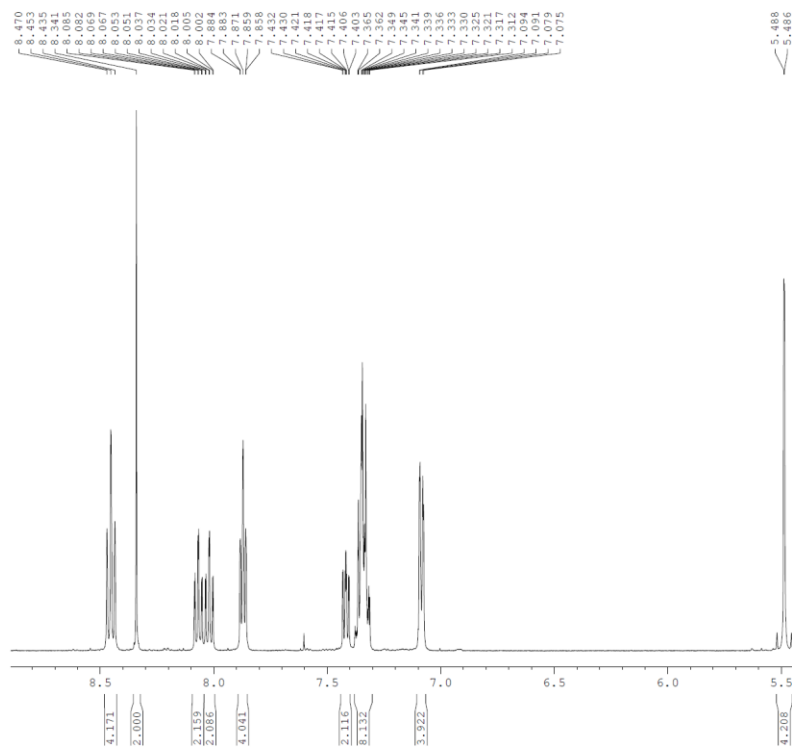


Supplementary Information for:

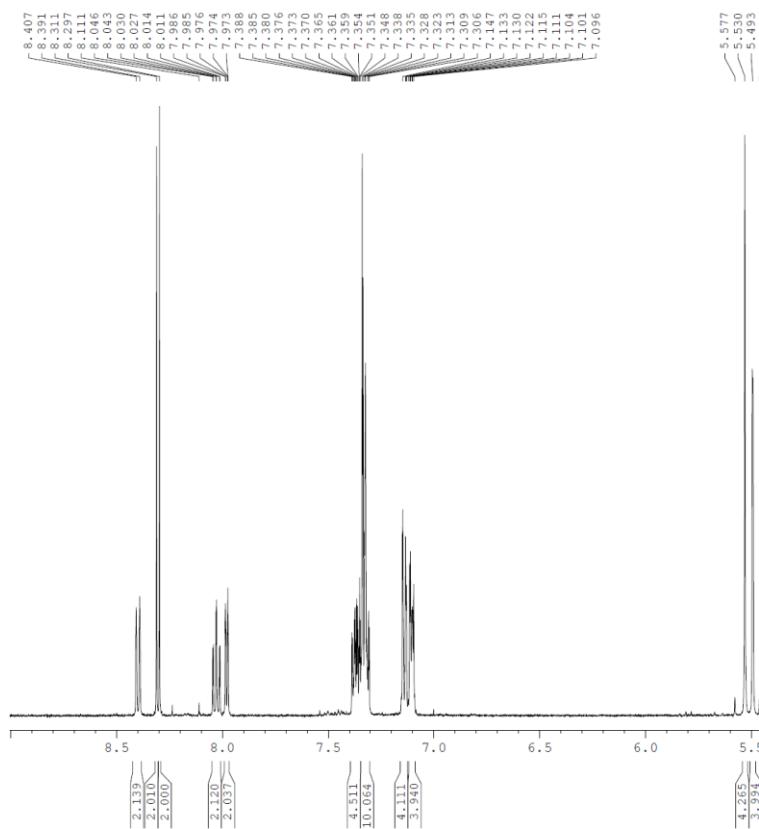
## Synthesis, characterisation and theoretical study of ruthenium 4,4'- bi-1,2,3-triazolyl complexes

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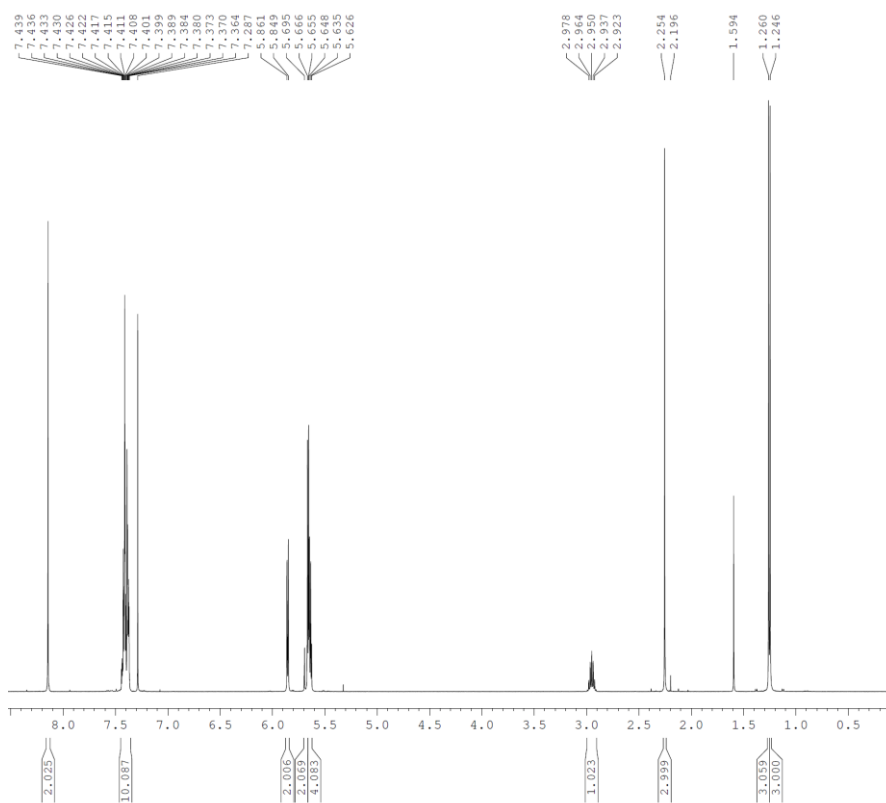
<b>Fig. S1</b> $^1\text{H}$ NMR spectrum of $[\text{Ru}(\text{bpy})_2(\text{btz})]\text{PF}_6$ .	S2
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NWChem TDDFT output for $[\text{Ru}(\text{btz})_3]^{2+}$	S27



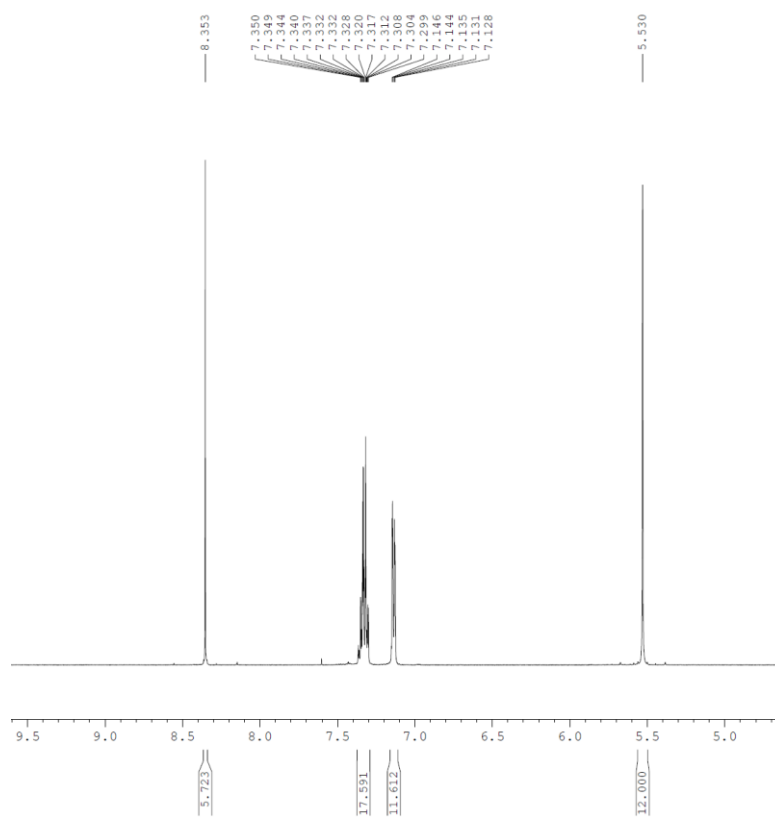
**Fig. S1**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\text{bpy})_2(\text{btz})]\text{PF}_6$  ( $\text{CD}_3\text{CN}$ ).



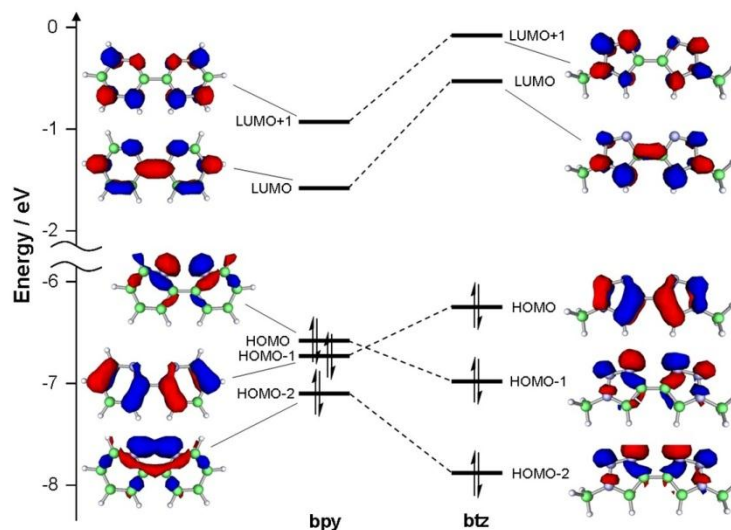
**Fig. S2**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\text{bpy})(\text{btz})_2]\text{PF}_6$  ( $\text{CD}_3\text{CN}$ ).



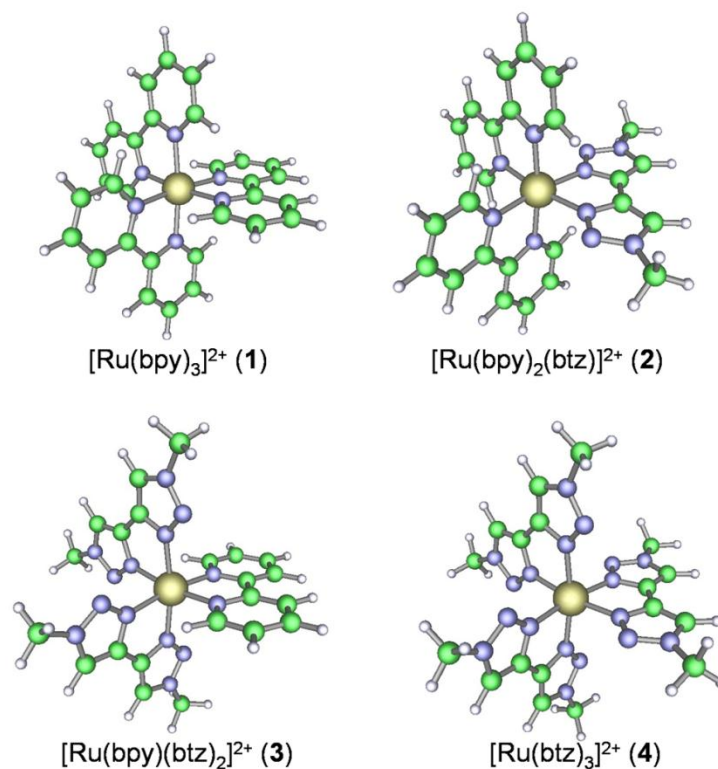
**Fig. S3**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\text{p-cymene})(\text{btz})\text{Cl}]\text{PF}_6$  ( $\text{CDCl}_3$ ).



