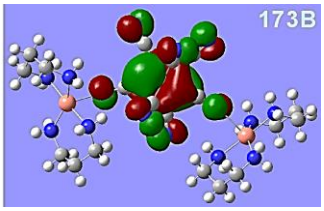
Excited State 65: 3.064-A 4.4240 eV 280.25 nm
f = 0.0226 $\langle S^2 \rangle$ = 2.097
148B ->173B -0.23903



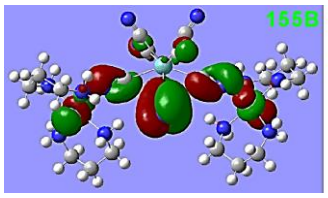


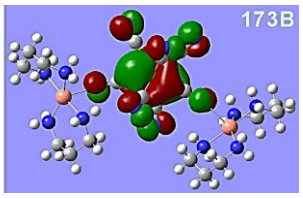
152B ->173B -0.27138



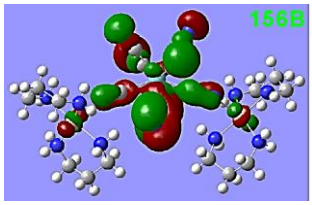


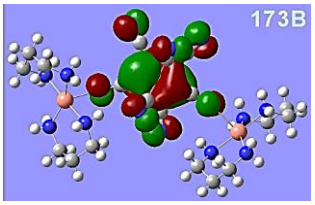
155B ->173B 0.83637



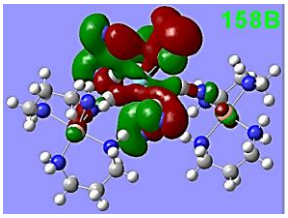


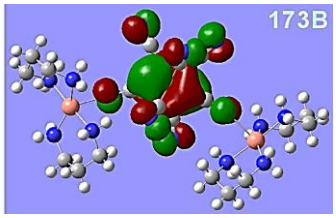
156B ->173B -0.26401



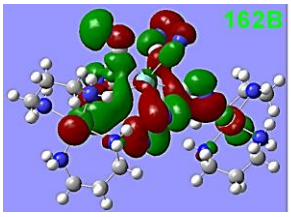


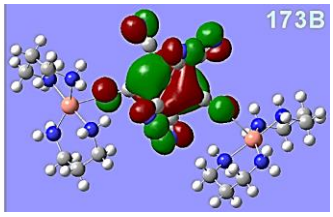
158B ->173B -0.11495





162B ->173B 0.19853

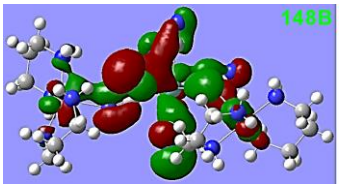


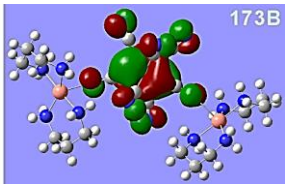


Excited State 68: 3.566-A 4.4450 eV 278.93 nm
f = 0.0004 $\langle S^2 \rangle$ = 2.929
172A ->175A 0.98598

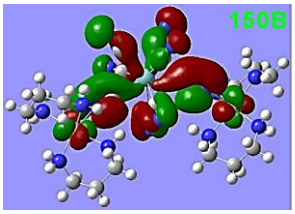
Excited State 72: 3.007-A 4.5467 eV 272.69 nm
f = 0.0002 $\langle S^2 \rangle$ = 2.011
141B ->172B 0.98938
149B ->172B 0.12234

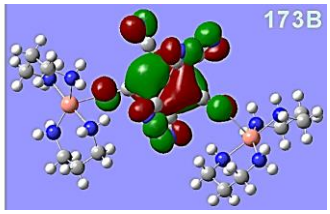
Excited State 80: 3.061-A 4.6499 eV 266.64 nm
f = 0.0062 $\langle S^2 \rangle$ = 2.093
146B ->173B 0.17547
148B ->173B 0.36576



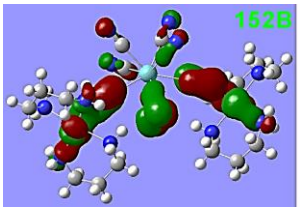


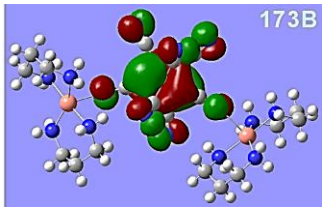
150B ->173B 0.40760



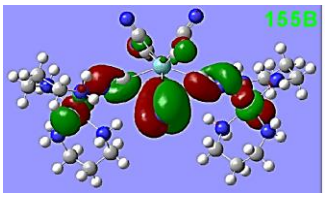


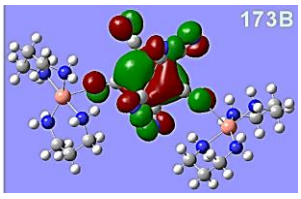
152B ->173B 0.71158





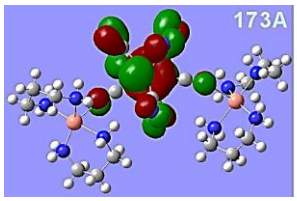
155B ->173B 0.29022

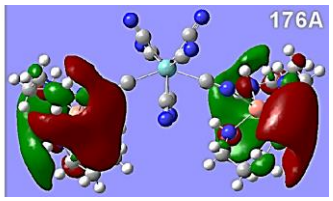




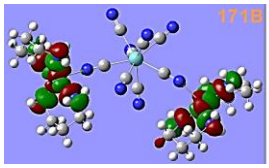
156B ->173B -0.10948
162B ->173B 0.12146

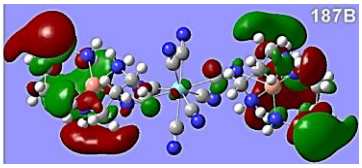
Excited State 84: 3.053-A 4.7025 eV 263.66 nm
f = 0.0027 <S^2> = 2.081
168A ->175A -0.17683
173A ->176A 0.95215



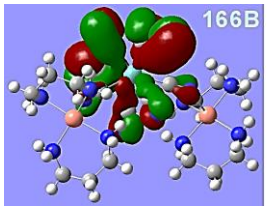


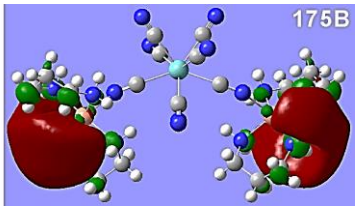
173A ->178A -0.16003
Excited State 89: 3.037-A 4.7214 eV 262.60 nm
f = 0.0006 <S^2> = 2.056
168A ->174A -0.10562
173A ->177A 0.96724
173A ->179A -0.15834
173A ->181A -0.12216
Excited State 92: 3.618-A 4.7856 eV 259.08 nm
f = 0.0007 <S^2> = 3.023
171B ->187B 0.96660



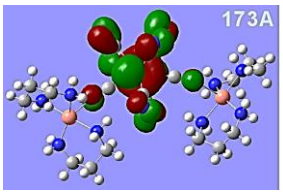


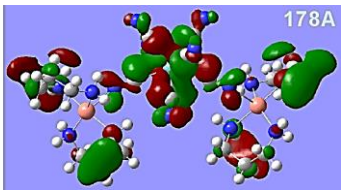
171B ->189B -0.21010
Excited State 94: 3.628-A 4.8560 eV 255.32 nm
f = 0.0004 <S^2> = 3.040
165B ->175B 0.21558
166B ->174B 0.96052
Excited State 95: 3.631-A 4.8675 eV 254.72 nm
f = 0.0014 <S^2> = 3.046
165B ->174B 0.25883
166B ->175B 0.94511



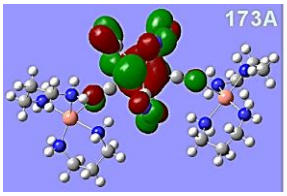


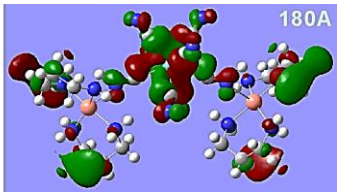
Excited State 96: 3.617-A 4.8775 eV 254.19 nm
f = 0.0002 <S^2> = 3.020
171B ->186B 0.30841
171B ->188B 0.93853
Excited State 98: 3.030-A 4.9068 eV 252.68 nm
f = 0.0007 <S^2> = 2.045
173A ->176A 0.15587
173A ->178A 0.59817



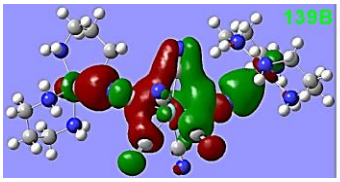


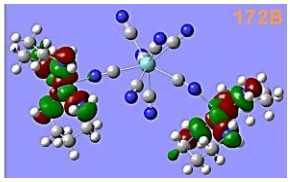
173A ->180A 0.61933





173A ->189A -0.10023
173A ->190A 0.35691
173A ->193A -0.10859
173A ->195A -0.12952
152B ->173B 0.10510
Excited State 100: 3.009-A 4.9359 eV 251.19 nm
f = 0.0008 <S^2> = 2.013
139B ->172B 0.97216

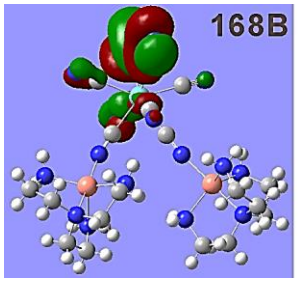


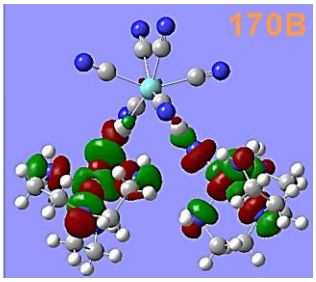


155B ->172B -0.11855

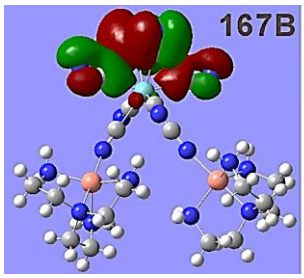
List of calculated excitation energies with non-zero oscillator strengths (*f*) for **4**

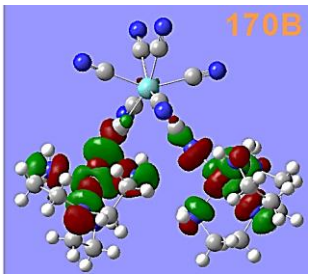
Excited State 2: 3.012-A 0.9170 eV 1352.07 nm
f = 0.0004 <S^2> = 2.019
168B ->170B 0.99921



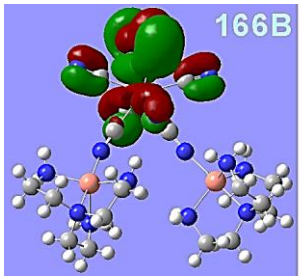


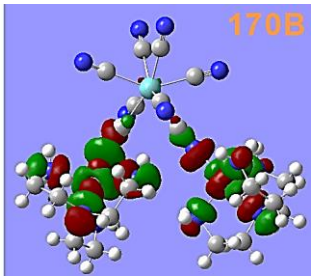
Excited State 3: 3.012-A 1.0694 eV 1159.39 nm
f = 0.0004 <S^2> = 2.019
167B ->170B 0.99673



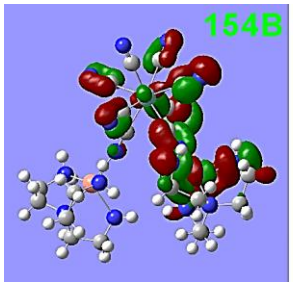


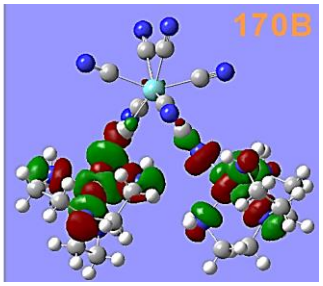
Excited State 4: 3.012-A 1.2076 eV 1026.72 nm
f = 0.0002 <S^2> = 2.018
166B ->170B 0.99347



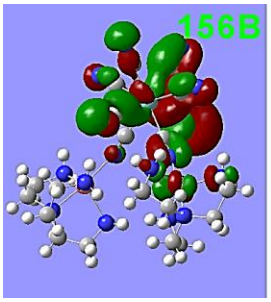


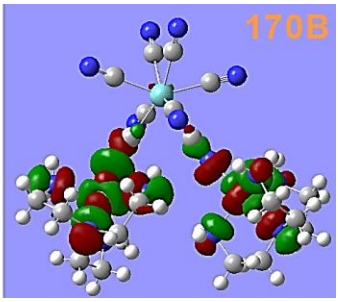
Excited State 6: 3.012-A 1.3279 eV 933.66 nm
f = 0.0005 <S^2> = 2.019
152B ->170B -0.15470
153B ->170B -0.30492
154B ->170B 0.76688





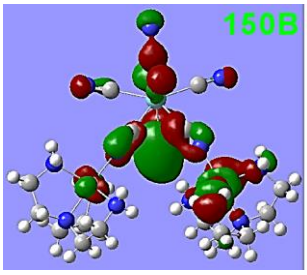
156B ->170B 0.35771

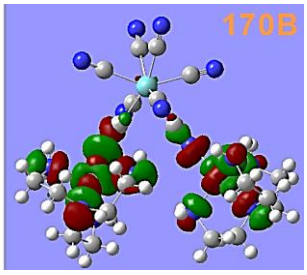




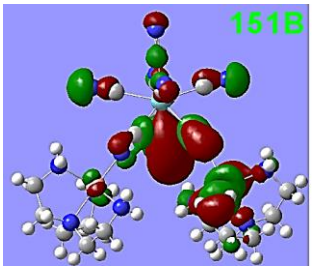
159B ->170B -0.16046
161B ->170B -0.18446
165B ->170B 0.11197

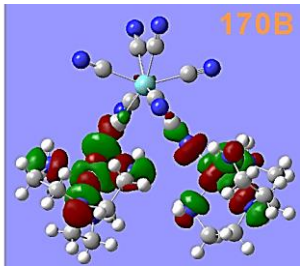
Excited State 7: 3.012-A 1.4391 eV 861.55 nm
f = 0.0006 <S^2> = 2.018
127B ->170B -0.11345
149B ->170B -0.16301
150B ->170B 0.46679



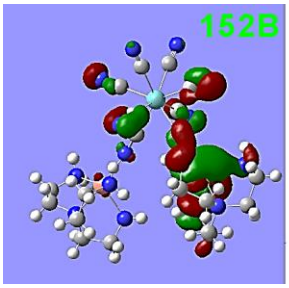


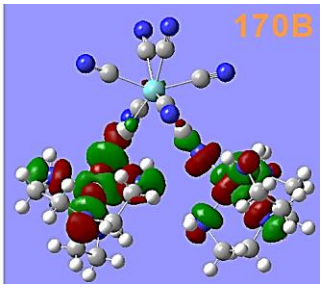
151B ->170B 0.61640





152B ->170B 0.44869



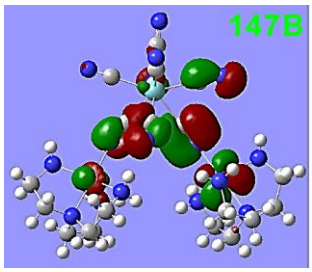


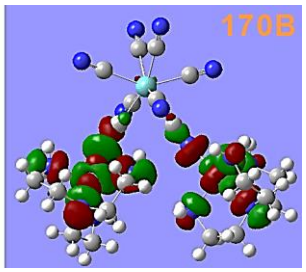
153B ->170B 0.11957
154B ->170B 0.18798
161B ->170B 0.17993
162B ->170B -0.11317
164B ->170B -0.10316

Excited State 8: 3.013-A 1.4592 eV 849.65 nm
f = 0.0003 <S^2> = 2.019
150B ->170B -0.35090
151B ->170B -0.32098
152B ->170B 0.72816
154B ->170B 0.11271
155B ->170B 0.32376
157B ->170B -0.15241
161B ->170B 0.11953
163B ->170B -0.15130

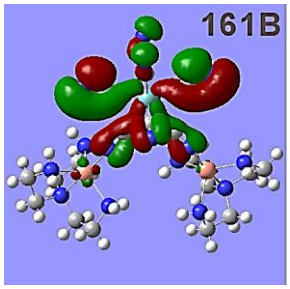
Excited State 9: 3.012-A 1.6135 eV 768.42 nm
f = 0.0004 <S^2> = 2.018
150B ->170B 0.10945
164B ->170B 0.98497

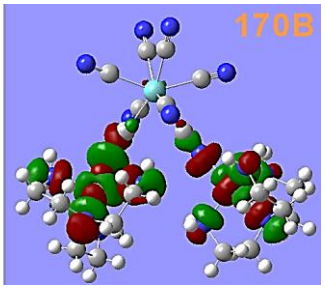
Excited State 11: 3.016-A 1.7968 eV 690.02 nm
f = 0.0009 <S^2> = 2.024
140B ->170B -0.18381
142B ->170B 0.13462
146B ->170B 0.15519
147B ->170B 0.59236



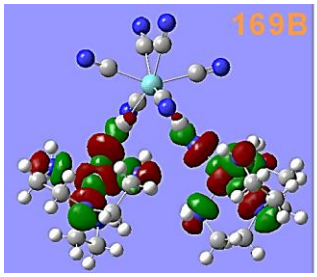


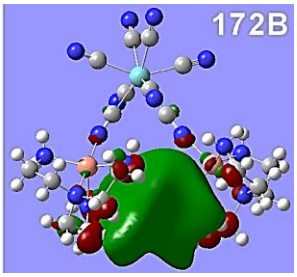
148B ->170B -0.27379
149B ->170B -0.10722
152B ->170B -0.24472
154B ->170B 0.10327
159B ->170B 0.10195
161B ->170B 0.58998



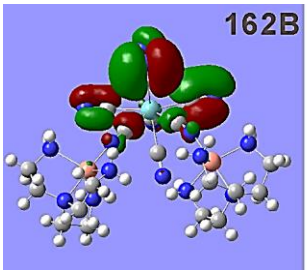


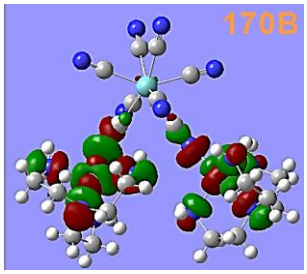
Excited State 12: 3.619-A 1.8274 eV 678.47 nm
f = 0.0028 <S^2> = 3.025
169B ->172B 0.99445



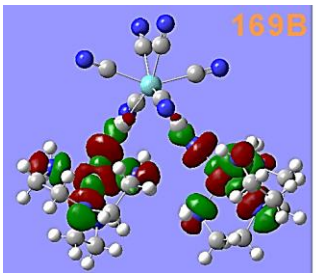


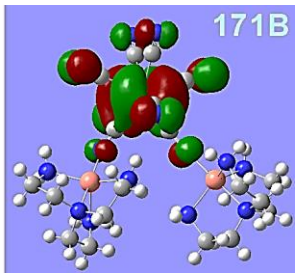
Excited State 14: 3.026-A 1.8763 eV 660.80 nm
f = 0.0020 <S^2> = 2.040
145B ->170B -0.15275
149B ->170B 0.10999
162B ->170B -0.22611





169B ->171B 0.94459





Excited State 15: 3.013-A 1.8881 eV 656.66 nm
f = 0.0011 <S^2> = 2.019
139B ->170B -0.13844
140B ->170B -0.10168
141B ->170B -0.13541
142B ->170B -0.16492
144B ->170B 0.31594
145B ->170B 0.17603
146B ->170B 0.37665
147B ->170B -0.26862
148B ->170B -0.23410
149B ->170B -0.10758
150B ->170B 0.18624
156B ->170B 0.11840
158B ->170B 0.15745
160B ->170B 0.35107
162B ->170B 0.38546
163B ->170B -0.25883
169B ->171B 0.18327

Excited State 16: 3.013-A 1.9579 eV 633.26 nm
f = 0.0006 <S^2> = 2.019
141B ->170B -0.15363
143B ->170B -0.15272
145B ->170B -0.49605
146B ->170B -0.37606
148B ->170B -0.13826
149B ->170B 0.20055
150B ->170B 0.13171
155B ->170B 0.15802
157B ->170B -0.10589
159B ->170B 0.12057
162B ->170B 0.61285

163B ->170B 0.15314

Excited State 17: 3.013-A 2.0373 eV 608.57 nm

f = 0.0009 <S^2> = 2.019

140B ->170B -0.12395
141B ->170B 0.10770
142B ->170B -0.20016
144B ->170B -0.51734
145B ->170B -0.14899
147B ->170B -0.31287
148B ->170B 0.22114
155B ->170B -0.16565
159B ->170B -0.21469
160B ->170B 0.24079
161B ->170B 0.52491
162B ->170B 0.12973
163B ->170B -0.17386

Excited State 18: 3.012-A 2.0503 eV 604.72 nm

f = 0.0010 <S^2> = 2.019

139B ->170B -0.14526
141B ->170B -0.14871
143B ->170B -0.46620
146B ->170B -0.39585
149B ->170B -0.21335
154B ->170B -0.10033
159B ->170B 0.12663
160B ->170B 0.57583
162B ->170B -0.36236

Excited State 19: 3.012-A 2.1296 eV 582.19 nm

f = 0.0005 <S^2> = 2.018

139B ->170B 0.16465
141B ->170B 0.22626
142B ->170B 0.16713
143B ->170B 0.41255
144B ->170B -0.12268
146B ->170B 0.18258
147B ->170B 0.24720
149B ->170B 0.14839
151B ->170B 0.11886
156B ->170B -0.13193
158B ->170B -0.13929
159B ->170B 0.20161
160B ->170B 0.63854
161B ->170B -0.20424

Excited State 20: 3.012-A 2.1603 eV 573.92 nm

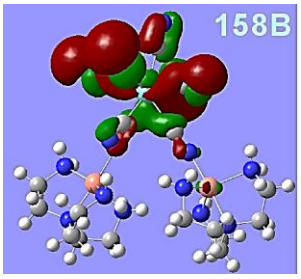
f = 0.0012 <S^2> = 2.018

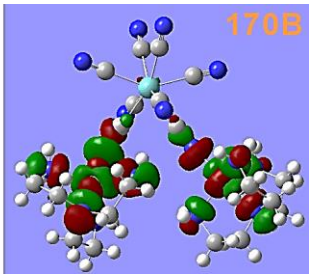
139B ->170B 0.14648
140B ->170B 0.42670
143B ->170B 0.21100
144B ->170B 0.45043
145B ->170B 0.11484
146B ->170B -0.12936
147B ->170B -0.33789
148B ->170B 0.11360
149B ->170B 0.11008
153B ->170B -0.10174
157B ->170B -0.12134
159B ->170B 0.26866
160B ->170B 0.14240
161B ->170B 0.45879