**Fig. S4**  $^1\text{H}$  NMR spectrum of  $[\text{Ru}(\text{btz})_3]\text{PF}_6$  ( $\text{CD}_3\text{CN}$ ).

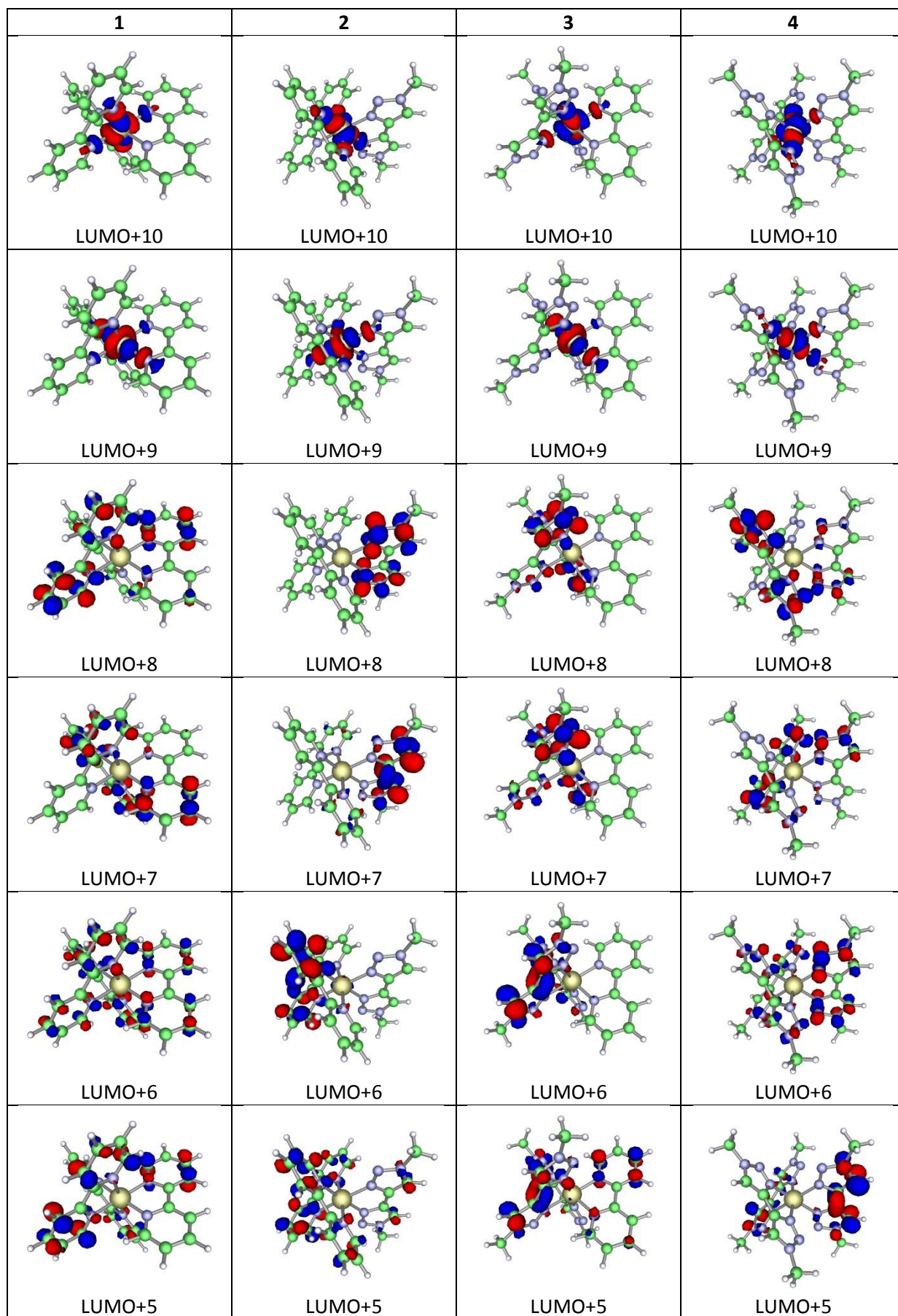


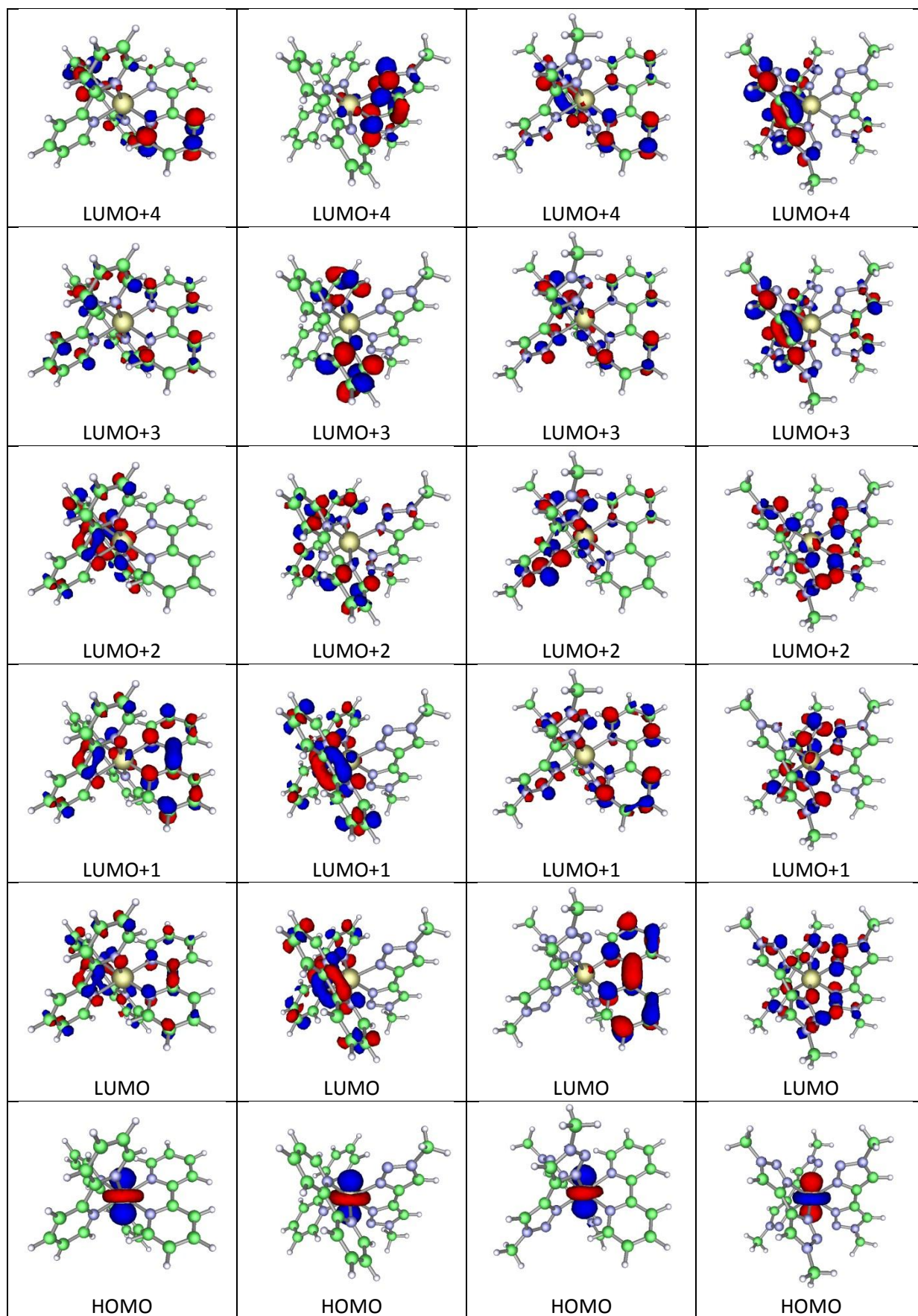
**Fig. S5** Molecular orbital energy level diagram for DFT optimised geometries of isolated bpy and btz ligands.

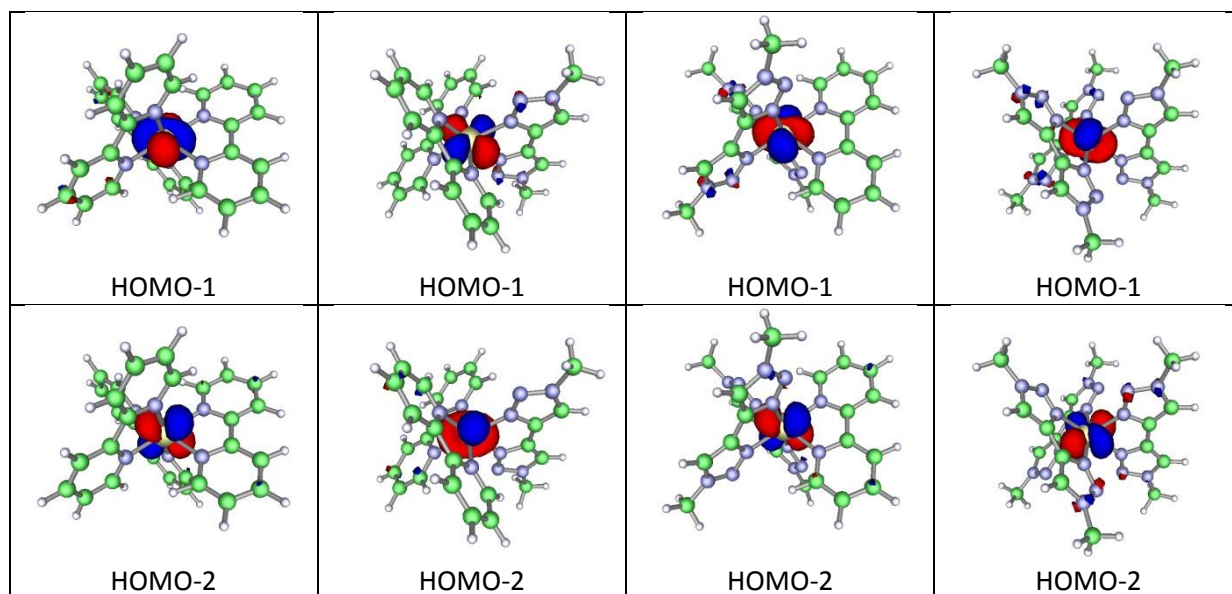


**Fig. S6** Optimised ground state geometries of complexes [Ru(bpy)<sub>3-n</sub>(btz)<sub>n</sub>]<sup>2+</sup> (benzyl substituents simplified to methyl).

**Fig. S7** Plots of molecular orbitals HOMO-2 to LUMO+10 for complexes [Ru(bpy)<sub>3-n</sub>(btz)<sub>n</sub>]<sup>2+</sup>.







**Fig. S8** Plots of molecular orbitals HOMO-2 to LUMO+10 for complexes  $[\text{Ru}(\text{bpy})_{3-n}(\text{btz})_n]^{2+}$ .

**Table S1** Energies (eV) for frontier molecular orbitals of DFT optimised singlet ground states of complexes **1'** to **4'**.

	<b>1'</b>	<b>2'</b>	<b>3'</b>	<b>4'</b>
LUMO+10	-5.3773	-5.1940	-5.0956	-4.7399
LUMO+9	-5.3799	-5.2007	-5.1071	-4.7595
LUMO+8	-6.4886	-6.1133	-5.8081	-5.558
LUMO+7	-6.4888	-6.1700	-5.8419	-5.5665
LUMO+6	-6.5602	-6.2343	-5.906	-5.6095
LUMO+5	-6.6475	-6.2658	-5.9724	-5.6819
LUMO+4	-6.6486	-6.3853	-5.9819	-5.6875
LUMO+3	-6.9609	-6.4345	-6.1154	-5.755
LUMO+2	-7.6025	-6.6389	-6.1274	-5.7844
LUMO+1	-7.6050	-7.3438	-6.283	-5.7943
LUMO	-7.7053	-7.4078	-7.0999	-5.9499
HOMO	-11.1435	-10.9875	-10.8314	-10.6603
HOMO-1	-11.3477	-11.1551	-10.9684	-10.815

**NWChem TDDFT output for [Ru(bpy)<sub>3</sub>]<sup>2+</sup>:**

```

-----
Root 1 singlet a      0.095806531 a.u. ( 2.6070295 eV)
-----
Transition Moments X  0.02989 Y  0.02433 Z  0.02428
Oscillator Strength                                0.00013

Occ.130 a --- Virt.131 a  -0.18359 X
Occ.130 a --- Virt.132 a  -0.82036 X
Occ.130 a --- Virt.133 a  -0.52035 X
Occ.130 a --- Virt.136 a   0.07756 X
Occ.130 a --- Virt.141 a   0.07822 X
-----
Root 2 singlet a      0.095849031 a.u. ( 2.6081860 eV)
-----
Transition Moments X  0.03075 Y -0.02510 Z -0.02993
Oscillator Strength                                0.00016

Occ.130 a --- Virt.131 a   0.23508 X
Occ.130 a --- Virt.132 a  -0.55088 X
Occ.130 a --- Virt.133 a   0.78718 X
Occ.130 a --- Virt.135 a   0.07664 X
Occ.130 a --- Virt.140 a   0.07631 X
-----
Root 3 singlet a      0.096032884 a.u. ( 2.6131888 eV)
-----
Transition Moments X  0.00321 Y  0.00428 Z -0.13115
Oscillator Strength                                0.00110

Occ.130 a --- Virt.131 a   0.95104 X
Occ.130 a --- Virt.133 a  -0.29528 X
Occ.130 a --- Virt.134 a   0.05448 X
-----
Root 4 singlet a      0.103789712 a.u. ( 2.8242630 eV)
-----
Transition Moments X  0.00284 Y  0.01437 Z -0.03303
Oscillator Strength                                0.00009

Occ.128 a --- Virt.132 a   0.22814 X
Occ.128 a --- Virt.133 a   0.64497 X
Occ.129 a --- Virt.132 a  -0.67243 X
Occ.129 a --- Virt.133 a   0.25233 X
-----
Root 5 singlet a      0.104811057 a.u. ( 2.8520552 eV)
-----
Transition Moments X -0.23691 Y  0.20008 Z -0.00148
    
```



```
Oscillator Strength 0.00672

Occ.128 a --- Virt.131 a 0.39823 X
Occ.128 a --- Virt.132 a -0.10198 X
Occ.128 a --- Virt.133 a 0.32998 X
Occ.129 a --- Virt.131 a 0.77564 X
Occ.129 a --- Virt.132 a 0.31370 X
Occ.129 a --- Virt.133 a 0.09826 X
Occ.130 a --- Virt.140 a -0.06030 X

-----
Root 6 singlet a 0.104945375 a.u. ( 2.8557102 eV)
-----
Transition Moments X 0.21548 Y 0.23238 Z 0.00283
Oscillator Strength 0.00703

Occ.128 a --- Virt.131 a 0.76682 X
Occ.128 a --- Virt.132 a -0.34524 X
Occ.128 a --- Virt.133 a -0.14387 X
Occ.129 a --- Virt.131 a -0.38789 X
Occ.129 a --- Virt.132 a -0.07571 X
Occ.129 a --- Virt.133 a 0.32139 X
Occ.130 a --- Virt.141 a 0.06148 X

-----
Root 7 singlet a 0.109517569 a.u. ( 2.9801260 eV)
-----
Transition Moments X 1.07556 Y 0.49628 Z 0.00189
Oscillator Strength 0.10244

Occ.128 a --- Virt.131 a 0.32040 X
Occ.128 a --- Virt.132 a 0.45287 X
Occ.128 a --- Virt.133 a 0.39736 X
Occ.129 a --- Virt.131 a -0.38428 X
Occ.129 a --- Virt.132 a 0.40039 X
Occ.129 a --- Virt.133 a -0.44418 X
Occ.130 a --- Virt.132 a -0.06485 X
Occ.130 a --- Virt.138 a 0.06112 X
Occ.130 a --- Virt.141 a -0.09271 X

-----
Root 8 singlet a 0.109630104 a.u. ( 2.9831882 eV)
-----
Transition Moments X -0.49900 Y 1.08434 Z -0.00296
Oscillator Strength 0.10413

Occ.128 a --- Virt.131 a 0.37450 X
Occ.128 a --- Virt.132 a 0.39555 X
Occ.128 a --- Virt.133 a -0.46231 X
Occ.129 a --- Virt.131 a 0.30101 X
Occ.129 a --- Virt.132 a -0.45124 X
Occ.129 a --- Virt.133 a -0.40796 X
Occ.130 a --- Virt.133 a -0.05837 X
Occ.130 a --- Virt.139 a 0.06270 X
Occ.130 a --- Virt.140 a 0.09483 X

-----
Root 9 singlet a 0.117193128 a.u. ( 3.1889886 eV)
-----
Transition Moments X 0.00110 Y 0.00086 Z -0.00011
Oscillator Strength 0.00000

Occ.128 a --- Virt.132 a 0.61956 X
Occ.128 a --- Virt.133 a -0.22910 X
Occ.128 a --- Virt.135 a 0.05441 X
Occ.128 a --- Virt.138 a -0.06722 X
Occ.128 a --- Virt.139 a 0.05105 X
Occ.128 a --- Virt.140 a -0.05532 X
Occ.129 a --- Virt.132 a 0.22325 X
Occ.129 a --- Virt.133 a 0.62134 X
Occ.129 a --- Virt.136 a 0.05363 X
Occ.129 a --- Virt.138 a -0.05270 X
Occ.129 a --- Virt.139 a -0.06650 X
Occ.129 a --- Virt.141 a -0.05738 X
Occ.130 a --- Virt.137 a -0.28634 X

-----
Root 10 singlet a 0.126571418 a.u. ( 3.4441850 eV)
-----
Transition Moments X -0.00486 Y 0.00278 Z 0.26008
Oscillator Strength 0.00571
```