Excited State 23: 3.014-A 2.3213 eV 534.11 nm

f = 0.0006 <S^2> = 2.021

143B ->170B 0.11074
151B ->170B 0.10159
158B ->170B 0.90664



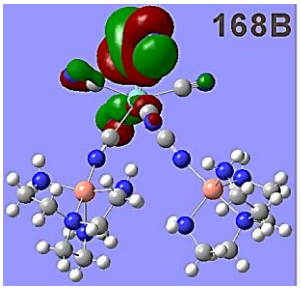


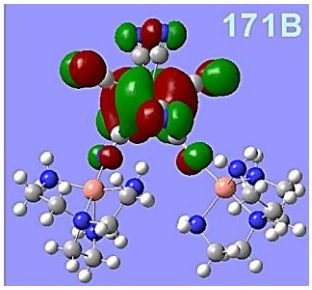
168B ->171B -0.28843

Excited State 24: 3.026-A 2.3312 eV 531.84 nm

f = 0.0015 <S^2> = 2.039

158B ->170B 0.27773
168B ->171B 0.94902

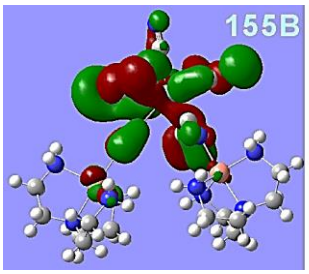


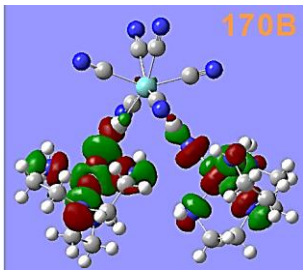


Excited State 25: 3.012-A 2.4260 eV 511.07 nm

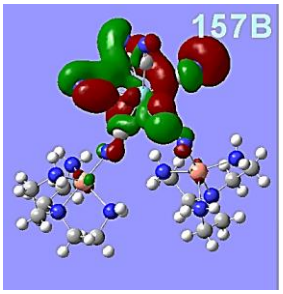
f = 0.0018 <S^2> = 2.019

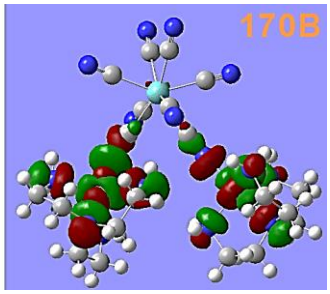
155B ->170B 0.28639



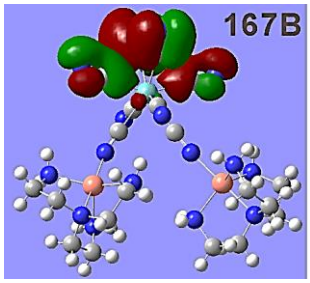


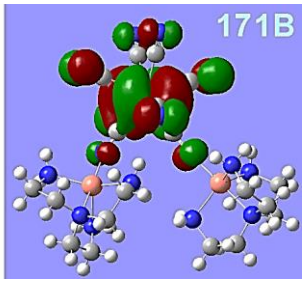
157B ->170B 0.93008





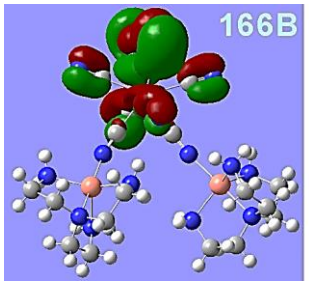
Excited State 26: 3.030-A 2.4943 eV 497.07 nm
f = 0.0037 <S^2> = 2.045
167B ->171B 0.98743

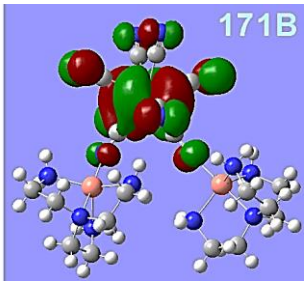




Excited State 27: 3.013-A 2.5142 eV 493.15 nm
f = 0.0002 <S^2> = 2.019
147B ->170B 0.10292
151B ->170B 0.10165
153B ->170B 0.11324
154B ->170B -0.35348
156B ->170B 0.88343

Excited State 28: 3.027-A 2.5639 eV 483.58 nm
f = 0.0009 <S^2> = 2.040
166B ->171B 0.98368

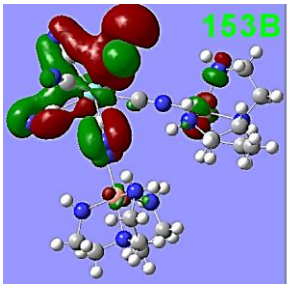


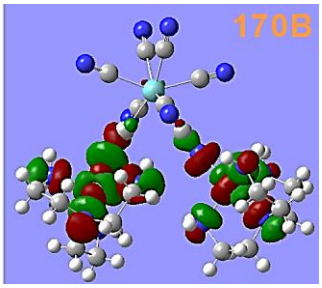


Excited State 29: 3.012-A 2.6052 eV 475.92 nm
f = 0.0009 <S^2> = 2.019
141B ->170B 0.15556
144B ->170B -0.16501
145B ->170B 0.14440
147B ->170B -0.12788
148B ->170B 0.13181
152B ->170B -0.30225
153B ->170B 0.12205
155B ->170B 0.83521
157B ->170B -0.20791

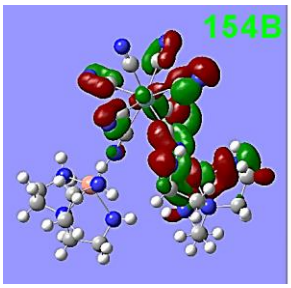
Excited State 30: 3.012-A 2.7071 eV 458.00 nm
f = 0.0021 <S^2> = 2.018
150B ->170B -0.10168
151B ->170B -0.11224
152B ->170B -0.10045

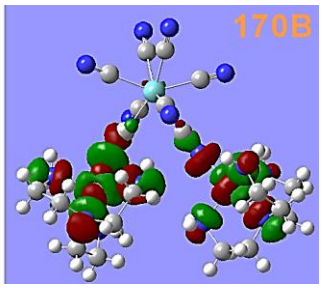
153B ->170B 0.90130





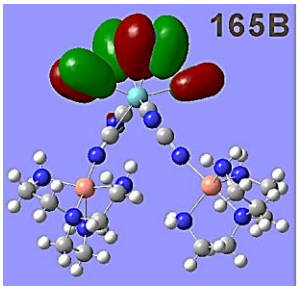
154B ->170B 0.31858

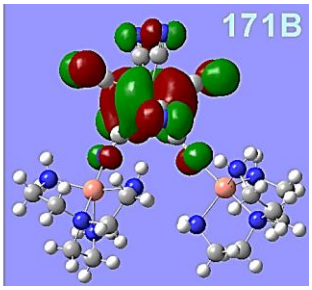




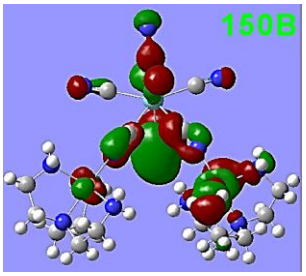
155B ->170B -0.11858

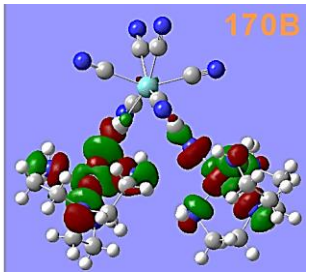
Excited State 31: 3.036-A 2.7899 eV 444.40 nm
f = 0.0039 <S^2> = 2.055
165B ->171B 0.98801



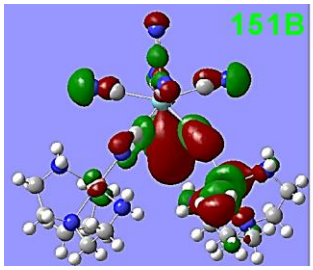


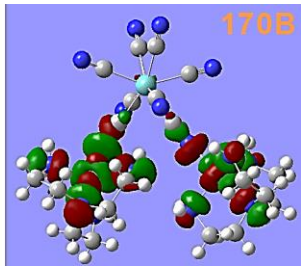
Excited State 32: 3.013-A 2.9665 eV 417.95 nm
f = 0.0038 <S^2> = 2.019
141B ->170B 0.14171
142B ->170B 0.10906
145B ->170B 0.16895
146B ->170B -0.16432
147B ->170B 0.11432
148B ->170B 0.17287
150B ->170B 0.67941





151B ->170B -0.59000

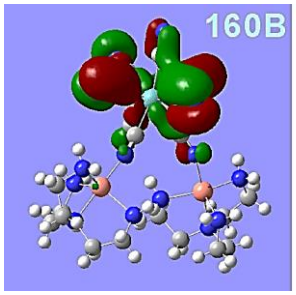


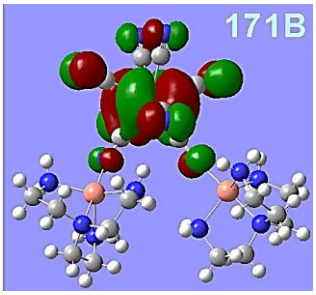


Excited State 33: 3.031-A 2.9984 eV 413.51 nm

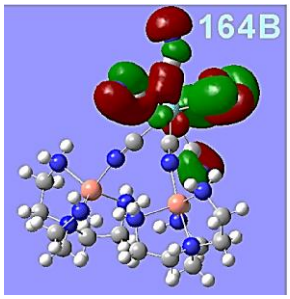
f = 0.0052 $\langle S^2 \rangle$ = 2.047

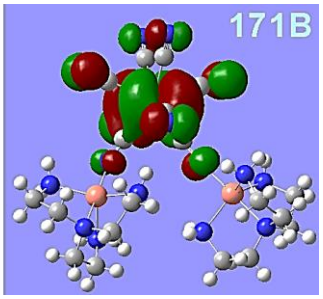
160B ->171B 0.11096





164B ->171B 0.97006

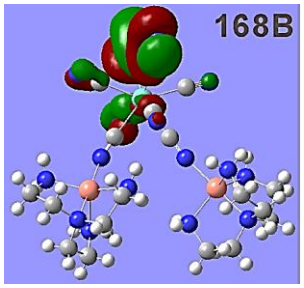


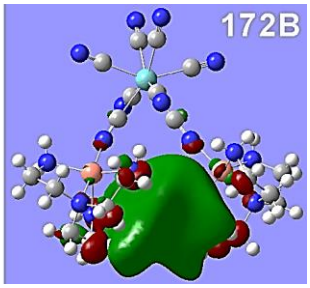


Excited State 34: 3.627-A 3.0640 eV 404.65 nm

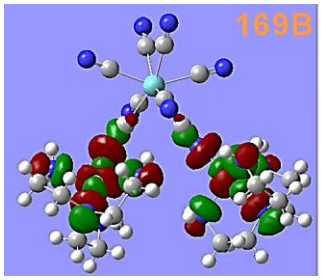
f = 0.0025 $\langle S^2 \rangle$ = 3.039

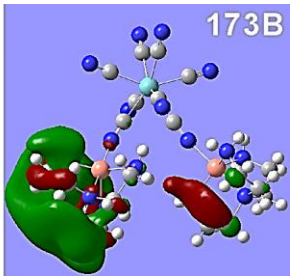
168B ->172B 0.10694





169B ->173B 0.98390





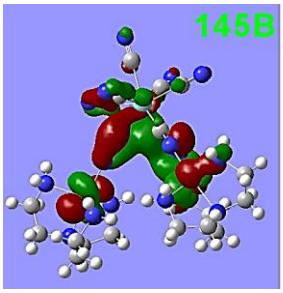
Excited State 37: 3.012-A 3.1215 eV 397.19 nm

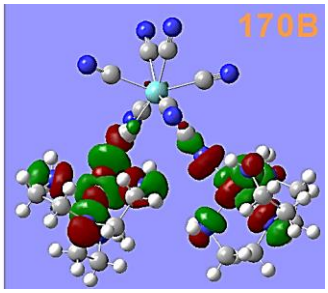
f = 0.0034 $\langle S^2 \rangle$ = 2.019

139B ->170B -0.18511

143B ->170B -0.24718

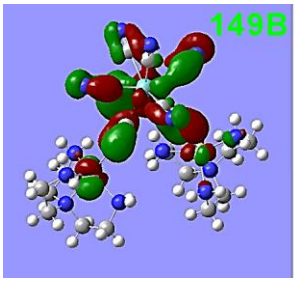
145B ->170B 0.41441

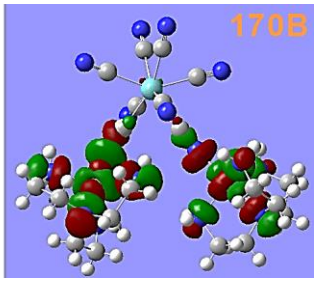




147B ->170B 0.11741

149B ->170B 0.81295





151B ->170B 0.11455

154B ->170B 0.12889

Excited State 38: 3.032-A 3.1401 eV 394.84 nm

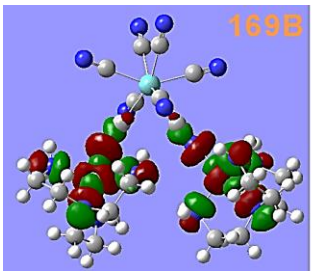
f = 0.0002 $\langle S^2 \rangle$ = 2.048

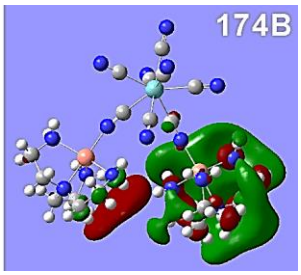
163B ->171B 0.98364

Excited State 41: 3.619-A 3.2939 eV 376.40 nm

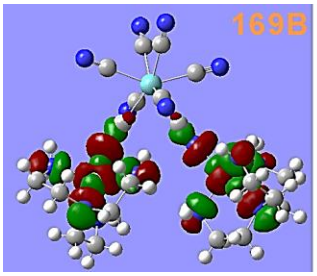
f = 0.0036 $\langle S^2 \rangle$ = 3.024

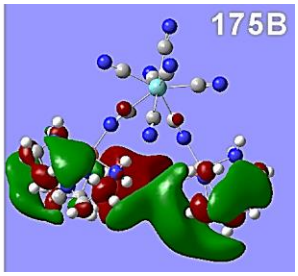
169B ->174B 0.97203





169B ->175B -0.21285





Excited State 42: 3.033-A 3.3476 eV 370.37 nm

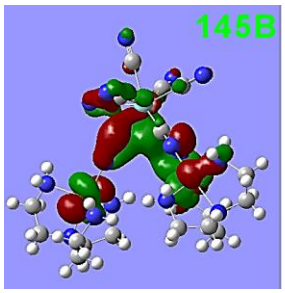
f = 0.0002 $\langle S^2 \rangle$ = 2.050

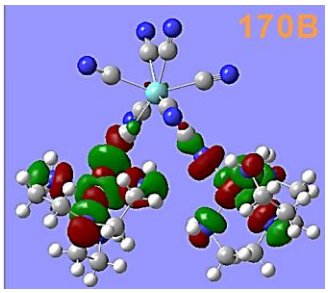
159B ->171B 0.11938

161B ->171B 0.93131

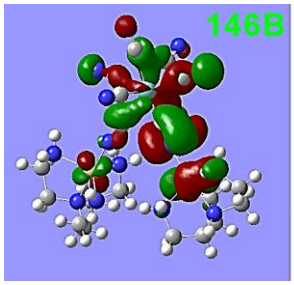
162B ->171B 0.27871

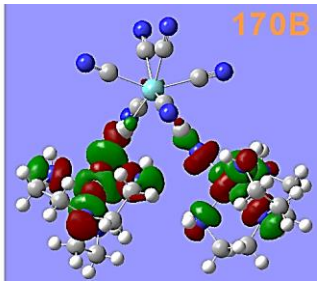
Excited State 43: 3.013-A 3.3581 eV 369.21 nm
f = 0.0017 $\langle S^2 \rangle$ = 2.020
141B ->170B -0.21136
143B ->170B -0.18425
144B ->170B 0.26240
145B ->170B -0.28289



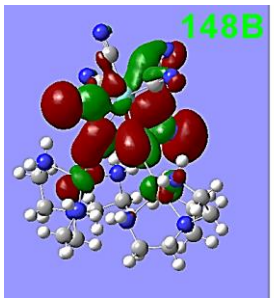


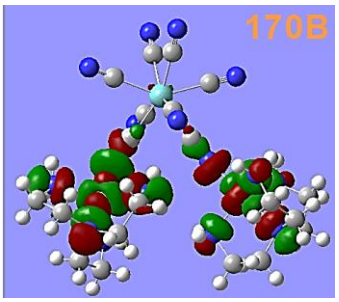
146B ->170B 0.27194



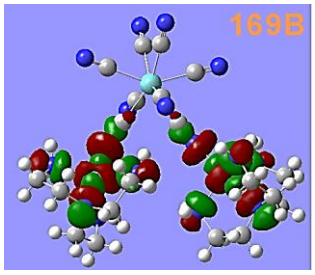


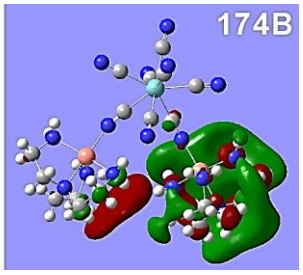
147B ->170B 0.20429
148B ->170B 0.77239



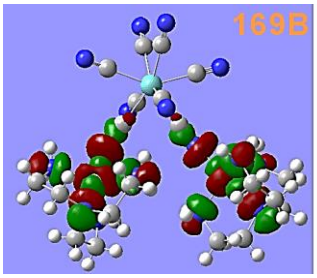


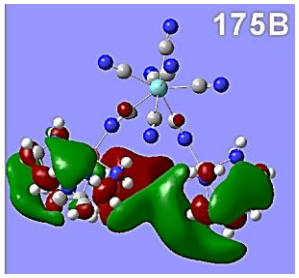
150B ->170B 0.12698
Excited State 46: 3.616-A 3.4131 eV 363.26 nm
f = 0.0026 $\langle S^2 \rangle$ = 3.019
169B ->174B 0.21589



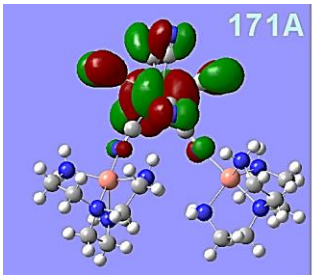


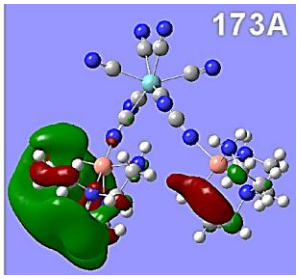
169B ->175B 0.96865



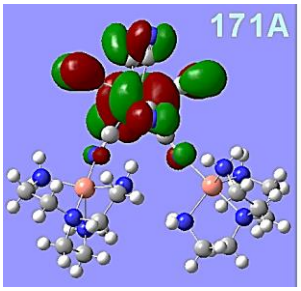


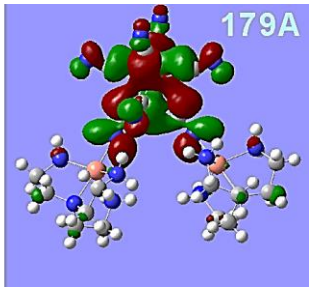
Excited State 47: 3.054-A 3.4344 eV 361.00 nm
f = 0.0154 $\langle S^2 \rangle$ = 2.081
171A ->173A 0.14486



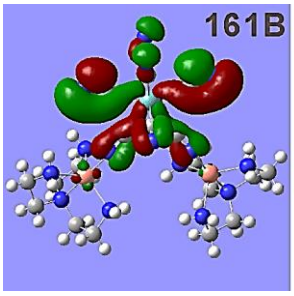


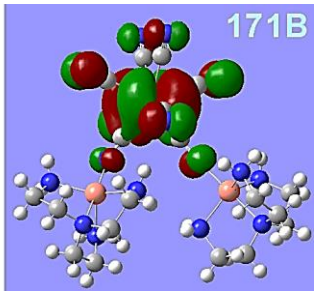
171A ->179A 0.10478



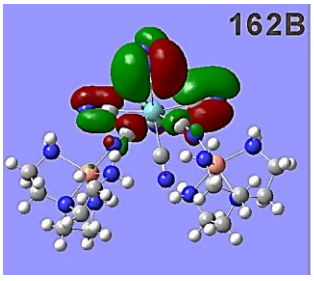


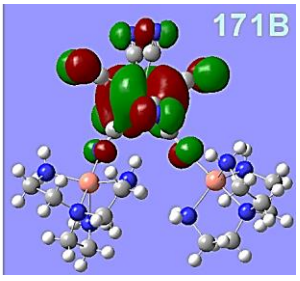
161B ->171B -0.27735



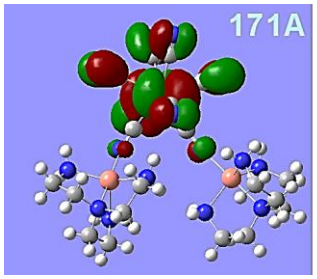


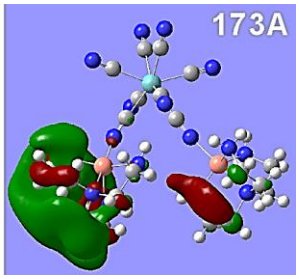
162B ->171B 0.90624



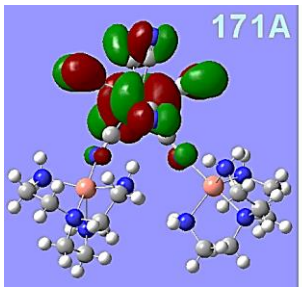


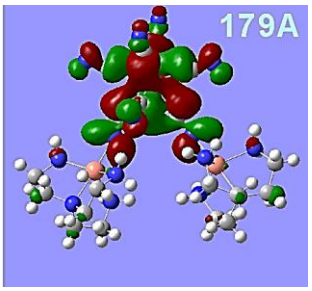
Excited State 48: 3.035-A 3.4478 eV 359.60 nm
f = 0.0007 <S^2> = 2.053
171A ->173A 0.97845



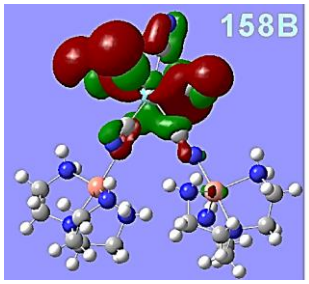


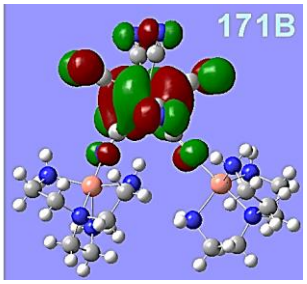
162B ->171B -0.15448
Excited State 50: 3.038-A 3.4781 eV 356.47 nm
f = 0.0080 <S^2> = 2.058
171A ->179A -0.30113