Occ.125	a	---	Virt.131	a	0.07203	X
Occ.126	a	---	Virt.133	a	-0.05917	X
Occ.127	a	---	Virt.132	a	-0.05920	X
Occ.130	a	---	Virt.131	a	0.05913	X
Occ.130	a	---	Virt.134	a	-0.98982	X
-----						
Root 11	singlet	a	0.132933862	a.u.	( 3.6173160	eV)
-----						
Transition Moments	X	-0.01330	Y	-0.00620	Z	-0.00030
Oscillator Strength						0.00002
Occ.119	a	---	Virt.140	a	-0.06225	X
Occ.128	a	---	Virt.133	a	0.06916	X
Occ.128	a	---	Virt.135	a	-0.07238	X
Occ.128	a	---	Virt.140	a	-0.29939	X
Occ.128	a	---	Virt.141	a	0.21026	X
Occ.129	a	---	Virt.132	a	0.06827	X
Occ.129	a	---	Virt.136	a	0.07436	X
Occ.129	a	---	Virt.140	a	0.21615	X
Occ.129	a	---	Virt.141	a	0.29915	X
Occ.130	a	---	Virt.132	a	0.05752	X
Occ.130	a	---	Virt.133	a	-0.05091	X
Occ.130	a	---	Virt.135	a	0.26914	X
Occ.130	a	---	Virt.136	a	0.11237	X
Occ.130	a	---	Virt.140	a	0.75771	X
Occ.130	a	---	Virt.143	a	-0.05096	X
Occ.130	a	---	Virt.147	a	-0.06304	X
Occ.130	a	---	Virt.148	a	0.05320	X
Occ.130	a	---	Virt.150	a	0.05132	X
-----						
Root 12	singlet	a	0.132987395	a.u.	( 3.6187727	eV)
-----						
Transition Moments	X	0.00258	Y	0.00385	Z	0.00007
Oscillator Strength						0.00000
Occ.119	a	---	Virt.141	a	-0.06187	X
Occ.128	a	---	Virt.132	a	0.06752	X
Occ.128	a	---	Virt.136	a	0.07365	X
Occ.128	a	---	Virt.140	a	0.21267	X
Occ.128	a	---	Virt.141	a	0.29488	X
Occ.129	a	---	Virt.133	a	-0.07080	X
Occ.129	a	---	Virt.135	a	0.07311	X
Occ.129	a	---	Virt.140	a	0.30277	X
Occ.129	a	---	Virt.141	a	-0.20656	X
Occ.130	a	---	Virt.132	a	0.05309	X
Occ.130	a	---	Virt.133	a	0.06035	X
Occ.130	a	---	Virt.135	a	-0.10661	X
Occ.130	a	---	Virt.136	a	0.28118	X
Occ.130	a	---	Virt.141	a	0.75623	X
Occ.130	a	---	Virt.147	a	0.05404	X
Occ.130	a	---	Virt.148	a	0.06245	X
Occ.130	a	---	Virt.149	a	-0.05128	X
-----						
Root 13	singlet	a	0.135102779	a.u.	( 3.6763352	eV)
-----						
Transition Moments	X	0.30229	Y	-0.10085	Z	0.00201
Oscillator Strength						0.00915
Occ.128	a	---	Virt.134	a	-0.05862	X
Occ.129	a	---	Virt.134	a	-0.98877	X
-----						
Root 14	singlet	a	0.135196164	a.u.	( 3.6788764	eV)
-----						
Transition Moments	X	0.10200	Y	0.30295	Z	-0.00064
Oscillator Strength						0.00921
Occ.128	a	---	Virt.134	a	0.98863	X
Occ.129	a	---	Virt.134	a	-0.05873	X
-----						
Root 15	singlet	a	0.137496162	a.u.	( 3.7414625	eV)
-----						
Transition Moments	X	0.06617	Y	-0.09047	Z	-0.00181
Oscillator Strength						0.00115
Occ.125	a	---	Virt.133	a	0.05510	X
Occ.126	a	---	Virt.131	a	-0.09178	X
Occ.128	a	---	Virt.140	a	-0.15229	X

Occ.129	a	---	Virt.140	a	0.05430	X
Occ.129	a	---	Virt.141	a	0.15160	X
Occ.130	a	---	Virt.133	a	0.05467	X
Occ.130	a	---	Virt.135	a	-0.93237	X
Occ.130	a	---	Virt.136	a	-0.06548	X
Occ.130	a	---	Virt.139	a	-0.06269	X
Occ.130	a	---	Virt.140	a	0.18446	X
-----						
Root 16 singlet a			0.137563266	a.u.	( 3.7432885	eV)
-----						
Transition Moments	X	0.08542	Y	0.06808	Z	-0.00001
Oscillator Strength						0.00109
Occ.125	a	---	Virt.132	a	-0.05219	X
Occ.127	a	---	Virt.131	a	0.08855	X
Occ.128	a	---	Virt.140	a	0.05621	X
Occ.128	a	---	Virt.141	a	0.15039	X
Occ.129	a	---	Virt.140	a	0.16746	X
Occ.130	a	---	Virt.132	a	-0.05355	X
Occ.130	a	---	Virt.135	a	0.06650	X
Occ.130	a	---	Virt.136	a	-0.92820	X
Occ.130	a	---	Virt.138	a	0.06625	X
Occ.130	a	---	Virt.140	a	0.05163	X
Occ.130	a	---	Virt.141	a	0.19373	X
-----						
Root 17 singlet a			0.138810982	a.u.	( 3.7772406	eV)
-----						
Transition Moments	X	0.00439	Y	0.00580	Z	-0.05268
Oscillator Strength						0.00026
Occ.115	a	---	Virt.141	a	-0.05445	X
Occ.116	a	---	Virt.140	a	-0.05394	X
Occ.128	a	---	Virt.135	a	0.06772	X
Occ.128	a	---	Virt.136	a	-0.08017	X
Occ.128	a	---	Virt.140	a	0.26449	X
Occ.128	a	---	Virt.141	a	-0.63053	X
Occ.128	a	---	Virt.147	a	-0.06705	X
Occ.129	a	---	Virt.135	a	0.07388	X
Occ.129	a	---	Virt.136	a	0.07752	X
Occ.129	a	---	Virt.140	a	0.62495	X
Occ.129	a	---	Virt.141	a	0.26620	X
Occ.129	a	---	Virt.143	a	-0.05314	X
Occ.129	a	---	Virt.148	a	0.06645	X
-----						
Root 18 singlet a			0.141212076	a.u.	( 3.8425777	eV)
-----						
Transition Moments	X	0.02031	Y	-0.00159	Z	-0.00204
Oscillator Strength						0.00004
Occ.128	a	---	Virt.132	a	-0.12573	X
Occ.128	a	---	Virt.135	a	-0.22183	X
Occ.128	a	---	Virt.136	a	-0.18200	X
Occ.128	a	---	Virt.138	a	0.13668	X
Occ.128	a	---	Virt.139	a	-0.10786	X
Occ.128	a	---	Virt.140	a	-0.10973	X
Occ.128	a	---	Virt.141	a	-0.05643	X
Occ.129	a	---	Virt.133	a	-0.12682	X
Occ.129	a	---	Virt.135	a	0.18491	X
Occ.129	a	---	Virt.136	a	-0.21862	X
Occ.129	a	---	Virt.138	a	0.11411	X
Occ.129	a	---	Virt.139	a	0.13988	X
Occ.129	a	---	Virt.141	a	-0.11449	X
Occ.130	a	---	Virt.137	a	-0.83433	X
-----						
Root 19 singlet a			0.142733142	a.u.	( 3.8839681	eV)
-----						
Transition Moments	X	-0.32515	Y	-0.40757	Z	0.00098
Oscillator Strength						0.02587
Occ.128	a	---	Virt.136	a	-0.13045	X
Occ.128	a	---	Virt.137	a	-0.09066	X
Occ.129	a	---	Virt.135	a	-0.13489	X
Occ.129	a	---	Virt.137	a	-0.19049	X
Occ.130	a	---	Virt.136	a	0.06372	X
Occ.130	a	---	Virt.138	a	0.83487	X
Occ.130	a	---	Virt.139	a	0.44619	X
-----						

Root 20 singlet a 0.142773218 a.u. ( 3.8850586 eV)

-----  
Transition Moments X 0.40969 Y -0.33255 Z 0.00075  
Oscillator Strength 0.02650

Occ.128 a --- Virt.135 a -0.11976 X  
Occ.128 a --- Virt.137 a 0.19108 X  
Occ.129 a --- Virt.136 a 0.14525 X  
Occ.129 a --- Virt.137 a -0.08610 X  
Occ.130 a --- Virt.135 a -0.06188 X  
Occ.130 a --- Virt.138 a -0.44512 X  
Occ.130 a --- Virt.139 a 0.83599 X

-----  
Root 21 singlet a 0.145066333 a.u. ( 3.9474574 eV)

-----  
Transition Moments X -0.02232 Y -0.01526 Z -0.02203  
Oscillator Strength 0.00012

Occ.125 a --- Virt.131 a -0.18562 X  
Occ.126 a --- Virt.132 a -0.06323 X  
Occ.126 a --- Virt.133 a 0.12666 X  
Occ.127 a --- Virt.132 a 0.12656 X  
Occ.127 a --- Virt.133 a 0.05997 X  
Occ.128 a --- Virt.133 a -0.05283 X  
Occ.128 a --- Virt.135 a 0.42235 X  
Occ.128 a --- Virt.136 a -0.49592 X  
Occ.128 a --- Virt.141 a 0.09056 X  
Occ.129 a --- Virt.132 a 0.05226 X  
Occ.129 a --- Virt.135 a 0.53767 X  
Occ.129 a --- Virt.136 a 0.42218 X  
Occ.129 a --- Virt.140 a -0.10004 X

-----  
Root 22 singlet a 0.146166618 a.u. ( 3.9773978 eV)

-----  
Transition Moments X 0.02330 Y 0.01510 Z 0.00010  
Oscillator Strength 0.00008

Occ.125 a --- Virt.133 a 0.08803 X  
Occ.126 a --- Virt.131 a -0.14022 X  
Occ.126 a --- Virt.133 a -0.06674 X  
Occ.127 a --- Virt.132 a 0.06971 X  
Occ.128 a --- Virt.135 a 0.41821 X  
Occ.128 a --- Virt.136 a 0.06193 X  
Occ.128 a --- Virt.137 a 0.46841 X  
Occ.128 a --- Virt.140 a -0.13760 X  
Occ.129 a --- Virt.135 a 0.05865 X  
Occ.129 a --- Virt.136 a -0.41111 X  
Occ.129 a --- Virt.137 a -0.58405 X  
Occ.129 a --- Virt.141 a 0.13151 X  
Occ.130 a --- Virt.140 a -0.05381 X

-----  
Root 23 singlet a 0.146222254 a.u. ( 3.9789117 eV)

-----  
Transition Moments X -0.01979 Y 0.00644 Z -0.00019  
Oscillator Strength 0.00004

Occ.125 a --- Virt.132 a 0.08277 X  
Occ.126 a --- Virt.132 a 0.07221 X  
Occ.127 a --- Virt.131 a -0.13442 X  
Occ.127 a --- Virt.133 a 0.06975 X  
Occ.128 a --- Virt.135 a -0.11825 X  
Occ.128 a --- Virt.136 a 0.42875 X  
Occ.128 a --- Virt.137 a -0.54661 X  
Occ.128 a --- Virt.141 a -0.13720 X  
Occ.129 a --- Virt.135 a 0.42028 X  
Occ.129 a --- Virt.136 a 0.07544 X  
Occ.129 a --- Virt.137 a -0.48624 X  
Occ.129 a --- Virt.140 a -0.13312 X

-----  
Root 24 singlet a 0.147087287 a.u. ( 4.0024504 eV)

-----  
Transition Moments X -0.24855 Y -0.70698 Z -0.00098  
Oscillator Strength 0.05507