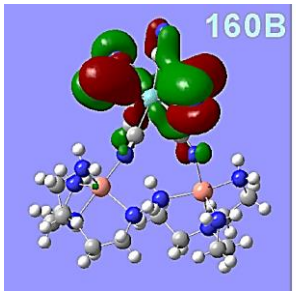


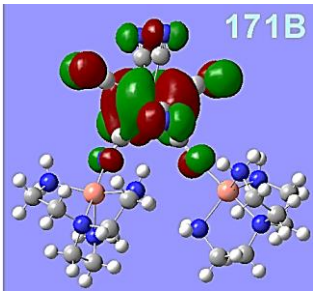
158B ->171B 0.31690



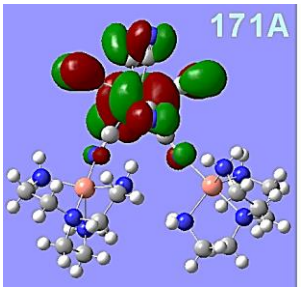


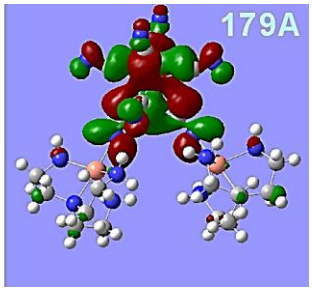
159B ->171B -0.21209
160B ->171B 0.80466



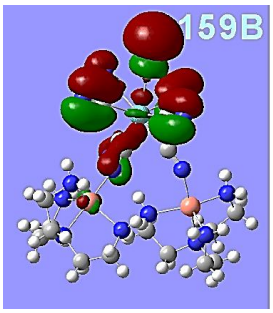


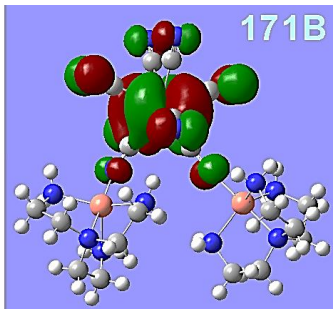
162B ->171B 0.15748
164B ->171B -0.13404
Excited State 52: 3.032-A 3.5838 eV 345.96 nm
f = 0.0063 <S^2> = 2.048
171A ->174A 0.24330
171A ->175A 0.12390
171A ->176A 0.18080
171A ->179A 0.63527



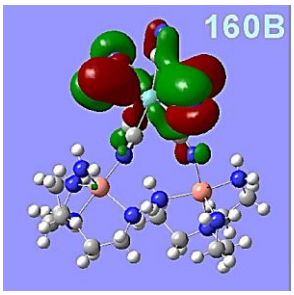


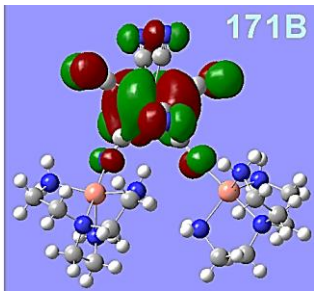
171A ->184A -0.12013
156B ->171B -0.18398
158B ->171B -0.17609
159B ->171B 0.26787



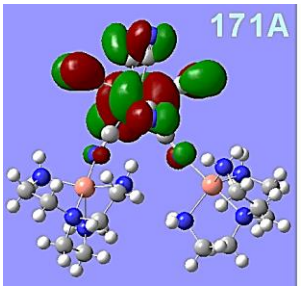


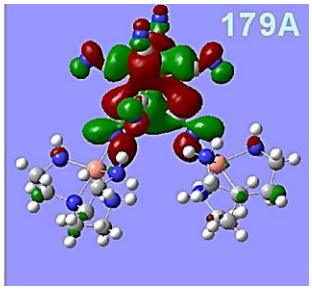
160B ->171B 0.49303





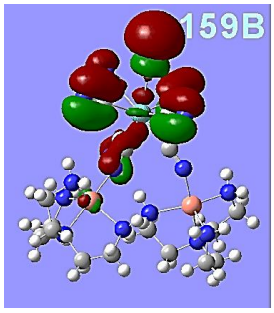
Excited State 53: 3.034-A 3.6550 eV 339.22 nm
f = 0.0077 <S^2> = 2.051
171A ->174A -0.17332
171A ->175A -0.14565
171A ->176A -0.10863
171A ->179A -0.37223

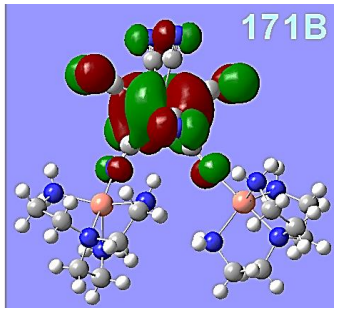




156B ->171B -0.10913
158B ->171B -0.23399

159B ->171B 0.81144



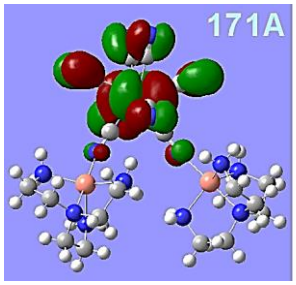


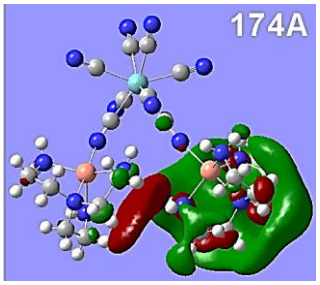
160B ->171B 0.11473

Excited State 54: 3.033-A 3.7102 eV 334.17 nm

f = 0.0019 $\langle S^2 \rangle$ = 2.049

171A ->174A 0.86871





171A ->175A -0.35982

171A ->179A -0.16517

171A ->182A -0.13586

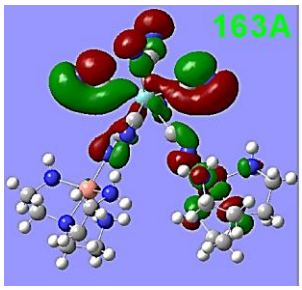
171A ->183A 0.14794

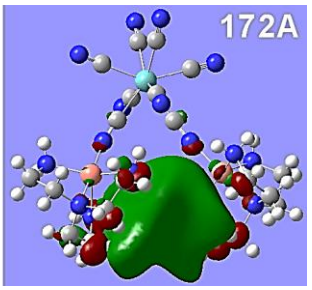
Excited State 55: 3.392-A 3.7384 eV 331.65 nm

f = 0.0023 $\langle S^2 \rangle$ = 2.626

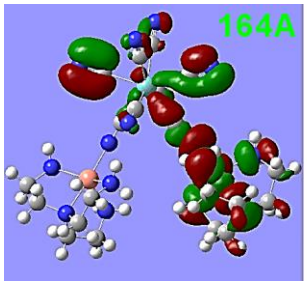
161A ->172A 0.11151

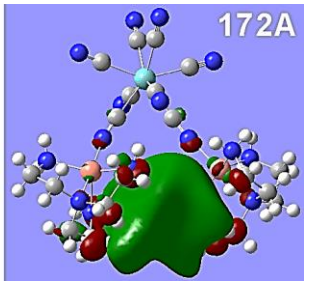
163A ->172A 0.31539



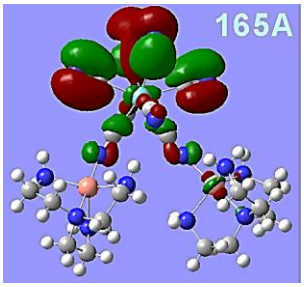


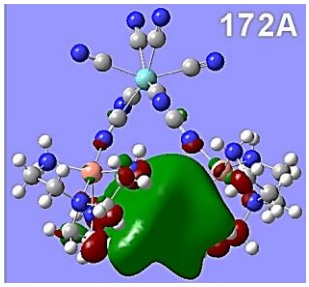
164A ->172A 0.81305





165A ->172A -0.34074





169B ->176B 0.22462

Excited State 56: 3.037-A 3.7448 eV 331.09 nm

f = 0.0006 $\langle S^2 \rangle$ = 2.056

171A ->175A 0.17617

171A ->179A 0.14893

156B ->171B 0.31037

158B ->171B 0.77035

159B ->171B 0.41391

160B ->171B -0.12070

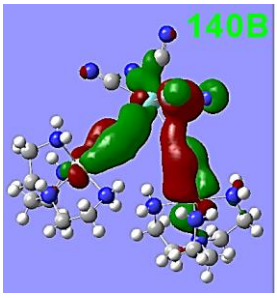
Excited State 57: 3.041-A 3.7601 eV 329.74 nm

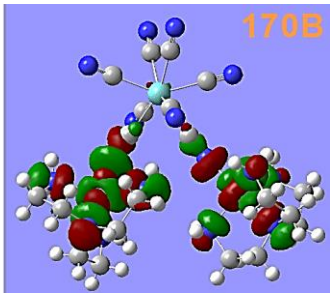
f = 0.0018 $\langle S^2 \rangle$ = 2.061

138B ->170B 0.12955

139B ->170B 0.10869

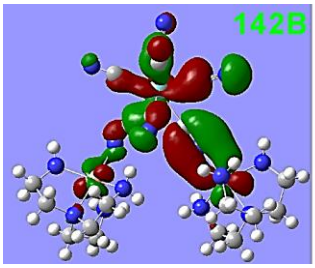
140B ->170B 0.66575

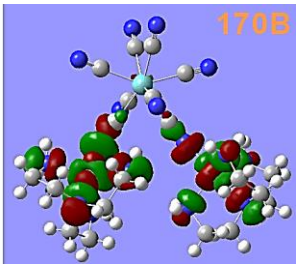




141B ->170B -0.14241

142B ->170B -0.36275

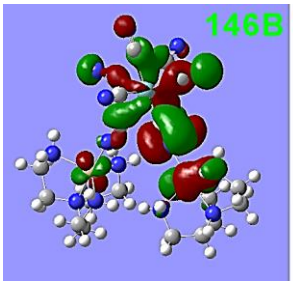


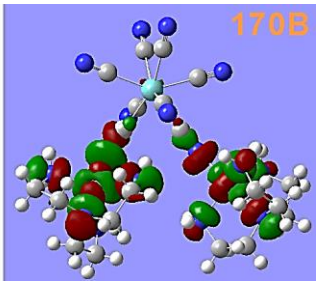


143B ->170B -0.14891

144B ->170B -0.29831

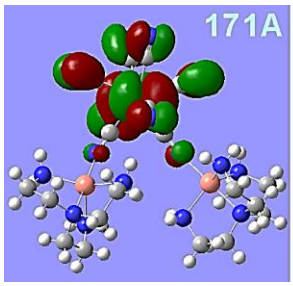
146B ->170B 0.30325

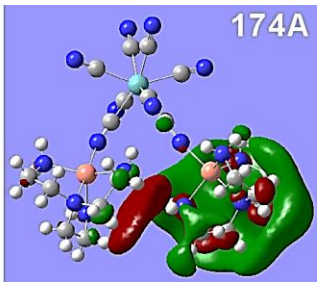




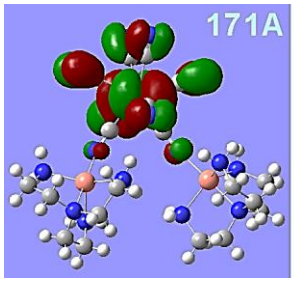
147B ->170B 0.24749

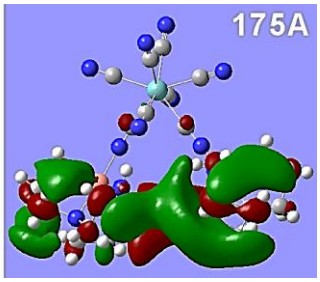
148B ->170B -0.13903
169B ->176B 0.19036
Excited State 58: 3.581-A 3.7664 eV 329.19 nm
f = 0.0003 <S^2> = 2.955
164A ->172A -0.21134
140B ->170B -0.11661
169B ->176B 0.93951
Excited State 59: 3.633-A 3.7746 eV 328.47 nm
f = 0.0002 <S^2> = 3.050
164B ->172B 0.99135
Excited State 60: 3.558-A 3.8222 eV 324.38 nm
f = 0.0003 <S^2> = 2.914
166A ->172A 0.96721
171A ->175A -0.16975
Excited State 61: 3.061-A 3.8291 eV 323.80 nm
f = 0.0018 <S^2> = 2.092
166A ->172A 0.21068
171A ->174A 0.30299





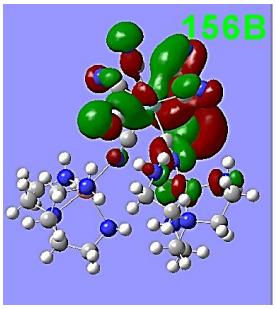
171A ->175A 0.81320

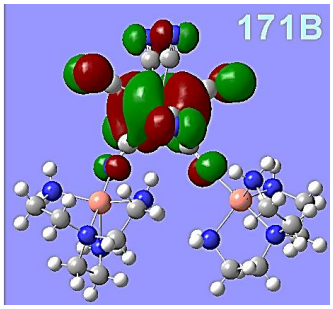




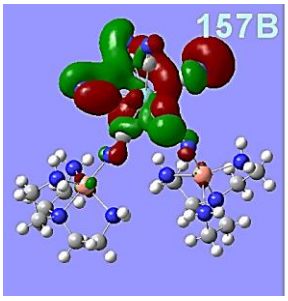
171A ->176A -0.13437
171A ->177A -0.12431
171A ->179A -0.24148
157B ->171B -0.14995
158B ->171B -0.20747
Excited State 62: 3.044-A 3.8402 eV 322.86 nm
f = 0.0015 <S^2> = 2.066
171A ->175A 0.24799
154B ->171B 0.16625
155B ->171B -0.19356

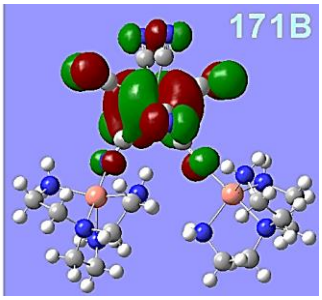
156B ->171B -0.42468



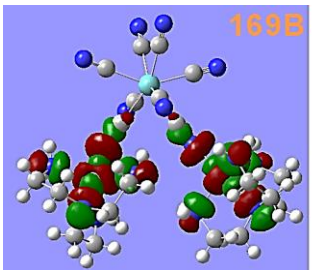


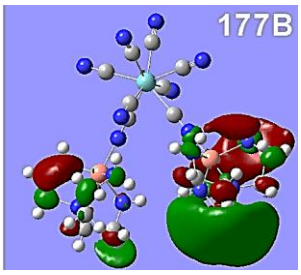
157B ->171B 0.78967





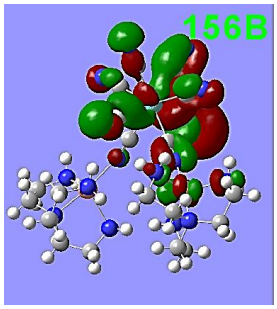
158B ->171B 0.13904
Excited State 63: 3.019-A 3.8656 eV 320.74 nm
f = 0.0006 <S^2> = 2.028
136B ->170B 0.10753
140B ->170B 0.16341
142B ->170B 0.73225
143B ->170B -0.40982
144B ->170B -0.13741
146B ->170B 0.34656
147B ->170B -0.24865
Excited State 64: 3.613-A 3.8774 eV 319.76 nm
f = 0.0007 <S^2> = 3.013
165A ->172A 0.10453
169B ->177B 0.95883

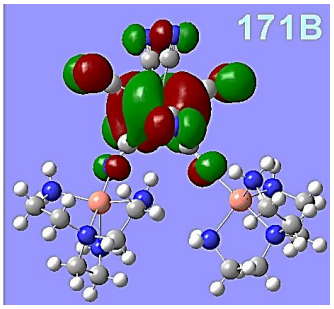




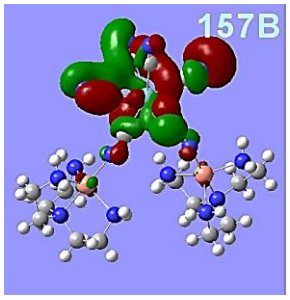
169B ->178B 0.21693
Excited State 66: 3.250-A 3.8952 eV 318.30 nm
f = 0.0004 <S^2> = 2.391
164A ->172A 0.32010
165A ->172A 0.86373
156B ->171B -0.10936
163B ->172B 0.30642

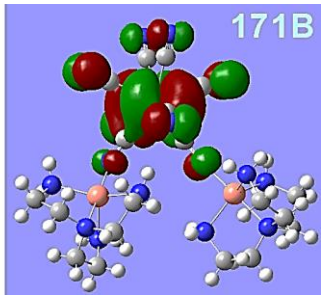
Excited State 67: 3.042-A 3.9130 eV 316.85 nm
f = 0.0040 <S^2> = 2.063
154B ->171B -0.14210
156B ->171B 0.73638



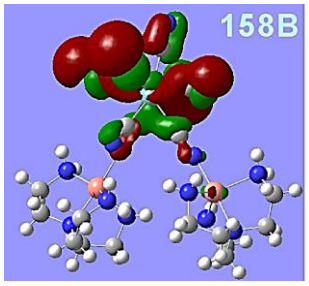


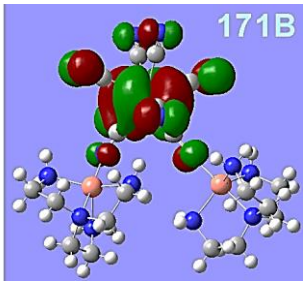
157B ->171B 0.52738



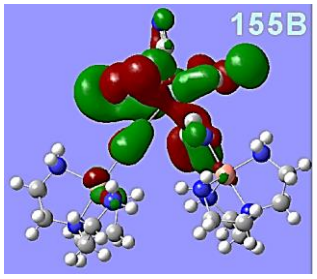


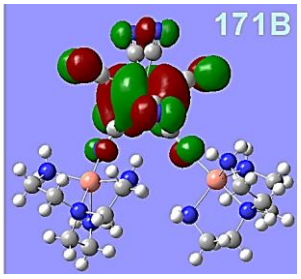
158B ->171B -0.29403



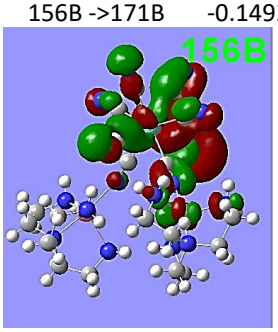


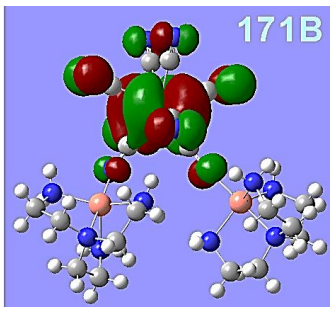
160B ->171B 0.13236
Excited State 68: 3.616-A 3.9286 eV 315.59 nm
f = 0.0011 <S^2> = 3.018
169B ->177B -0.21752
169B ->178B 0.97199
Excited State 69: 3.045-A 3.9770 eV 311.75 nm
f = 0.0087 <S^2> = 2.068
152B ->171B -0.11810
155B ->171B 0.93476



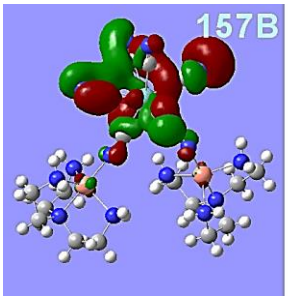


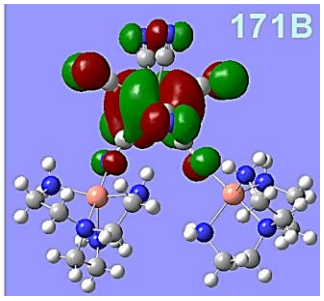
156B ->171B -0.14924



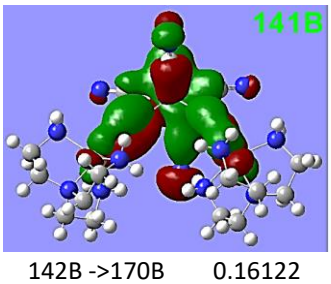


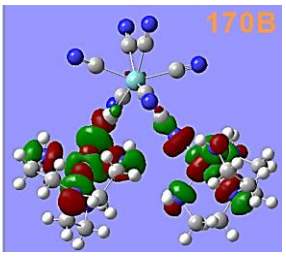
157B ->171B 0.14555





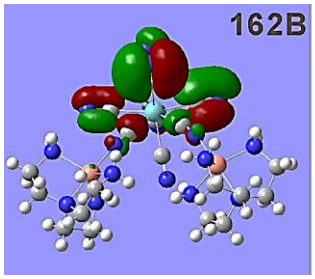
158B ->171B 0.11510
Excited State 70: 3.019-A 4.0234 eV 308.16 nm
f = 0.0009 <S^2> = 2.029
171A ->174A -0.18649
171A ->176A 0.18609
171A ->178A -0.27673
171A ->180A -0.21059
171A ->181A -0.18663
171A ->182A -0.34215
171A ->183A 0.21344
171A ->184A 0.10078
171A ->185A 0.40958
171A ->186A -0.29914
171A ->187A 0.42007
171A ->189A -0.13416
171A ->190A 0.13114
171A ->191A -0.17199
155B ->171B 0.10625
Excited State 71: 3.393-A 4.0845 eV 303.55 nm
f = 0.0008 <S^2> = 2.628
159A ->172A -0.18000
141B ->170B -0.49955