Occ.125 a --- Virt.133 a -0.07555 X  
Occ.126 a --- Virt.131 a 0.06307 X  
Occ.126 a --- Virt.132 a -0.05554 X

```
Occ.126 a --- Virt.133 a 0.05729 X
Occ.127 a --- Virt.131 a 0.08573 X
Occ.127 a --- Virt.132 a -0.06755 X
Occ.127 a --- Virt.133 a -0.06235 X
Occ.128 a --- Virt.134 a -0.07402 X
Occ.128 a --- Virt.135 a 0.25949 X
Occ.128 a --- Virt.136 a 0.42360 X
Occ.128 a --- Virt.137 a 0.06622 X
Occ.129 a --- Virt.135 a 0.46374 X
Occ.129 a --- Virt.136 a -0.35006 X
Occ.129 a --- Virt.137 a 0.52899 X
Occ.130 a --- Virt.138 a 0.17128 X
Occ.130 a --- Virt.139 a 0.18873 X
Occ.130 a --- Virt.141 a -0.07554 X
-----
Root 25 singlet a 0.147182602 a.u. ( 4.0050441 eV)
-----
Transition Moments X -0.70727 Y 0.25039 Z -0.00315
Oscillator Strength 0.05524

Occ.125 a --- Virt.132 a -0.08314 X
Occ.126 a --- Virt.131 a -0.09389 X
Occ.126 a --- Virt.132 a -0.06780 X
Occ.126 a --- Virt.133 a -0.05821 X
Occ.127 a --- Virt.131 a 0.06997 X
Occ.127 a --- Virt.132 a 0.05096 X
Occ.127 a --- Virt.133 a -0.06882 X
Occ.128 a --- Virt.135 a -0.42401 X
Occ.128 a --- Virt.136 a 0.29115 X
Occ.128 a --- Virt.137 a 0.58041 X
Occ.129 a --- Virt.134 a 0.07418 X
Occ.129 a --- Virt.135 a 0.26695 X
Occ.129 a --- Virt.136 a 0.43738 X
Occ.130 a --- Virt.138 a 0.19058 X
Occ.130 a --- Virt.139 a -0.17119 X
Occ.130 a --- Virt.140 a -0.08227 X
-----
Root 26 singlet a 0.147593336 a.u. ( 4.0162207 eV)
-----
Transition Moments X 0.01270 Y 0.05767 Z -0.00176
Oscillator Strength 0.00034

Occ.128 a --- Virt.135 a -0.45321 X
Occ.128 a --- Virt.136 a -0.38687 X
Occ.128 a --- Virt.138 a -0.33179 X
Occ.128 a --- Virt.139 a 0.25145 X
Occ.129 a --- Virt.135 a 0.30397 X
Occ.129 a --- Virt.136 a -0.38815 X
Occ.129 a --- Virt.138 a -0.26808 X
Occ.129 a --- Virt.139 a -0.33177 X
Occ.130 a --- Virt.137 a 0.18571 X
-----
Root 27 singlet a 0.149267753 a.u. ( 4.0617840 eV)
-----
Transition Moments X 0.18599 Y -0.13308 Z -0.00576
Oscillator Strength 0.00521

Occ.125 a --- Virt.132 a -0.10952 X
Occ.125 a --- Virt.133 a 0.10849 X
Occ.126 a --- Virt.131 a -0.22847 X
Occ.126 a --- Virt.133 a -0.08711 X
Occ.127 a --- Virt.131 a 0.08072 X
Occ.127 a --- Virt.132 a 0.06405 X
Occ.128 a --- Virt.139 a -0.58834 X
Occ.128 a --- Virt.140 a 0.16102 X
Occ.128 a --- Virt.141 a -0.10271 X
Occ.129 a --- Virt.138 a -0.66008 X
Occ.129 a --- Virt.139 a 0.06021 X
Occ.129 a --- Virt.140 a -0.08368 X
Occ.129 a --- Virt.141 a -0.14745 X
Occ.130 a --- Virt.140 a 0.16992 X
-----
Root 28 singlet a 0.149271614 a.u. ( 4.0618890 eV)
-----
Transition Moments X 0.13816 Y 0.17850 Z -0.00309
Oscillator Strength 0.00507
```

```
Occ.125 a --- Virt.132 a -0.10484 X
Occ.125 a --- Virt.133 a -0.10832 X
Occ.126 a --- Virt.131 a 0.08332 X
Occ.126 a --- Virt.132 a -0.08148 X
Occ.127 a --- Virt.131 a 0.22706 X
Occ.127 a --- Virt.132 a -0.06062 X
Occ.127 a --- Virt.133 a -0.09182 X
Occ.128 a --- Virt.138 a -0.61065 X
Occ.128 a --- Virt.140 a -0.09268 X
Occ.128 a --- Virt.141 a -0.15775 X
Occ.129 a --- Virt.139 a 0.64093 X
Occ.129 a --- Virt.140 a -0.14687 X
Occ.129 a --- Virt.141 a 0.09478 X
Occ.130 a --- Virt.141 a 0.16693 X
-----
Root 29 singlet a 0.149876858 a.u. ( 4.0783585 eV)
-----
Transition Moments X 0.01277 Y 0.00018 Z 0.10829
Oscillator Strength 0.00119

Occ.125 a --- Virt.131 a -0.22903 X
Occ.126 a --- Virt.132 a -0.08345 X
Occ.126 a --- Virt.133 a 0.14933 X
Occ.127 a --- Virt.132 a 0.16357 X
Occ.127 a --- Virt.133 a 0.06934 X
Occ.128 a --- Virt.136 a 0.05752 X
Occ.128 a --- Virt.138 a -0.43041 X
Occ.128 a --- Virt.139 a -0.56576 X
Occ.129 a --- Virt.135 a -0.05561 X
Occ.129 a --- Virt.138 a 0.46388 X
Occ.129 a --- Virt.139 a -0.37976 X
-----
Root 30 singlet a 0.156165114 a.u. ( 4.2494708 eV)
-----
Transition Moments X 0.09297 Y 0.07109 Z -0.00838
Oscillator Strength 0.00143

Occ.125 a --- Virt.132 a 0.20946 X
Occ.125 a --- Virt.133 a 0.11997 X
Occ.126 a --- Virt.131 a 0.06689 X
Occ.126 a --- Virt.132 a 0.27547 X
Occ.126 a --- Virt.133 a -0.06063 X
Occ.127 a --- Virt.131 a 0.85421 X
Occ.127 a --- Virt.132 a 0.10561 X
Occ.127 a --- Virt.133 a 0.30233 X
Occ.128 a --- Virt.138 a 0.07405 X
Occ.129 a --- Virt.139 a -0.08108 X
```

### NWChem TDDFT output for [Ru(bpy)<sub>2</sub>(btz)]<sup>2+</sup>:

```
-----
Root 1 singlet a 0.099887946 a.u. ( 2.7180905 eV)
-----
Transition Moments X 0.02515 Y -0.05919 Z 0.10347
Oscillator Strength 0.00099

Occ.132 a --- Virt.133 a 0.97489 X
Occ.132 a --- Virt.134 a -0.18247 X
Occ.132 a --- Virt.137 a -0.06920 X
-----
Root 2 singlet a 0.100423251 a.u. ( 2.7326569 eV)
-----
Transition Moments X -0.07424 Y -0.01007 Z 0.02670
Oscillator Strength 0.00042

Occ.130 a --- Virt.134 a 0.07955 X
Occ.132 a --- Virt.133 a 0.18393 X
Occ.132 a --- Virt.134 a 0.97163 X
Occ.132 a --- Virt.136 a -0.06277 X
Occ.132 a --- Virt.143 a -0.05182 X
-----
Root 3 singlet a 0.106975651 a.u. ( 2.9109568 eV)
-----
Transition Moments X -0.00716 Y -0.08917 Z 0.01385
```

Oscillator Strength					0.00058
Occ.130	a	---	Virt.133	a	-0.60543 X
Occ.130	a	---	Virt.134	a	0.06716 X
Occ.130	a	---	Virt.137	a	0.05511 X
Occ.131	a	---	Virt.133	a	-0.08756 X
Occ.131	a	---	Virt.134	a	0.77775 X
Occ.131	a	---	Virt.136	a	-0.05419 X
Occ.132	a	---	Virt.133	a	0.05040 X
-----					
Root 4 singlet a					0.107679672 a.u. ( 2.9301142 eV)
-----					
Transition Moments	X	0.10342	Y	-0.01436	Z -0.00092
Oscillator Strength					0.00078
Occ.130	a	---	Virt.134	a	-0.42780 X
Occ.131	a	---	Virt.133	a	0.88330 X
Occ.131	a	---	Virt.134	a	0.13669 X
Occ.131	a	---	Virt.135	a	-0.05113 X
Occ.132	a	---	Virt.134	a	0.06078 X
Occ.132	a	---	Virt.143	a	0.05546 X
-----					
Root 5 singlet a					0.112158562 a.u. ( 3.0519911 eV)
-----					
Transition Moments	X	0.05642	Y	-1.21385	Z -0.22218
Oscillator Strength					0.11410
Occ.130	a	---	Virt.133	a	-0.78367 X
Occ.131	a	---	Virt.133	a	0.07316 X
Occ.131	a	---	Virt.134	a	-0.59264 X
Occ.132	a	---	Virt.137	a	-0.05310 X
Occ.132	a	---	Virt.138	a	0.06735 X
Occ.132	a	---	Virt.142	a	-0.07077 X
Occ.132	a	---	Virt.143	a	-0.06168 X
-----					
Root 6 singlet a					0.117049291 a.u. ( 3.1850746 eV)
-----					
Transition Moments	X	-0.71841	Y	-0.06089	Z 0.00244
Oscillator Strength					0.04056
Occ.130	a	---	Virt.134	a	-0.86006 X
Occ.130	a	---	Virt.139	a	-0.05473 X
Occ.131	a	---	Virt.133	a	-0.42485 X
Occ.131	a	---	Virt.137	a	-0.12219 X
Occ.131	a	---	Virt.138	a	0.05511 X
Occ.132	a	---	Virt.134	a	0.06806 X
Occ.132	a	---	Virt.136	a	-0.09683 X
Occ.132	a	---	Virt.139	a	0.14414 X
-----					
Root 7 singlet a					0.126780718 a.u. ( 3.4498803 eV)
-----					
Transition Moments	X	-0.01929	Y	0.22491	Z -0.10534
Oscillator Strength					0.00524
Occ.130	a	---	Virt.133	a	0.05966 X
Occ.130	a	---	Virt.137	a	0.14406 X
Occ.130	a	---	Virt.142	a	0.11549 X
Occ.130	a	---	Virt.143	a	0.11026 X
Occ.131	a	---	Virt.134	a	0.06352 X
Occ.131	a	---	Virt.142	a	-0.09205 X
Occ.131	a	---	Virt.143	a	0.09276 X
Occ.132	a	---	Virt.133	a	-0.05928 X
Occ.132	a	---	Virt.135	a	0.30760 X
Occ.132	a	---	Virt.136	a	0.08582 X
Occ.132	a	---	Virt.137	a	-0.74331 X
Occ.132	a	---	Virt.138	a	0.10285 X
Occ.132	a	---	Virt.142	a	-0.37631 X
Occ.132	a	---	Virt.143	a	-0.31398 X
-----					
Root 8 singlet a					0.132109335 a.u. ( 3.5948794 eV)
-----					
Transition Moments	X	-0.05027	Y	-0.00020	Z 0.22090
Oscillator Strength					0.00452
Occ.128	a	---	Virt.133	a	-0.07500 X
Occ.129	a	---	Virt.134	a	0.07376 X
Occ.130	a	---	Virt.135	a	-0.05752 X

```
Occ.130 a --- Virt.137 a 0.14126 X
Occ.130 a --- Virt.142 a 0.05102 X
Occ.130 a --- Virt.143 a 0.18254 X
Occ.131 a --- Virt.137 a -0.05520 X
Occ.131 a --- Virt.142 a -0.17193 X
Occ.132 a --- Virt.133 a -0.05820 X
Occ.132 a --- Virt.135 a -0.84041 X
Occ.132 a --- Virt.136 a 0.05729 X
Occ.132 a --- Virt.142 a -0.39057 X
Occ.132 a --- Virt.143 a -0.08710 X
-----
Root 9 singlet a 0.132575349 a.u. ( 3.6075603 eV)
-----
Transition Moments X 0.19758 Y 0.00904 Z 0.05383
Oscillator Strength 0.00371

Occ.130 a --- Virt.136 a -0.06856 X
Occ.130 a --- Virt.137 a 0.05493 X
Occ.130 a --- Virt.142 a 0.29906 X
Occ.130 a --- Virt.143 a -0.21726 X
Occ.130 a --- Virt.144 a 0.05512 X
Occ.130 a --- Virt.146 a 0.08566 X
Occ.131 a --- Virt.137 a 0.18393 X
Occ.131 a --- Virt.142 a 0.27052 X
Occ.131 a --- Virt.143 a 0.29306 X
Occ.132 a --- Virt.135 a -0.22985 X
Occ.132 a --- Virt.136 a -0.19065 X
Occ.132 a --- Virt.139 a 0.11952 X
Occ.132 a --- Virt.142 a 0.37090 X
Occ.132 a --- Virt.143 a -0.57472 X
Occ.132 a --- Virt.144 a 0.09669 X
Occ.132 a --- Virt.146 a 0.16288 X
Occ.132 a --- Virt.147 a 0.06354 X
-----
Root 10 singlet a 0.134893643 a.u. ( 3.6706443 eV)
-----
Transition Moments X 0.00060 Y 0.10367 Z 0.03504
Oscillator Strength 0.00108

Occ.130 a --- Virt.135 a 0.20659 X
Occ.130 a --- Virt.137 a -0.40725 X
Occ.130 a --- Virt.138 a 0.07101 X
Occ.130 a --- Virt.142 a -0.28392 X
Occ.130 a --- Virt.143 a -0.26063 X
Occ.131 a --- Virt.142 a 0.06072 X
Occ.132 a --- Virt.135 a -0.33446 X
Occ.132 a --- Virt.136 a 0.06598 X
Occ.132 a --- Virt.137 a -0.57797 X
Occ.132 a --- Virt.142 a 0.30379 X
Occ.132 a --- Virt.143 a 0.25448 X
-----
Root 11 singlet a 0.136783121 a.u. ( 3.7220597 eV)
-----
Transition Moments X -0.02539 Y 0.06313 Z 0.08144
Oscillator Strength 0.00103

Occ.130 a --- Virt.135 a -0.31131 X
Occ.130 a --- Virt.137 a 0.39625 X
Occ.130 a --- Virt.138 a -0.05262 X
Occ.130 a --- Virt.142 a 0.21689 X
Occ.130 a --- Virt.143 a 0.16110 X
Occ.131 a --- Virt.136 a -0.09489 X
Occ.131 a --- Virt.139 a 0.07315 X
Occ.131 a --- Virt.141 a 0.06627 X
Occ.131 a --- Virt.142 a 0.41289 X
Occ.131 a --- Virt.143 a -0.51217 X
Occ.131 a --- Virt.144 a 0.10010 X
Occ.131 a --- Virt.146 a 0.15593 X
Occ.131 a --- Virt.147 a 0.06560 X
Occ.132 a --- Virt.135 a -0.09616 X
Occ.132 a --- Virt.137 a -0.22850 X
Occ.132 a --- Virt.142 a 0.21906 X
Occ.132 a --- Virt.143 a 0.20496 X
-----
Root 12 singlet a 0.139107742 a.u. ( 3.7853159 eV)
-----
Transition Moments X -0.07998 Y -0.13093 Z -0.05496
```