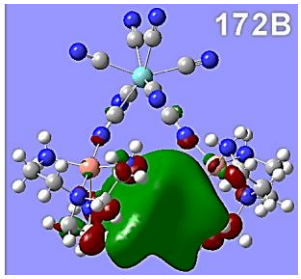




142B ->170B 0.16122
143B ->170B 0.22275
144B ->170B -0.20389
145B ->170B 0.10803

162B ->172B 0.73841



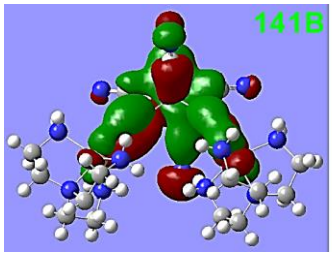


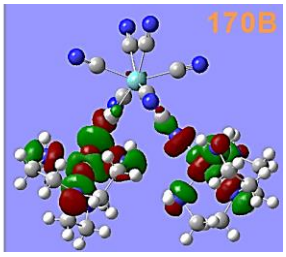
Excited State 72: 3.303-A 4.0868 eV 303.38 nm

f = 0.0012 $\langle S^2 \rangle$ = 2.477

159A ->172A 0.28070

141B ->170B 0.54069





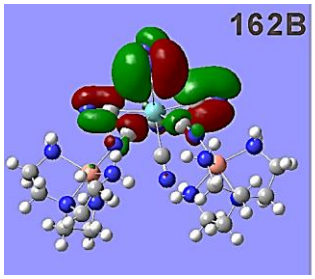
142B ->170B -0.17316

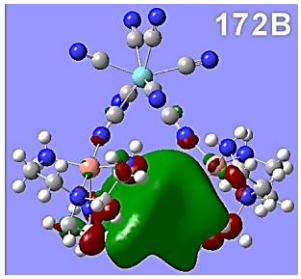
143B ->170B -0.24501

144B ->170B 0.22302

145B ->170B -0.12490

162B ->172B 0.65196

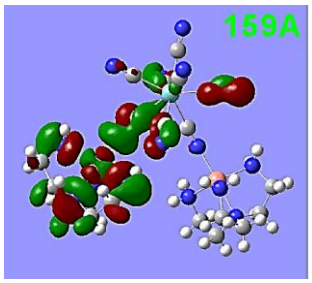


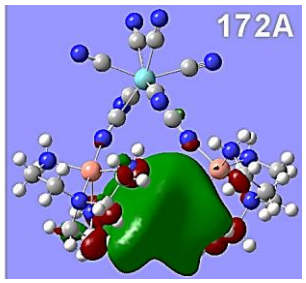


Excited State 73: 3.307-A 4.0924 eV 302.96 nm

f = 0.0018 $\langle S^2 \rangle$ = 2.484

159A ->172A 0.88525





160A ->172A -0.14771

162A ->172A 0.13321

163A ->172A -0.10800

141B ->170B -0.27732

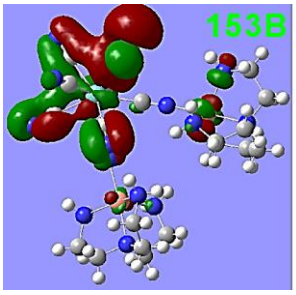
143B ->170B 0.11706

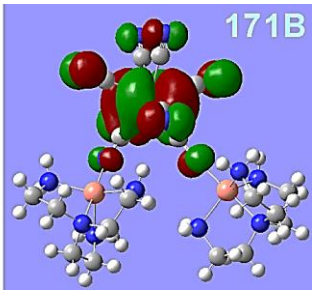
144B ->170B -0.10818

Excited State 74: 3.476-A 4.1194 eV 300.97 nm

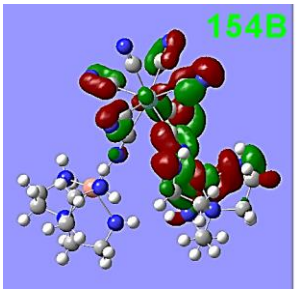
f = 0.0067 $\langle S^2 \rangle$ = 2.770

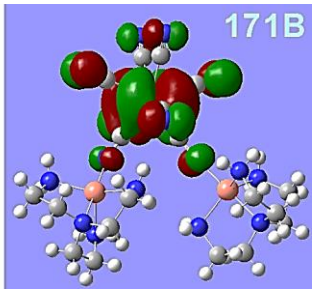
153B ->171B 0.56408



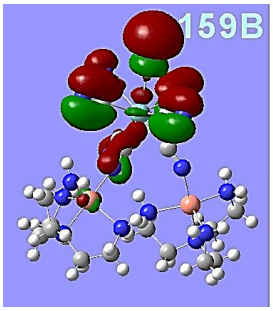


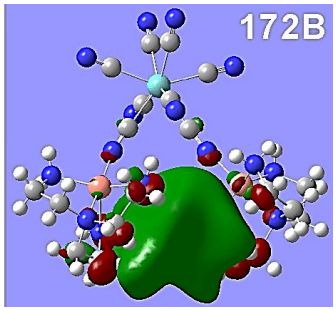
154B ->171B 0.25995



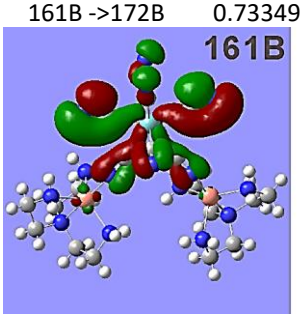


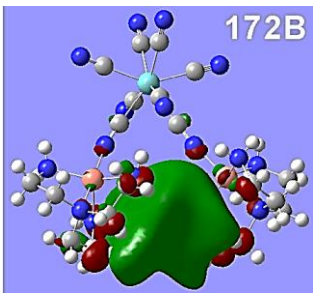
159B ->172B 0.10809





161B ->172B 0.73349

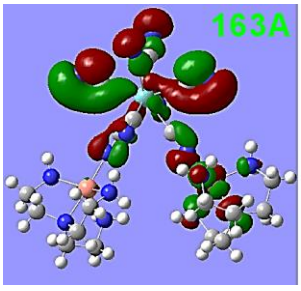


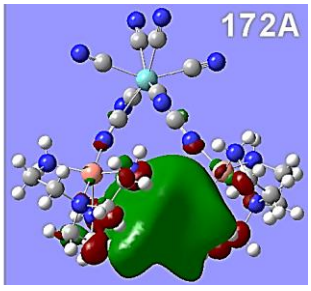


Excited State 75: 3.428-A 4.1204 eV 300.90 nm

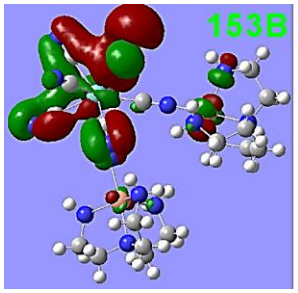
f = 0.0111 $\langle S^2 \rangle$ = 2.688

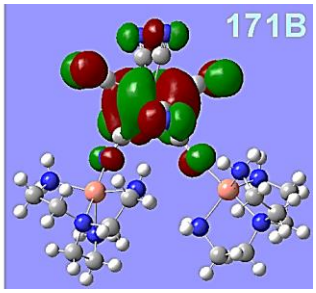
163A ->172A -0.15035



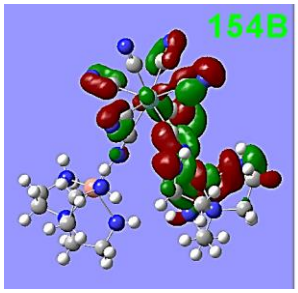


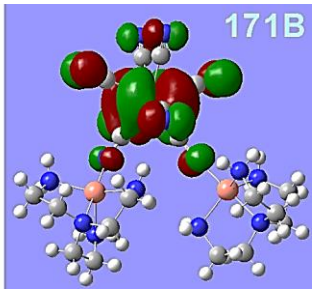
153B ->171B 0.66394



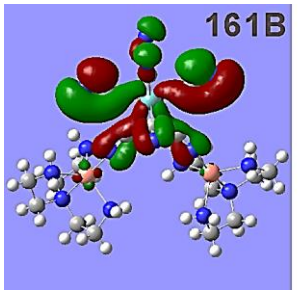


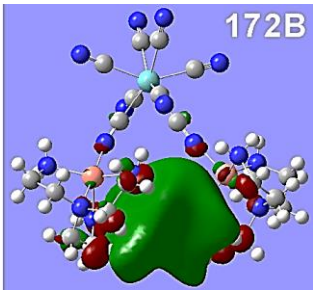
154B ->171B 0.30357



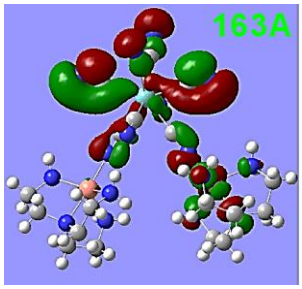


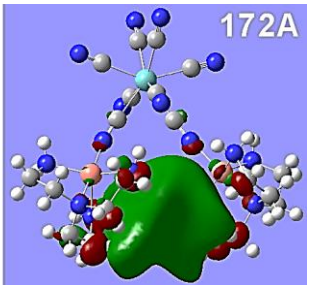
161B ->172B -0.59907



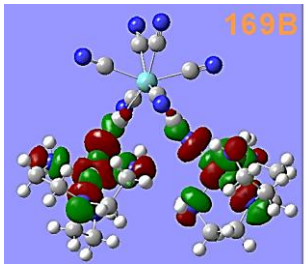


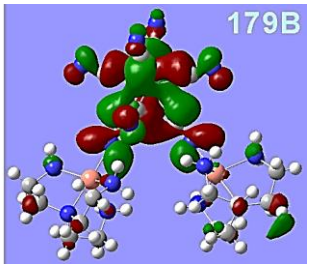
Excited State 76: 3.463-A 4.1529 eV 298.55 nm
f = 0.0038 <S^2> = 2.747
161A ->172A 0.13539
163A ->172A 0.61151





164A ->172A -0.25673
161B ->172B -0.19219
169B ->179B 0.67914



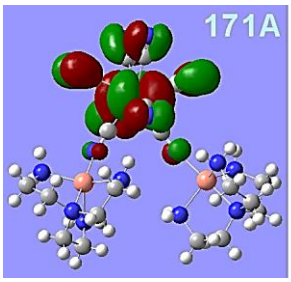


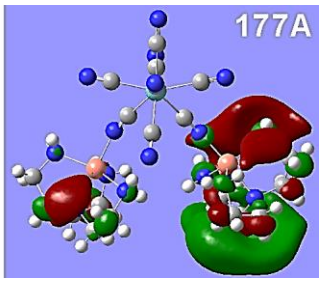
Excited State 77: 3.560-A 4.1546 eV 298.42 nm
f = 0.0006 <S^2> = 2.918
161A ->172A -0.13139
163A ->172A -0.61798
164A ->172A 0.25648
169B ->179B 0.70407

Excited State 80: 3.095-A 4.2021 eV 295.05 nm
f = 0.0004 <S^2> = 2.145
170A ->173A -0.31335
171A ->176A 0.86863
171A ->177A 0.11837
171A ->178A 0.14776
171A ->179A -0.23751

Excited State 81: 3.633-A 4.2250 eV 293.45 nm
f = 0.0002 <S^2> = 3.050
158B ->172B 0.14858
159B ->172B -0.12160
160B ->172B 0.95858
161B ->172B 0.13480

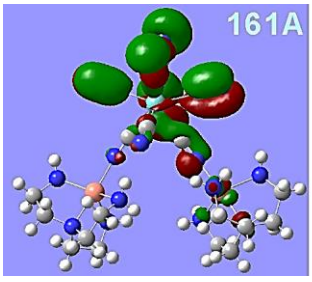
Excited State 83: 3.035-A 4.2659 eV 290.64 nm
f = 0.0017 <S^2> = 2.053
171A ->175A 0.14672
171A ->176A -0.18690
171A ->177A 0.79347

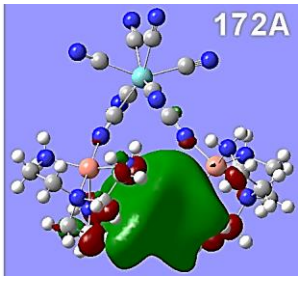




171A ->182A -0.28686
171A ->183A 0.33522
171A ->187A -0.11662
171A ->188A -0.11075
171A ->190A -0.15907

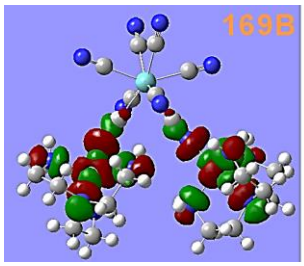
Excited State 84: 3.612-A 4.2937 eV 288.76 nm
f = 0.0008 <S^2> = 3.012
158A ->172A 0.16029
160A ->172A -0.25940
161A ->172A 0.89803

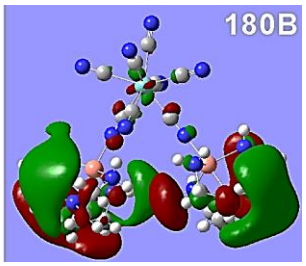




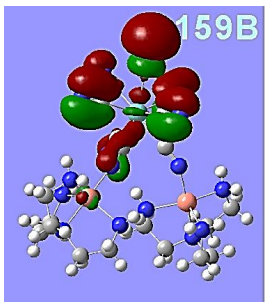
162A ->172A 0.17412
163A ->172A -0.21344

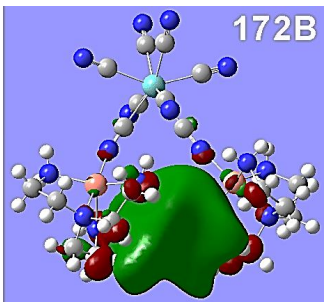
Excited State 85: 3.615-A 4.3118 eV 287.55 nm
f = 0.0012 <S^2> = 3.017
169B ->179B 0.10901
169B ->180B 0.98853





Excited State 86: 3.617-A 4.3201 eV 287.00 nm
f = 0.0016 <S^2> = 3.021
154B ->172B -0.18163
156B ->172B -0.15979
158B ->172B -0.17062
159B ->172B 0.90417

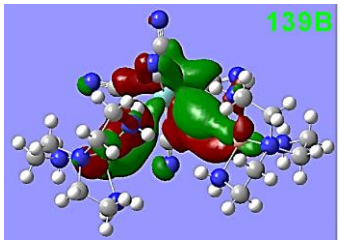


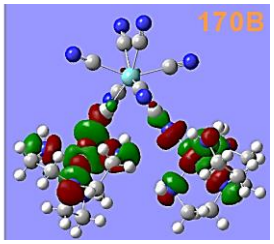


160B ->172B 0.18162
161B ->172B -0.14161
162B ->172B -0.11840

Excited State 88: 3.036-A 4.3548 eV 284.71 nm
f = 0.0006 <S^2> = 2.054
171A ->177A -0.28365
171A ->178A 0.80864
171A ->179A 0.15311
171A ->182A -0.25813
171A ->183A 0.25821
154B ->171B -0.14687

Excited State 89: 3.047-A 4.3687 eV 283.80 nm
f = 0.0021 <S^2> = 2.071
171A ->177A -0.13269
171A ->178A -0.29600
138B ->170B 0.10182
139B ->170B 0.57446



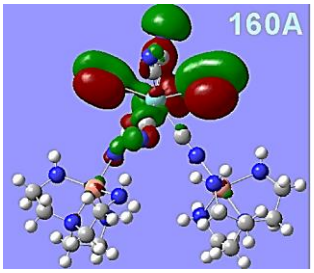


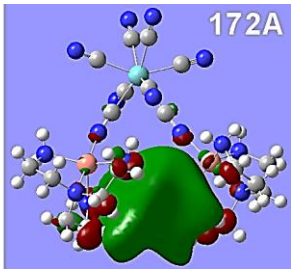
140B ->170B -0.20905
141B ->170B -0.13177
143B ->170B -0.14309
145B ->170B 0.14867
150B ->171B -0.27619
151B ->171B 0.27215
153B ->171B 0.19785
154B ->171B -0.36854

Excited State 90: 3.043-A 4.3716 eV 283.61 nm
f = 0.0005 <S^2> = 2.065
171A ->177A 0.31733
171A ->178A 0.31062
171A ->180A -0.10465
171A ->182A 0.14940
171A ->183A -0.21102
171A ->185A 0.16535
171A ->187A 0.19100
171A ->190A 0.18177
171A ->191A -0.13146
139B ->170B 0.53506
140B ->170B -0.20186
141B ->170B -0.13077
143B ->170B -0.12921
145B ->170B 0.13127
150B ->171B 0.17977
151B ->171B -0.19843
153B ->171B -0.11541
154B ->171B 0.21492
154B ->172B 0.10552

Excited State 91: 3.048-A 4.3777 eV 283.22 nm
f = 0.0061 <S^2> = 2.073
160A ->172A -0.10760
171A ->177A -0.31784
171A ->178A -0.20928
171A ->180A 0.10872
171A ->182A -0.22142
171A ->183A 0.28177
171A ->185A -0.16017
171A ->187A -0.20416
171A ->190A -0.20481
171A ->191A 0.13767
139B ->170B 0.23546
149B ->171B 0.12579
150B ->171B 0.31829
151B ->171B -0.30173
153B ->171B -0.19767
154B ->171B 0.38466
156B ->171B 0.13283

Excited State 92: 3.580-A 4.3841 eV 282.80 nm
f = 0.0013 <S^2> = 2.954
160A ->172A 0.90075



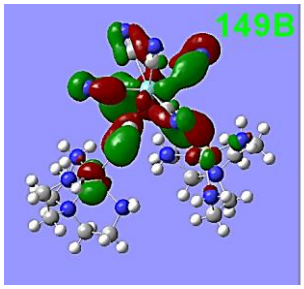


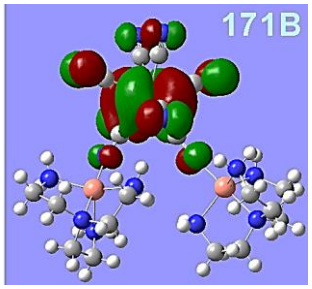
161A ->172A 0.17047
162A ->172A 0.26526
163A ->172A -0.13187
169A ->173A 0.18077

Excited State 99: 3.087-A 4.4905 eV 276.10 nm

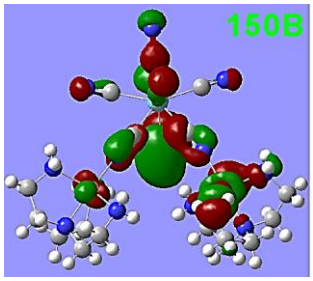
f = 0.0040 $\langle S^2 \rangle$ = 2.133

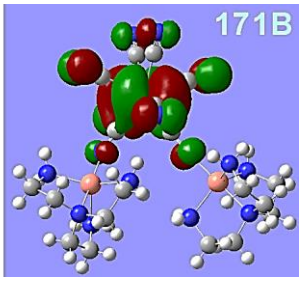
149B ->171B 0.56201



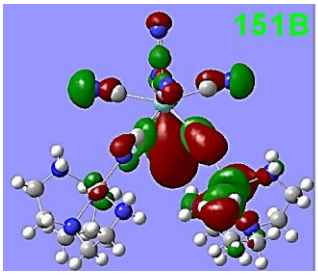


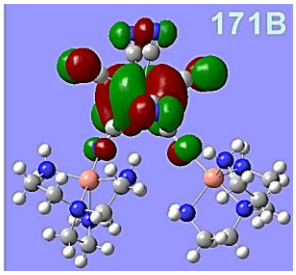
150B ->171B -0.35835



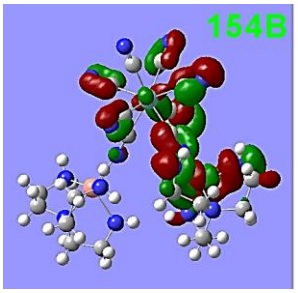


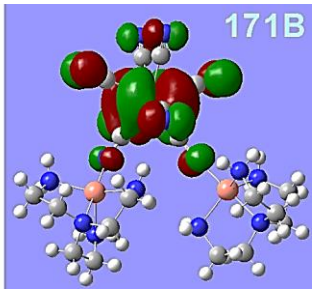
151B ->171B 0.53860





153B ->171B -0.18276
154B ->171B 0.38378





Photomagnetic properties

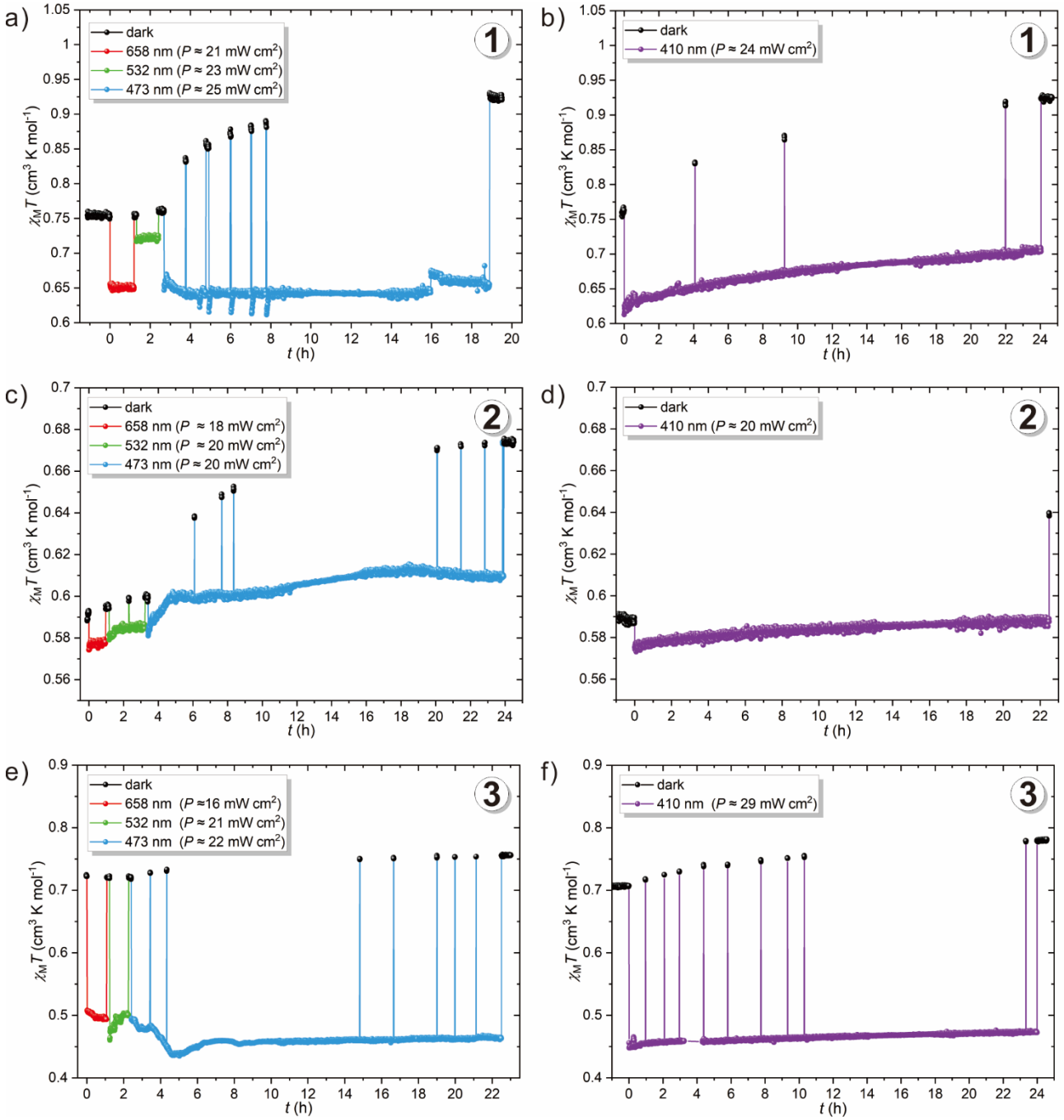


Figure S7. Time dependence of the $\chi_M T$ products of **1** – **3** (H_{dc} = 5 kOe, T = 10 K) after consecutive irradiation with the 658, 532 and 473 nm laser lights (**a**, **c** and **e**) and the 410 nm laser line (**b**, **d** and **f**). Steps on the graphs are associated to the laser light induced thermalisation effects. The black symbols indicate the actual signal gain measured in the dark.

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