Oscillator Strength				0.00246
Occ.130	a	---	Virt.135 a	0.69208 X
Occ.130	a	---	Virt.137 a	-0.29587 X
Occ.130	a	---	Virt.142 a	0.41429 X
Occ.130	a	---	Virt.143 a	0.31323 X
Occ.131	a	---	Virt.135 a	0.09888 X
Occ.131	a	---	Virt.136 a	-0.05710 X
Occ.131	a	---	Virt.139 a	0.06156 X
Occ.131	a	---	Virt.142 a	0.18581 X
Occ.131	a	---	Virt.143 a	-0.24127 X
Occ.131	a	---	Virt.146 a	0.07341 X
Occ.132	a	---	Virt.136 a	0.07063 X
Occ.132	a	---	Virt.137 a	0.06844 X
Occ.132	a	---	Virt.142 a	-0.08521 X
Occ.132	a	---	Virt.143 a	-0.08277 X
-----				
Root 13 singlet a	0.139329897 a.u. ( 3.7913610 eV)			
-----				
Transition Moments X				-0.36725 Y 0.00059 Z 0.01395
Oscillator Strength				0.01255
Occ.129	a	---	Virt.133 a	-0.05375 X
Occ.130	a	---	Virt.142 a	-0.06792 X
Occ.131	a	---	Virt.135 a	0.95964 X
Occ.131	a	---	Virt.142 a	-0.05024 X
Occ.132	a	---	Virt.136 a	-0.21004 X
Occ.132	a	---	Virt.141 a	0.07447 X
-----				
Root 14 singlet a	0.139474232 a.u. ( 3.7952886 eV)			
-----				
Transition Moments X				-0.32642 Y -0.00343 Z 0.00463
Oscillator Strength				0.00991
Occ.128	a	---	Virt.134 a	0.06531 X
Occ.129	a	---	Virt.133 a	-0.09500 X
Occ.130	a	---	Virt.134 a	-0.05961 X
Occ.130	a	---	Virt.135 a	-0.06953 X
Occ.130	a	---	Virt.136 a	-0.05068 X
Occ.130	a	---	Virt.142 a	0.09282 X
Occ.130	a	---	Virt.143 a	-0.18851 X
Occ.131	a	---	Virt.135 a	0.17165 X
Occ.131	a	---	Virt.137 a	-0.17842 X
Occ.131	a	---	Virt.138 a	0.05590 X
Occ.131	a	---	Virt.143 a	0.09475 X
Occ.132	a	---	Virt.134 a	0.06486 X
Occ.132	a	---	Virt.136 a	0.89637 X
Occ.132	a	---	Virt.137 a	0.09836 X
Occ.132	a	---	Virt.141 a	0.09207 X
Occ.132	a	---	Virt.142 a	0.09047 X
Occ.132	a	---	Virt.143 a	-0.08620 X
-----				
Root 15 singlet a	0.142371390 a.u. ( 3.8741243 eV)			
-----				
Transition Moments X				-0.01704 Y 0.26719 Z 0.02032
Oscillator Strength				0.00684
Occ.128	a	---	Virt.133 a	0.05055 X
Occ.130	a	---	Virt.135 a	-0.57886 X
Occ.130	a	---	Virt.136 a	0.09493 X
Occ.130	a	---	Virt.137 a	-0.67816 X
Occ.130	a	---	Virt.138 a	0.05208 X
Occ.130	a	---	Virt.142 a	0.26412 X
Occ.130	a	---	Virt.143 a	0.21494 X
Occ.131	a	---	Virt.134 a	0.05950 X
Occ.131	a	---	Virt.136 a	0.20327 X
Occ.132	a	---	Virt.138 a	-0.07038 X
Occ.132	a	---	Virt.142 a	-0.05219 X
-----				
Root 16 singlet a	0.143473131 a.u. ( 3.9041042 eV)			
-----				
Transition Moments X				0.39788 Y 0.03647 Z -0.00765
Oscillator Strength				0.01527
Occ.128	a	---	Virt.134 a	0.09875 X
Occ.129	a	---	Virt.133 a	-0.12336 X
Occ.130	a	---	Virt.141 a	-0.07021 X

Occ.130	a	---	Virt.142	a	-0.14598	X
Occ.130	a	---	Virt.143	a	0.19694	X
Occ.130	a	---	Virt.146	a	-0.05645	X
Occ.131	a	---	Virt.135	a	0.06654	X
Occ.131	a	---	Virt.136	a	-0.08563	X
Occ.131	a	---	Virt.137	a	0.58496	X
Occ.131	a	---	Virt.138	a	-0.09318	X
Occ.131	a	---	Virt.142	a	0.05813	X
Occ.132	a	---	Virt.136	a	0.16492	X
Occ.132	a	---	Virt.138	a	-0.07305	X
Occ.132	a	---	Virt.139	a	0.61610	X
Occ.132	a	---	Virt.141	a	-0.31847	X
Occ.132	a	---	Virt.142	a	-0.07084	X
Occ.132	a	---	Virt.143	a	0.05992	X
-----						
Root 17	singlet	a	0.145163974	a.u.	( 3.9501144	eV)
-----						
Transition Moments	X	0.01592	Y	0.12438	Z	0.03608
Oscillator Strength						0.00165
Occ.128	a	---	Virt.133	a	0.13305	X
Occ.129	a	---	Virt.134	a	-0.11089	X
Occ.130	a	---	Virt.137	a	0.07653	X
Occ.131	a	---	Virt.136	a	0.59657	X
Occ.131	a	---	Virt.137	a	0.08202	X
Occ.131	a	---	Virt.139	a	-0.10262	X
Occ.131	a	---	Virt.142	a	0.06876	X
Occ.131	a	---	Virt.143	a	-0.05830	X
Occ.132	a	---	Virt.137	a	0.07163	X
Occ.132	a	---	Virt.138	a	0.72295	X
Occ.132	a	---	Virt.139	a	0.07523	X
Occ.132	a	---	Virt.140	a	-0.18764	X
Occ.132	a	---	Virt.142	a	0.05166	X
-----						
Root 18	singlet	a	0.146454190	a.u.	( 3.9852230	eV)
-----						
Transition Moments	X	0.15909	Y	-0.02954	Z	-0.01316
Oscillator Strength						0.00257
Occ.128	a	---	Virt.134	a	-0.08421	X
Occ.129	a	---	Virt.133	a	0.10504	X
Occ.130	a	---	Virt.134	a	-0.06289	X
Occ.130	a	---	Virt.136	a	-0.85055	X
Occ.130	a	---	Virt.137	a	-0.08317	X
Occ.130	a	---	Virt.139	a	0.08546	X
Occ.130	a	---	Virt.141	a	-0.09971	X
Occ.130	a	---	Virt.142	a	-0.06199	X
Occ.130	a	---	Virt.143	a	0.07036	X
Occ.131	a	---	Virt.136	a	0.05242	X
Occ.131	a	---	Virt.137	a	0.27303	X
Occ.131	a	---	Virt.142	a	-0.14017	X
Occ.131	a	---	Virt.143	a	-0.12390	X
Occ.132	a	---	Virt.136	a	0.07231	X
Occ.132	a	---	Virt.139	a	-0.26968	X
Occ.132	a	---	Virt.141	a	-0.11845	X
Occ.132	a	---	Virt.142	a	0.05347	X
Occ.132	a	---	Virt.143	a	-0.05082	X
-----						
Root 19	singlet	a	0.147045819	a.u.	( 4.0013220	eV)
-----						
Transition Moments	X	0.01598	Y	-0.81723	Z	-0.16465
Oscillator Strength						0.06815
Occ.128	a	---	Virt.133	a	0.11166	X
Occ.129	a	---	Virt.134	a	-0.13610	X
Occ.130	a	---	Virt.133	a	-0.06293	X
Occ.130	a	---	Virt.135	a	0.16104	X
Occ.130	a	---	Virt.136	a	0.05728	X
Occ.130	a	---	Virt.137	a	0.14939	X
Occ.130	a	---	Virt.138	a	-0.14688	X
Occ.131	a	---	Virt.136	a	0.68995	X
Occ.132	a	---	Virt.137	a	-0.05422	X
Occ.132	a	---	Virt.138	a	-0.62510	X
Occ.132	a	---	Virt.140	a	0.06675	X
-----						
Root 20	singlet	a	0.148269193	a.u.	( 4.0346117	eV)
-----						

Transition Moments X 0.26170 Y 0.03762 Z 0.00993  
Oscillator Strength 0.00692

Occ.130	a	---	Virt.134	a	0.06975	X
Occ.130	a	---	Virt.136	a	-0.28379	X
Occ.130	a	---	Virt.139	a	0.37708	X
Occ.131	a	---	Virt.135	a	-0.06992	X
Occ.131	a	---	Virt.137	a	-0.18401	X
Occ.131	a	---	Virt.138	a	-0.17024	X
Occ.131	a	---	Virt.140	a	0.11049	X
Occ.132	a	---	Virt.136	a	-0.07219	X
Occ.132	a	---	Virt.139	a	0.51255	X
Occ.132	a	---	Virt.141	a	0.63240	X
Occ.132	a	---	Virt.142	a	-0.05777	X
Occ.132	a	---	Virt.143	a	0.06803	X

-----  
Root 21 singlet a 0.150475045 a.u. ( 4.0946361 eV)  
-----

Transition Moments X 0.00560 Y -0.15634 Z -0.04459  
Oscillator Strength 0.00265

Occ.130	a	---	Virt.138	a	0.11036	X
Occ.130	a	---	Virt.140	a	-0.06873	X
Occ.130	a	---	Virt.142	a	0.21309	X
Occ.130	a	---	Virt.143	a	0.19497	X
Occ.131	a	---	Virt.134	a	-0.08348	X
Occ.131	a	---	Virt.136	a	-0.08750	X
Occ.131	a	---	Virt.138	a	0.12960	X
Occ.131	a	---	Virt.139	a	-0.83953	X
Occ.131	a	---	Virt.142	a	-0.12975	X
Occ.131	a	---	Virt.143	a	0.12369	X
Occ.131	a	---	Virt.146	a	-0.05091	X
Occ.132	a	---	Virt.137	a	-0.08012	X
Occ.132	a	---	Virt.138	a	-0.07508	X
Occ.132	a	---	Virt.140	a	-0.19654	X
Occ.132	a	---	Virt.142	a	0.19043	X
Occ.132	a	---	Virt.143	a	0.16507	X

-----  
Root 22 singlet a 0.151084977 a.u. ( 4.1112331 eV)  
-----

Transition Moments X -0.09031 Y -0.17576 Z 0.18266  
Oscillator Strength 0.00729

Occ.128	a	---	Virt.133	a	0.15663	X
Occ.128	a	---	Virt.134	a	-0.08438	X
Occ.129	a	---	Virt.133	a	0.11896	X
Occ.129	a	---	Virt.134	a	-0.12392	X
Occ.130	a	---	Virt.138	a	-0.35123	X
Occ.130	a	---	Virt.139	a	0.17117	X
Occ.130	a	---	Virt.140	a	0.08581	X
Occ.130	a	---	Virt.141	a	0.10083	X
Occ.130	a	---	Virt.142	a	0.07655	X
Occ.131	a	---	Virt.138	a	0.20304	X
Occ.131	a	---	Virt.139	a	-0.14187	X
Occ.131	a	---	Virt.140	a	-0.05258	X
Occ.131	a	---	Virt.141	a	-0.13609	X
Occ.131	a	---	Virt.143	a	0.09353	X
Occ.132	a	---	Virt.135	a	-0.06234	X
Occ.132	a	---	Virt.138	a	0.17490	X
Occ.132	a	---	Virt.139	a	0.06465	X
Occ.132	a	---	Virt.140	a	0.75964	X
Occ.132	a	---	Virt.141	a	-0.17098	X
Occ.132	a	---	Virt.143	a	0.10841	X

-----  
Root 23 singlet a 0.151209156 a.u. ( 4.1146122 eV)  
-----

Transition Moments X -0.34244 Y 0.11717 Z -0.05999  
Oscillator Strength 0.01357

Occ.128	a	---	Virt.134	a	-0.18670	X
Occ.129	a	---	Virt.133	a	0.29548	X
Occ.129	a	---	Virt.134	a	0.06726	X
Occ.130	a	---	Virt.134	a	0.05877	X
Occ.130	a	---	Virt.139	a	0.50590	X
Occ.130	a	---	Virt.141	a	0.30680	X
Occ.130	a	---	Virt.143	a	-0.10985	X
Occ.131	a	---	Virt.135	a	0.07521	X

```
Occ.131 a --- Virt.137 a -0.16730 X
Occ.131 a --- Virt.138 a 0.26860 X
Occ.131 a --- Virt.139 a 0.11530 X
Occ.131 a --- Virt.142 a 0.18108 X
Occ.131 a --- Virt.143 a 0.11720 X
Occ.132 a --- Virt.138 a -0.08501 X
Occ.132 a --- Virt.139 a 0.11384 X
Occ.132 a --- Virt.140 a -0.35536 X
Occ.132 a --- Virt.141 a -0.37897 X
Occ.132 a --- Virt.142 a -0.13948 X
Occ.132 a --- Virt.143 a 0.07388 X
-----
Root 24 singlet a 0.151643687 a.u. ( 4.1264364 eV)
-----
Transition Moments X -0.53656 Y -0.03832 Z 0.02380
Oscillator Strength 0.02931

Occ.128 a --- Virt.134 a 0.05020 X
Occ.129 a --- Virt.133 a -0.08875 X
Occ.130 a --- Virt.136 a -0.14890 X
Occ.130 a --- Virt.138 a -0.05864 X
Occ.130 a --- Virt.141 a 0.22860 X
Occ.131 a --- Virt.137 a -0.32261 X
Occ.131 a --- Virt.138 a -0.74197 X
Occ.131 a --- Virt.139 a -0.12418 X
Occ.131 a --- Virt.140 a 0.25396 X
Occ.131 a --- Virt.143 a 0.05548 X
Occ.132 a --- Virt.141 a -0.40243 X
-----
Root 25 singlet a 0.151951068 a.u. ( 4.1348007 eV)
-----
Transition Moments X -0.02502 Y -0.55624 Z -0.18376
Oscillator Strength 0.03483

Occ.128 a --- Virt.133 a -0.26598 X
Occ.129 a --- Virt.134 a 0.17982 X
Occ.130 a --- Virt.137 a 0.12494 X
Occ.130 a --- Virt.138 a 0.76314 X
Occ.130 a --- Virt.139 a 0.09805 X
Occ.130 a --- Virt.140 a -0.21483 X
Occ.130 a --- Virt.142 a 0.05967 X
Occ.131 a --- Virt.136 a 0.18691 X
Occ.131 a --- Virt.139 a 0.06471 X
Occ.131 a --- Virt.141 a -0.08429 X
Occ.132 a --- Virt.140 a 0.41477 X
Occ.132 a --- Virt.141 a -0.05157 X
```

### NWChem TDDFT output for $[\text{Ru}(\text{bpy})(\text{btz})_2]^{2+}$ :

```
-----
Root 1 singlet a 0.104900451 a.u. ( 2.8544877 eV)
-----
Transition Moments X 0.00256 Y 0.00471 Z 0.09391
Oscillator Strength 0.00062

Occ.133 a --- Virt.135 a 0.09634 X
Occ.134 a --- Virt.135 a 0.98917 X
Occ.134 a --- Virt.138 a 0.06702 X
-----
Root 2 singlet a 0.110224530 a.u. ( 2.9993633 eV)
-----
Transition Moments X 0.03475 Y 0.00058 Z 0.00293
Oscillator Strength 0.00009

Occ.133 a --- Virt.135 a -0.98575 X
Occ.133 a --- Virt.138 a -0.06593 X
Occ.134 a --- Virt.135 a 0.10155 X
Occ.134 a --- Virt.144 a -0.06475 X
-----
Root 3 singlet a 0.118167882 a.u. ( 3.2155130 eV)
-----
Transition Moments X -0.03439 Y 1.03648 Z -0.00031
Oscillator Strength 0.08472
```

Occ.132	a	---	Virt.135	a	0.97409	X
Occ.132	a	---	Virt.138	a	-0.05682	X
Occ.133	a	---	Virt.137	a	-0.05372	X
Occ.133	a	---	Virt.140	a	0.06491	X
Occ.133	a	---	Virt.145	a	-0.05070	X
Occ.134	a	---	Virt.139	a	-0.06717	X
Occ.134	a	---	Virt.140	a	-0.09976	X
Occ.134	a	---	Virt.145	a	-0.07508	X
-----						
Root	4	singlet	a	0.126460428	a.u.	( 3.4411648 eV)
-----						
Transition Moments		X	-0.00525	Y	-0.09002	Z 0.00868
Oscillator Strength						0.00069
Occ.123	a	---	Virt.145	a	0.05237	X
Occ.132	a	---	Virt.135	a	-0.07702	X
Occ.132	a	---	Virt.138	a	0.07335	X
Occ.132	a	---	Virt.144	a	0.29385	X
Occ.132	a	---	Virt.145	a	-0.11365	X
Occ.133	a	---	Virt.137	a	-0.07062	X
Occ.133	a	---	Virt.144	a	0.08115	X
Occ.133	a	---	Virt.145	a	0.21579	X
Occ.134	a	---	Virt.137	a	0.41233	X
Occ.134	a	---	Virt.138	a	-0.05483	X
Occ.134	a	---	Virt.139	a	-0.07679	X
Occ.134	a	---	Virt.140	a	-0.10407	X
Occ.134	a	---	Virt.144	a	-0.43408	X
Occ.134	a	---	Virt.145	a	-0.64314	X
Occ.134	a	---	Virt.146	a	0.10164	X
-----						
Root	5	singlet	a	0.128042436	a.u.	( 3.4842134 eV)
-----						
Transition Moments		X	0.06448	Y	0.00311	Z -0.07390
Oscillator Strength						0.00082
Occ.129	a	---	Virt.144	a	-0.06518	X
Occ.132	a	---	Virt.137	a	0.13222	X
Occ.132	a	---	Virt.144	a	-0.15491	X
Occ.132	a	---	Virt.145	a	-0.32171	X
Occ.133	a	---	Virt.144	a	0.46205	X
Occ.133	a	---	Virt.145	a	-0.22899	X
Occ.133	a	---	Virt.148	a	0.05335	X
Occ.134	a	---	Virt.136	a	-0.12850	X
Occ.134	a	---	Virt.138	a	0.13200	X
Occ.134	a	---	Virt.143	a	0.07264	X
Occ.134	a	---	Virt.144	a	0.57768	X
Occ.134	a	---	Virt.145	a	-0.41025	X
Occ.134	a	---	Virt.148	a	0.06977	X
-----						
Root	6	singlet	a	0.132833258	a.u.	( 3.6145784 eV)
-----						
Transition Moments		X	-0.03571	Y	-0.01141	Z -0.04010
Oscillator Strength						0.00027
Occ.132	a	---	Virt.137	a	0.16340	X
Occ.132	a	---	Virt.144	a	-0.30761	X
Occ.132	a	---	Virt.145	a	-0.54026	X
Occ.132	a	---	Virt.146	a	0.08224	X
Occ.133	a	---	Virt.143	a	-0.09657	X
Occ.133	a	---	Virt.144	a	-0.60941	X
Occ.133	a	---	Virt.145	a	0.32003	X
Occ.133	a	---	Virt.148	a	-0.07003	X
Occ.134	a	---	Virt.136	a	-0.17104	X
Occ.134	a	---	Virt.138	a	0.12776	X
Occ.134	a	---	Virt.144	a	0.08449	X
Occ.134	a	---	Virt.145	a	-0.05651	X
-----						
Root	7	singlet	a	0.134442556	a.u.	( 3.6583696 eV)
-----						
Transition Moments		X	-0.18170	Y	-0.02801	Z -0.17312
Oscillator Strength						0.00572
Occ.132	a	---	Virt.144	a	0.07799	X
Occ.132	a	---	Virt.145	a	0.27759	X
Occ.133	a	---	Virt.136	a	-0.06799	X
Occ.133	a	---	Virt.138	a	0.05490	X
Occ.133	a	---	Virt.145	a	-0.05827	X

```
Occ.134 a --- Virt.136 a -0.74324 X
Occ.134 a --- Virt.137 a 0.22409 X
Occ.134 a --- Virt.138 a 0.48691 X
Occ.134 a --- Virt.139 a 0.09825 X
Occ.134 a --- Virt.140 a -0.15270 X
Occ.134 a --- Virt.144 a -0.05650 X
Occ.134 a --- Virt.145 a 0.10952 X
-----
Root 8 singlet a 0.135202518 a.u. ( 3.6790493 eV)
-----
Transition Moments X -0.04404 Y 0.08330 Z -0.03881
Oscillator Strength 0.00094

Occ.132 a --- Virt.144 a 0.27787 X
Occ.132 a --- Virt.145 a -0.10206 X
Occ.133 a --- Virt.137 a -0.06085 X
Occ.133 a --- Virt.144 a 0.08724 X
Occ.133 a --- Virt.145 a 0.22753 X
Occ.134 a --- Virt.136 a -0.15572 X
Occ.134 a --- Virt.137 a -0.77575 X
Occ.134 a --- Virt.138 a 0.21589 X
Occ.134 a --- Virt.139 a 0.20759 X
Occ.134 a --- Virt.140 a 0.18335 X
Occ.134 a --- Virt.141 a -0.06387 X
Occ.134 a --- Virt.142 a 0.10108 X
Occ.134 a --- Virt.144 a -0.14895 X
Occ.134 a --- Virt.145 a -0.21265 X
-----
Root 9 singlet a 0.140877407 a.u. ( 3.8334709 eV)
-----
Transition Moments X -0.17026 Y -0.00267 Z 0.17882
Oscillator Strength 0.00573

Occ.132 a --- Virt.136 a -0.33915 X
Occ.132 a --- Virt.137 a 0.59704 X
Occ.132 a --- Virt.138 a 0.14479 X
Occ.132 a --- Virt.139 a -0.07805 X
Occ.132 a --- Virt.140 a -0.21266 X
Occ.132 a --- Virt.141 a 0.05634 X
Occ.132 a --- Virt.142 a -0.07760 X
Occ.132 a --- Virt.145 a 0.18689 X
Occ.133 a --- Virt.136 a 0.49841 X
Occ.133 a --- Virt.137 a -0.16052 X
Occ.133 a --- Virt.138 a -0.32161 X
Occ.133 a --- Virt.139 a -0.06221 X
Occ.133 a --- Virt.140 a 0.10915 X
Occ.133 a --- Virt.145 a -0.05658 X
-----
Root 10 singlet a 0.141371991 a.u. ( 3.8469292 eV)
-----
Transition Moments X 0.10950 Y -0.01571 Z -0.08071
Oscillator Strength 0.00177

Occ.132 a --- Virt.136 a -0.66578 X
Occ.132 a --- Virt.137 a -0.22279 X
Occ.132 a --- Virt.138 a 0.46394 X
Occ.132 a --- Virt.139 a 0.18243 X
Occ.132 a --- Virt.143 a -0.05393 X
Occ.132 a --- Virt.144 a -0.13247 X
Occ.133 a --- Virt.136 a -0.24659 X
Occ.133 a --- Virt.137 a -0.27592 X
Occ.133 a --- Virt.138 a 0.20603 X
Occ.133 a --- Virt.139 a 0.11832 X
Occ.133 a --- Virt.144 a -0.09021 X
Occ.133 a --- Virt.145 a -0.11689 X
Occ.134 a --- Virt.137 a -0.06661 X
-----
Root 11 singlet a 0.141791266 a.u. ( 3.8583383 eV)
-----
Transition Moments X -0.14417 Y 0.00036 Z -0.03508
Oscillator Strength 0.00208

Occ.131 a --- Virt.135 a -0.17507 X
Occ.132 a --- Virt.137 a -0.10012 X
Occ.132 a --- Virt.144 a -0.06697 X
Occ.132 a --- Virt.145 a -0.10976 X
Occ.133 a --- Virt.136 a 0.07293 X
```

```
Occ.133 a --- Virt.138 a -0.07941 X
Occ.133 a --- Virt.144 a 0.07464 X
Occ.134 a --- Virt.135 a 0.07688 X
Occ.134 a --- Virt.136 a -0.57805 X
Occ.134 a --- Virt.137 a -0.10305 X
Occ.134 a --- Virt.138 a -0.74049 X
Occ.134 a --- Virt.143 a 0.06675 X
Occ.134 a --- Virt.144 a -0.05789 X
-----
Root 12 singlet a 0.145095038 a.u. ( 3.9482386 eV)
-----
Transition Moments X -0.67784 Y 0.03050 Z 0.24637
Oscillator Strength 0.05041

Occ.131 a --- Virt.135 a -0.06380 X
Occ.132 a --- Virt.137 a -0.55800 X
Occ.132 a --- Virt.138 a 0.07406 X
Occ.132 a --- Virt.139 a 0.08583 X
Occ.132 a --- Virt.140 a 0.08739 X
Occ.132 a --- Virt.144 a -0.11309 X
Occ.132 a --- Virt.145 a -0.14183 X
Occ.133 a --- Virt.136 a 0.71951 X
Occ.133 a --- Virt.139 a -0.08621 X
Occ.133 a --- Virt.140 a 0.08281 X
Occ.133 a --- Virt.144 a 0.08216 X
Occ.133 a --- Virt.145 a -0.05348 X
Occ.134 a --- Virt.138 a 0.22800 X
Occ.134 a --- Virt.143 a 0.10973 X
Occ.134 a --- Virt.144 a -0.06813 X
-----
Root 13 singlet a 0.145863943 a.u. ( 3.9691615 eV)
-----
Transition Moments X -0.00789 Y -0.64125 Z 0.01308
Oscillator Strength 0.04001

Occ.132 a --- Virt.136 a -0.19574 X
Occ.132 a --- Virt.138 a 0.10763 X
Occ.132 a --- Virt.143 a 0.07872 X
Occ.132 a --- Virt.144 a 0.31194 X
Occ.132 a --- Virt.145 a -0.15619 X
Occ.133 a --- Virt.136 a 0.05590 X
Occ.133 a --- Virt.137 a 0.53096 X
Occ.133 a --- Virt.139 a -0.14723 X
Occ.133 a --- Virt.140 a -0.17639 X
Occ.133 a --- Virt.141 a 0.07215 X
Occ.133 a --- Virt.142 a -0.07837 X
Occ.133 a --- Virt.144 a -0.10006 X
Occ.133 a --- Virt.145 a -0.17974 X
Occ.134 a --- Virt.137 a -0.19262 X
Occ.134 a --- Virt.139 a -0.25385 X
Occ.134 a --- Virt.140 a -0.34711 X
Occ.134 a --- Virt.141 a 0.05360 X
Occ.134 a --- Virt.142 a -0.43491 X
-----
Root 14 singlet a 0.147155033 a.u. ( 4.0042939 eV)
-----
Transition Moments X -0.40065 Y -0.05083 Z 0.09431
Oscillator Strength 0.01687

Occ.131 a --- Virt.135 a 0.16342 X
Occ.132 a --- Virt.137 a -0.11061 X
Occ.132 a --- Virt.142 a -0.05106 X
Occ.132 a --- Virt.144 a -0.12713 X
Occ.132 a --- Virt.145 a -0.25597 X
Occ.133 a --- Virt.135 a 0.09699 X
Occ.133 a --- Virt.136 a -0.31737 X
Occ.133 a --- Virt.137 a -0.06715 X
Occ.133 a --- Virt.138 a -0.74911 X
Occ.133 a --- Virt.139 a -0.09255 X
Occ.133 a --- Virt.140 a 0.05634 X
Occ.133 a --- Virt.143 a 0.14031 X
Occ.133 a --- Virt.144 a 0.16939 X
Occ.133 a --- Virt.145 a -0.11440 X
Occ.134 a --- Virt.138 a 0.16547 X
Occ.134 a --- Virt.139 a -0.07533 X
Occ.134 a --- Virt.143 a 0.05885 X
Occ.134 a --- Virt.144 a -0.23973 X
```

```
Occ.134 a --- Virt.145 a 0.13048 X
-----
Root 15 singlet a 0.148048772 a.u. ( 4.0286138 eV)
-----
Transition Moments X 0.02681 Y 0.19646 Z -0.00947
Oscillator Strength 0.00389

Occ.132 a --- Virt.135 a -0.07173 X
Occ.132 a --- Virt.136 a 0.54342 X
Occ.132 a --- Virt.137 a 0.08786 X
Occ.132 a --- Virt.138 a 0.43549 X
Occ.132 a --- Virt.143 a -0.13073 X
Occ.132 a --- Virt.144 a -0.12585 X
Occ.132 a --- Virt.145 a 0.08819 X
Occ.133 a --- Virt.137 a -0.18879 X
Occ.133 a --- Virt.139 a 0.06636 X
Occ.133 a --- Virt.140 a 0.05724 X
Occ.133 a --- Virt.142 a 0.11898 X
Occ.133 a --- Virt.144 a -0.17606 X
Occ.133 a --- Virt.145 a -0.30741 X
Occ.134 a --- Virt.137 a -0.22761 X
Occ.134 a --- Virt.139 a -0.21501 X
Occ.134 a --- Virt.140 a -0.33232 X
Occ.134 a --- Virt.141 a -0.11251 X
Occ.134 a --- Virt.142 a 0.05170 X
Occ.134 a --- Virt.144 a -0.09280 X
Occ.134 a --- Virt.145 a -0.16606 X
-----
Root 16 singlet a 0.150949197 a.u. ( 4.1075384 eV)
-----
Transition Moments X 0.06142 Y -0.08333 Z -0.04625
Oscillator Strength 0.00129

Occ.132 a --- Virt.136 a -0.10013 X
Occ.132 a --- Virt.138 a -0.12410 X
Occ.132 a --- Virt.143 a 0.05862 X
Occ.132 a --- Virt.144 a 0.08686 X
Occ.133 a --- Virt.137 a -0.35574 X
Occ.133 a --- Virt.139 a -0.27599 X
Occ.133 a --- Virt.140 a -0.40549 X
Occ.133 a --- Virt.141 a -0.11762 X
Occ.133 a --- Virt.142 a -0.12804 X
Occ.133 a --- Virt.144 a 0.11418 X
Occ.133 a --- Virt.145 a 0.24729 X
Occ.134 a --- Virt.137 a -0.05138 X
Occ.134 a --- Virt.139 a -0.43135 X
Occ.134 a --- Virt.140 a -0.33844 X
Occ.134 a --- Virt.141 a -0.17523 X
Occ.134 a --- Virt.142 a 0.31562 X
Occ.134 a --- Virt.144 a 0.11957 X
Occ.134 a --- Virt.145 a 0.16445 X
-----
Root 17 singlet a 0.151518648 a.u. ( 4.1230340 eV)
-----
Transition Moments X -0.28410 Y -0.01949 Z 0.25077
Oscillator Strength 0.01454

Occ.131 a --- Virt.135 a -0.09672 X
Occ.132 a --- Virt.139 a -0.07613 X
Occ.132 a --- Virt.140 a -0.10331 X
Occ.132 a --- Virt.142 a -0.11409 X
Occ.132 a --- Virt.144 a -0.06131 X
Occ.132 a --- Virt.145 a -0.14877 X
Occ.133 a --- Virt.136 a 0.06490 X
Occ.133 a --- Virt.137 a -0.06805 X
Occ.133 a --- Virt.139 a -0.09387 X
Occ.133 a --- Virt.140 a -0.07076 X
Occ.133 a --- Virt.143 a 0.11353 X
Occ.133 a --- Virt.144 a 0.12051 X
Occ.134 a --- Virt.136 a 0.11773 X
Occ.134 a --- Virt.138 a -0.10030 X
Occ.134 a --- Virt.139 a 0.62724 X
Occ.134 a --- Virt.140 a -0.55658 X
Occ.134 a --- Virt.141 a 0.05414 X
Occ.134 a --- Virt.143 a -0.34766 X
Occ.134 a --- Virt.144 a -0.11574 X
Occ.134 a --- Virt.145 a 0.10702 X
```



-----  
Root 18 singlet a 0.152992815 a.u. ( 4.1631481 eV)  
-----

Transition Moments X 0.04342 Y -0.89519 Z -0.00467  
Oscillator Strength 0.08193

Occ.132 a --- Virt.135 a -0.08238 X  
Occ.132 a --- Virt.136 a -0.26923 X  
Occ.132 a --- Virt.138 a -0.40892 X  
Occ.132 a --- Virt.139 a -0.05345 X  
Occ.132 a --- Virt.143 a -0.10494 X  
Occ.132 a --- Virt.144 a -0.26059 X  
Occ.132 a --- Virt.145 a 0.11675 X  
Occ.133 a --- Virt.137 a 0.34631 X  
Occ.133 a --- Virt.139 a 0.18566 X  
Occ.133 a --- Virt.140 a 0.25731 X  
Occ.133 a --- Virt.142 a 0.17583 X  
Occ.133 a --- Virt.145 a -0.12567 X  
Occ.134 a --- Virt.137 a -0.14159 X  
Occ.134 a --- Virt.139 a -0.17839 X  
Occ.134 a --- Virt.140 a -0.27584 X  
Occ.134 a --- Virt.141 a -0.12760 X  
Occ.134 a --- Virt.142 a 0.43013 X  
Occ.134 a --- Virt.144 a -0.12998 X  
Occ.134 a --- Virt.145 a -0.16181 X

-----  
Root 19 singlet a 0.153222898 a.u. ( 4.1694090 eV)  
-----

Transition Moments X -0.04975 Y -0.01732 Z 0.30514  
Oscillator Strength 0.00979

Occ.131 a --- Virt.135 a -0.38870 X  
Occ.132 a --- Virt.137 a -0.34863 X  
Occ.132 a --- Virt.139 a -0.37996 X  
Occ.132 a --- Virt.140 a -0.51817 X  
Occ.132 a --- Virt.141 a -0.13911 X  
Occ.132 a --- Virt.144 a 0.09583 X  
Occ.132 a --- Virt.145 a 0.19253 X  
Occ.133 a --- Virt.136 a -0.12908 X  
Occ.133 a --- Virt.138 a -0.26990 X  
Occ.133 a --- Virt.143 a -0.10767 X  
Occ.133 a --- Virt.144 a -0.16187 X  
Occ.133 a --- Virt.145 a 0.08814 X  
Occ.134 a --- Virt.136 a 0.06260 X  
Occ.134 a --- Virt.143 a 0.09759 X  
Occ.134 a --- Virt.144 a 0.24847 X  
Occ.134 a --- Virt.145 a -0.13825 X

-----  
Root 20 singlet a 0.154068103 a.u. ( 4.1924082 eV)  
-----

Transition Moments X -0.22162 Y -0.06408 Z 0.09272  
Oscillator Strength 0.00635

Occ.131 a --- Virt.135 a 0.25059 X  
Occ.132 a --- Virt.137 a -0.11339 X  
Occ.132 a --- Virt.139 a 0.26839 X  
Occ.132 a --- Virt.140 a 0.37509 X  
Occ.132 a --- Virt.142 a 0.12153 X  
Occ.132 a --- Virt.144 a 0.14475 X  
Occ.132 a --- Virt.145 a 0.27743 X  
Occ.133 a --- Virt.138 a -0.31672 X  
Occ.133 a --- Virt.143 a -0.15158 X  
Occ.133 a --- Virt.144 a -0.22609 X  
Occ.133 a --- Virt.145 a 0.08320 X  
Occ.134 a --- Virt.138 a -0.11505 X  
Occ.134 a --- Virt.139 a 0.32786 X  
Occ.134 a --- Virt.140 a -0.22928 X  
Occ.134 a --- Virt.141 a -0.06376 X  
Occ.134 a --- Virt.143 a 0.26238 X  
Occ.134 a --- Virt.144 a 0.33692 X  
Occ.134 a --- Virt.145 a -0.19522 X

-----  
Root 21 singlet a 0.155088275 a.u. ( 4.2201685 eV)  
-----

Transition Moments X -0.04502 Y -0.23778 Z 0.01535  
Oscillator Strength 0.00608

Occ.132	a	---	Virt.136	a	0.06183	X
Occ.132	a	---	Virt.138	a	0.44557	X
Occ.132	a	---	Virt.139	a	-0.07628	X
Occ.132	a	---	Virt.140	a	0.09900	X
Occ.132	a	---	Virt.143	a	0.32034	X
Occ.132	a	---	Virt.144	a	0.05629	X
Occ.133	a	---	Virt.137	a	0.24470	X
Occ.133	a	---	Virt.139	a	0.23035	X
Occ.133	a	---	Virt.140	a	0.36604	X
Occ.133	a	---	Virt.141	a	0.18302	X
Occ.133	a	---	Virt.142	a	-0.23424	X
Occ.133	a	---	Virt.144	a	0.18731	X
Occ.133	a	---	Virt.145	a	0.35612	X
Occ.134	a	---	Virt.139	a	-0.07993	X
Occ.134	a	---	Virt.140	a	-0.14382	X
Occ.134	a	---	Virt.142	a	0.27361	X
Occ.134	a	---	Virt.143	a	-0.05724	X
Occ.134	a	---	Virt.144	a	0.13606	X
Occ.134	a	---	Virt.145	a	0.19291	X

-----  
Root 22 singlet a 0.155300934 a.u. ( 4.2259552 eV)  
-----

Transition Moments X 0.23408 Y -0.30283 Z -0.01116  
Oscillator Strength 0.01518

Occ.131	a	---	Virt.135	a	-0.07917	X
Occ.132	a	---	Virt.137	a	0.07249	X
Occ.132	a	---	Virt.139	a	-0.06244	X
Occ.132	a	---	Virt.142	a	0.09046	X
Occ.132	a	---	Virt.145	a	-0.06674	X
Occ.133	a	---	Virt.137	a	0.10148	X
Occ.133	a	---	Virt.138	a	0.08572	X
Occ.133	a	---	Virt.141	a	0.06774	X
Occ.133	a	---	Virt.142	a	-0.17128	X
Occ.133	a	---	Virt.143	a	0.07312	X
Occ.133	a	---	Virt.145	a	-0.10296	X
Occ.134	a	---	Virt.137	a	0.11678	X
Occ.134	a	---	Virt.139	a	0.20182	X
Occ.134	a	---	Virt.140	a	0.06426	X
Occ.134	a	---	Virt.141	a	-0.87399	X
Occ.134	a	---	Virt.143	a	0.23306	X
Occ.134	a	---	Virt.144	a	-0.09636	X
Occ.134	a	---	Virt.145	a	0.05424	X

-----  
Root 23 singlet a 0.156064814 a.u. ( 4.2467415 eV)  
-----

Transition Moments X 0.40471 Y 0.13563 Z 0.03577  
Oscillator Strength 0.01909

Occ.131	a	---	Virt.135	a	-0.15559	X
Occ.132	a	---	Virt.137	a	0.14713	X
Occ.132	a	---	Virt.141	a	-0.07385	X
Occ.132	a	---	Virt.142	a	0.26078	X
Occ.133	a	---	Virt.136	a	-0.06984	X
Occ.133	a	---	Virt.138	a	0.16985	X
Occ.133	a	---	Virt.139	a	-0.11323	X
Occ.133	a	---	Virt.140	a	0.09436	X
Occ.133	a	---	Virt.142	a	0.06166	X
Occ.133	a	---	Virt.143	a	0.16590	X
Occ.133	a	---	Virt.144	a	0.08578	X
Occ.134	a	---	Virt.136	a	0.06304	X
Occ.134	a	---	Virt.139	a	0.12766	X
Occ.134	a	---	Virt.140	a	-0.16638	X
Occ.134	a	---	Virt.141	a	0.31967	X
Occ.134	a	---	Virt.142	a	0.06394	X
Occ.134	a	---	Virt.143	a	0.75020	X
Occ.134	a	---	Virt.144	a	-0.17727	X
Occ.134	a	---	Virt.145	a	0.12912	X

-----  
Root 24 singlet a 0.157383306 a.u. ( 4.2826195 eV)  
-----

Transition Moments X -0.16190 Y -0.03301 Z -0.26573  
Oscillator Strength 0.01027

Occ.130	a	---	Virt.137	a	0.05302	X
Occ.132	a	---	Virt.139	a	0.10007	X
Occ.132	a	---	Virt.142	a	-0.14009	X

```
Occ.132 a --- Virt.145 a 0.05890 X
Occ.133 a --- Virt.136 a -0.12774 X
Occ.133 a --- Virt.138 a 0.14254 X
Occ.133 a --- Virt.139 a -0.75377 X
Occ.133 a --- Virt.140 a 0.52389 X
Occ.133 a --- Virt.141 a -0.05261 X
Occ.133 a --- Virt.143 a 0.16131 X
Occ.133 a --- Virt.144 a -0.06344 X
Occ.134 a --- Virt.143 a -0.13068 X
Occ.134 a --- Virt.144 a 0.08439 X
Occ.134 a --- Virt.145 a -0.06263 X
```

-----  
Root 25 singlet a 0.157875852 a.u. ( 4.2960223 eV)  
-----

Transition Moments X 0.04576 Y -0.17039 Z 0.03549  
Oscillator Strength 0.00341

```
Occ.132 a --- Virt.136 a 0.08140 X
Occ.132 a --- Virt.138 a -0.13092 X
Occ.132 a --- Virt.139 a 0.60218 X
Occ.132 a --- Virt.140 a -0.45058 X
Occ.132 a --- Virt.141 a 0.07877 X
Occ.132 a --- Virt.143 a -0.33027 X
Occ.132 a --- Virt.144 a -0.09017 X
Occ.132 a --- Virt.145 a 0.05381 X
Occ.133 a --- Virt.139 a 0.14208 X
Occ.133 a --- Virt.140 a 0.14393 X
Occ.133 a --- Virt.141 a 0.05799 X
Occ.133 a --- Virt.142 a -0.25194 X
Occ.133 a --- Virt.144 a 0.14747 X
Occ.133 a --- Virt.145 a 0.26936 X
Occ.134 a --- Virt.139 a -0.07316 X
Occ.134 a --- Virt.140 a -0.13482 X
Occ.134 a --- Virt.141 a -0.05245 X
Occ.134 a --- Virt.142 a -0.20243 X
```

### NWChem TDDFT output for $[\text{Ru}(\text{btz})_3]^{2+}$ :

-----  
Root 1 singlet a 0.134156757 a.u. ( 3.6505927 eV)  
-----

Transition Moments X -0.01379 Y -0.01344 Z 0.01640  
Oscillator Strength 0.00006

```
Occ.122 a --- Virt.146 a 0.06564 X
Occ.131 a --- Virt.146 a 0.08483 X
Occ.134 a --- Virt.146 a 0.20908 X
Occ.134 a --- Virt.147 a -0.28703 X
Occ.135 a --- Virt.146 a 0.35440 X
Occ.135 a --- Virt.147 a 0.19770 X
Occ.136 a --- Virt.139 a -0.11721 X
Occ.136 a --- Virt.146 a 0.79831 X
Occ.136 a --- Virt.147 a 0.13656 X
```

-----  
Root 2 singlet a 0.134560375 a.u. ( 3.6615757 eV)  
-----

Transition Moments X 0.02500 Y 0.00217 Z -0.01305  
Oscillator Strength 0.00007

```
Occ.122 a --- Virt.147 a 0.06924 X
Occ.131 a --- Virt.147 a 0.08697 X
Occ.134 a --- Virt.146 a -0.32898 X
Occ.134 a --- Virt.147 a -0.16788 X
Occ.135 a --- Virt.146 a 0.20884 X
Occ.135 a --- Virt.147 a -0.32009 X
Occ.136 a --- Virt.138 a -0.17664 X
Occ.136 a --- Virt.146 a -0.13088 X
Occ.136 a --- Virt.147 a 0.79223 X
```

-----  
Root 3 singlet a 0.137898022 a.u. ( 3.7523977 eV)  
-----

Transition Moments X 0.00757 Y -0.01338 Z 0.29775  
Oscillator Strength 0.00817

Occ.136	a	---	Virt.137	a	0.95239	X
Occ.136	a	---	Virt.139	a	-0.07799	X
Occ.136	a	---	Virt.140	a	0.25422	X
Occ.136	a	---	Virt.142	a	-0.05373	X
-----						
Root	4	singlet	a	0.139368637	a.u. (	3.7924152 eV)
-----						
Transition Moments	X	0.01148	Y	0.02270	Z	-0.04807
Oscillator Strength						0.00027
Occ.117	a	---	Virt.146	a	-0.05011	X
Occ.134	a	---	Virt.147	a	-0.39664	X
Occ.135	a	---	Virt.139	a	-0.16679	X
Occ.135	a	---	Virt.146	a	-0.62136	X
Occ.136	a	---	Virt.138	a	-0.46490	X
Occ.136	a	---	Virt.139	a	-0.40086	X
Occ.136	a	---	Virt.140	a	-0.06427	X
Occ.136	a	---	Virt.142	a	-0.13430	X
-----						
Root	5	singlet	a	0.139695430	a.u. (	3.8013077 eV)
-----						
Transition Moments	X	0.03070	Y	0.04472	Z	-0.00076
Oscillator Strength						0.00027
Occ.134	a	---	Virt.138	a	0.11413	X
Occ.134	a	---	Virt.147	a	0.57880	X
Occ.135	a	---	Virt.146	a	0.32241	X
Occ.136	a	---	Virt.137	a	-0.08767	X
Occ.136	a	---	Virt.138	a	-0.50290	X
Occ.136	a	---	Virt.139	a	-0.47529	X
Occ.136	a	---	Virt.140	a	-0.07144	X
Occ.136	a	---	Virt.142	a	-0.15063	X
Occ.136	a	---	Virt.147	a	-0.07815	X
-----						
Root	6	singlet	a	0.139852848	a.u. (	3.8055912 eV)
-----						
Transition Moments	X	0.04297	Y	0.01061	Z	-0.01832
Oscillator Strength						0.00021
Occ.134	a	---	Virt.139	a	-0.10107	X
Occ.134	a	---	Virt.146	a	-0.15403	X
Occ.135	a	---	Virt.138	a	-0.06364	X
Occ.135	a	---	Virt.147	a	-0.17220	X
Occ.136	a	---	Virt.138	a	0.61650	X
Occ.136	a	---	Virt.139	a	-0.69040	X
Occ.136	a	---	Virt.141	a	0.19120	X
Occ.136	a	---	Virt.144	a	-0.10873	X
Occ.136	a	---	Virt.145	a	0.10294	X
-----						
Root	7	singlet	a	0.144428613	a.u. (	3.9301042 eV)
-----						
Transition Moments	X	-0.12055	Y	-0.07987	Z	0.04560
Oscillator Strength						0.00221
Occ.134	a	---	Virt.138	a	-0.09802	X
Occ.134	a	---	Virt.139	a	0.20978	X
Occ.134	a	---	Virt.146	a	0.07717	X
Occ.134	a	---	Virt.147	a	-0.13591	X
Occ.135	a	---	Virt.137	a	-0.80979	X
Occ.135	a	---	Virt.138	a	0.28028	X
Occ.135	a	---	Virt.139	a	0.31408	X
Occ.135	a	---	Virt.140	a	-0.17596	X
Occ.135	a	---	Virt.142	a	0.11780	X
Occ.135	a	---	Virt.147	a	0.07299	X
Occ.136	a	---	Virt.139	a	-0.11621	X
Occ.136	a	---	Virt.142	a	-0.05478	X
Occ.136	a	---	Virt.146	a	-0.06679	X
-----						
Root	8	singlet	a	0.144937694	a.u. (	3.9439570 eV)
-----						
Transition Moments	X	-0.09299	Y	0.13384	Z	0.01336
Oscillator Strength						0.00258
Occ.134	a	---	Virt.137	a	0.77870	X
Occ.134	a	---	Virt.138	a	0.28727	X
Occ.134	a	---	Virt.139	a	0.24030	X
Occ.134	a	---	Virt.140	a	0.22556	X

Occ.134	a	---	Virt.142	a	0.05268	X
Occ.134	a	---	Virt.146	a	0.10789	X
Occ.134	a	---	Virt.147	a	0.11194	X
Occ.135	a	---	Virt.138	a	0.25599	X
Occ.135	a	---	Virt.139	a	-0.24077	X
Occ.135	a	---	Virt.141	a	0.06771	X
Occ.135	a	---	Virt.146	a	-0.05016	X
Occ.135	a	---	Virt.147	a	0.09747	X
Occ.136	a	---	Virt.138	a	0.10981	X
Occ.136	a	---	Virt.141	a	0.05127	X
Occ.136	a	---	Virt.147	a	0.07759	X

-----  
Root 9 singlet a 0.145764108 a.u. ( 3.9664449 eV)  
-----

Transition Moments X -0.04400 Y -0.02383 Z -0.15639  
Oscillator Strength 0.00262

Occ.134	a	---	Virt.138	a	-0.65345	X
Occ.134	a	---	Virt.139	a	0.18994	X
Occ.134	a	---	Virt.141	a	-0.12269	X
Occ.134	a	---	Virt.142	a	-0.05949	X
Occ.134	a	---	Virt.144	a	0.06848	X
Occ.134	a	---	Virt.145	a	-0.09194	X
Occ.134	a	---	Virt.147	a	0.12583	X
Occ.135	a	---	Virt.137	a	-0.15279	X
Occ.135	a	---	Virt.138	a	-0.10668	X
Occ.135	a	---	Virt.139	a	-0.63081	X
Occ.135	a	---	Virt.140	a	-0.09777	X
Occ.135	a	---	Virt.141	a	0.06678	X
Occ.135	a	---	Virt.142	a	-0.11703	X
Occ.135	a	---	Virt.146	a	0.12683	X

-----  
Root 10 singlet a 0.149788519 a.u. ( 4.0759547 eV)  
-----

Transition Moments X 0.63699 Y -0.54054 Z -0.01603  
Oscillator Strength 0.06972

Occ.134	a	---	Virt.137	a	-0.50660	X
Occ.134	a	---	Virt.138	a	0.25612	X
Occ.134	a	---	Virt.139	a	0.33958	X
Occ.134	a	---	Virt.140	a	-0.10713	X
Occ.134	a	---	Virt.142	a	0.14155	X
Occ.134	a	---	Virt.145	a	0.05335	X
Occ.134	a	---	Virt.146	a	0.22808	X
Occ.134	a	---	Virt.147	a	0.09358	X
Occ.135	a	---	Virt.137	a	0.15090	X
Occ.135	a	---	Virt.138	a	0.38685	X
Occ.135	a	---	Virt.139	a	-0.24808	X
Occ.135	a	---	Virt.141	a	0.13433	X
Occ.135	a	---	Virt.143	a	0.12742	X
Occ.135	a	---	Virt.144	a	-0.07802	X
Occ.135	a	---	Virt.145	a	0.06027	X
Occ.135	a	---	Virt.146	a	-0.07892	X
Occ.135	a	---	Virt.147	a	0.20372	X
Occ.136	a	---	Virt.138	a	0.15320	X
Occ.136	a	---	Virt.139	a	-0.09076	X
Occ.136	a	---	Virt.144	a	0.16725	X
Occ.136	a	---	Virt.145	a	-0.15097	X
Occ.136	a	---	Virt.146	a	-0.06910	X
Occ.136	a	---	Virt.147	a	0.19521	X

-----  
Root 11 singlet a 0.150176921 a.u. ( 4.0865237 eV)  
-----

Transition Moments X 0.56193 Y 0.66364 Z -0.06436  
Oscillator Strength 0.07612

Occ.134	a	---	Virt.137	a	0.13285	X
Occ.134	a	---	Virt.138	a	-0.40746	X
Occ.134	a	---	Virt.139	a	0.23154	X
Occ.134	a	---	Virt.141	a	-0.10160	X
Occ.134	a	---	Virt.143	a	0.13784	X
Occ.134	a	---	Virt.144	a	0.11950	X
Occ.134	a	---	Virt.145	a	-0.10983	X
Occ.134	a	---	Virt.146	a	0.12457	X
Occ.134	a	---	Virt.147	a	-0.23940	X
Occ.135	a	---	Virt.137	a	0.43657	X
Occ.135	a	---	Virt.138	a	0.27131	X

Occ.135	a	---	Virt.139	a	0.34480	X
Occ.135	a	---	Virt.140	a	0.15516	X
Occ.135	a	---	Virt.142	a	0.11316	X
Occ.135	a	---	Virt.143	a	-0.05078	X
Occ.135	a	---	Virt.145	a	0.06323	X
Occ.135	a	---	Virt.146	a	0.21512	X
Occ.135	a	---	Virt.147	a	0.07011	X
Occ.136	a	---	Virt.138	a	-0.08313	X
Occ.136	a	---	Virt.139	a	-0.15836	X
Occ.136	a	---	Virt.142	a	0.05660	X
Occ.136	a	---	Virt.143	a	0.06489	X
Occ.136	a	---	Virt.144	a	0.17803	X
Occ.136	a	---	Virt.145	a	0.17310	X
Occ.136	a	---	Virt.146	a	-0.19595	X
Occ.136	a	---	Virt.147	a	-0.06851	X
-----						
Root 12 singlet a			0.151641274	a.u. (	4.1263708	eV)
-----						
Transition Moments	X	0.05246	Y	0.05304	Z	-0.00547
Oscillator Strength						0.00057
Occ.134	a	---	Virt.138	a	0.05747	X
Occ.134	a	---	Virt.139	a	0.35997	X
Occ.134	a	---	Virt.140	a	0.05044	X
Occ.134	a	---	Virt.141	a	-0.05211	X
Occ.134	a	---	Virt.142	a	0.08736	X
Occ.134	a	---	Virt.146	a	-0.24969	X
Occ.135	a	---	Virt.138	a	-0.30082	X
Occ.135	a	---	Virt.139	a	0.10412	X
Occ.135	a	---	Virt.141	a	-0.08432	X
Occ.135	a	---	Virt.147	a	0.28012	X
Occ.136	a	---	Virt.141	a	-0.09330	X
Occ.136	a	---	Virt.142	a	-0.07197	X
Occ.136	a	---	Virt.143	a	-0.74755	X
Occ.136	a	---	Virt.144	a	-0.06713	X
Occ.136	a	---	Virt.145	a	0.11719	X
-----						
Root 13 singlet a			0.154223174	a.u. (	4.1966279	eV)
-----						
Transition Moments	X	0.06849	Y	0.05857	Z	0.33891
Oscillator Strength						0.01264
Occ.136	a	---	Virt.137	a	0.26039	X
Occ.136	a	---	Virt.139	a	0.06882	X
Occ.136	a	---	Virt.140	a	-0.95333	X
-----						
Root 14 singlet a			0.156272472	a.u. (	4.2523921	eV)
-----						
Transition Moments	X	0.37296	Y	0.03136	Z	-0.04581
Oscillator Strength						0.01481
Occ.134	a	---	Virt.137	a	-0.05585	X
Occ.134	a	---	Virt.142	a	0.05334	X
Occ.134	a	---	Virt.143	a	0.13010	X
Occ.134	a	---	Virt.144	a	0.12938	X
Occ.134	a	---	Virt.146	a	0.08110	X
Occ.135	a	---	Virt.137	a	0.09355	X
Occ.135	a	---	Virt.143	a	0.12820	X
Occ.135	a	---	Virt.145	a	0.11008	X
Occ.135	a	---	Virt.147	a	0.08730	X
Occ.136	a	---	Virt.138	a	-0.05813	X
Occ.136	a	---	Virt.139	a	0.17654	X
Occ.136	a	---	Virt.141	a	0.55613	X
Occ.136	a	---	Virt.142	a	-0.46514	X
Occ.136	a	---	Virt.143	a	0.06988	X
Occ.136	a	---	Virt.144	a	-0.56451	X
Occ.136	a	---	Virt.146	a	-0.08949	X
-----						
Root 15 singlet a			0.156447177	a.u. (	4.2571461	eV)
-----						
Transition Moments	X	0.03520	Y	-0.36135	Z	0.01954
Oscillator Strength						0.01379
Occ.134	a	---	Virt.137	a	-0.09746	X
Occ.134	a	---	Virt.144	a	-0.05079	X
Occ.134	a	---	Virt.145	a	0.12028	X
Occ.134	a	---	Virt.147	a	0.07829	X

Occ.135	a	---	Virt.143	a	0.18614	X
Occ.135	a	---	Virt.144	a	-0.10762	X
Occ.135	a	---	Virt.146	a	-0.07687	X
Occ.136	a	---	Virt.138	a	-0.19641	X
Occ.136	a	---	Virt.141	a	0.36931	X
Occ.136	a	---	Virt.142	a	0.62078	X
Occ.136	a	---	Virt.144	a	-0.09359	X
Occ.136	a	---	Virt.145	a	0.56318	X
Occ.136	a	---	Virt.147	a	0.07426	X
-----						
Root 16	singlet	a	0.157835417	a.u.	( 4.2949220	eV)
-----						
Transition Moments	X	-0.24186	Y	0.15561	Z	0.00294
Oscillator Strength						0.00870
Occ.134	a	---	Virt.143	a	-0.11287	X
Occ.135	a	---	Virt.141	a	-0.05411	X
Occ.135	a	---	Virt.143	a	-0.32372	X
Occ.135	a	---	Virt.147	a	-0.05874	X
Occ.136	a	---	Virt.138	a	-0.05243	X
Occ.136	a	---	Virt.141	a	0.68870	X
Occ.136	a	---	Virt.142	a	0.07439	X
Occ.136	a	---	Virt.143	a	-0.20006	X
Occ.136	a	---	Virt.144	a	0.46488	X
Occ.136	a	---	Virt.145	a	-0.35034	X
-----						
Root 17	singlet	a	0.158342601	a.u.	( 4.3087232	eV)
-----						
Transition Moments	X	-0.13804	Y	-0.20370	Z	0.01287
Oscillator Strength						0.00641
Occ.134	a	---	Virt.143	a	-0.34289	X
Occ.134	a	---	Virt.144	a	-0.09668	X
Occ.134	a	---	Virt.145	a	0.08924	X
Occ.134	a	---	Virt.147	a	0.08283	X
Occ.135	a	---	Virt.143	a	0.13416	X
Occ.135	a	---	Virt.145	a	-0.06588	X
Occ.135	a	---	Virt.146	a	-0.08468	X
Occ.136	a	---	Virt.138	a	0.05354	X
Occ.136	a	---	Virt.139	a	0.10403	X
Occ.136	a	---	Virt.141	a	0.05151	X
Occ.136	a	---	Virt.142	a	-0.55597	X
Occ.136	a	---	Virt.143	a	0.07172	X
Occ.136	a	---	Virt.144	a	0.43961	X
Occ.136	a	---	Virt.145	a	0.52805	X
Occ.136	a	---	Virt.146	a	0.09823	X
-----						
Root 18	singlet	a	0.159803517	a.u.	( 4.3484768	eV)
-----						
Transition Moments	X	0.18706	Y	-0.14920	Z	0.01060
Oscillator Strength						0.00611
Occ.134	a	---	Virt.137	a	-0.07746	X
Occ.134	a	---	Virt.139	a	-0.25792	X
Occ.134	a	---	Virt.140	a	0.16797	X
Occ.134	a	---	Virt.142	a	0.06526	X
Occ.134	a	---	Virt.144	a	0.35493	X
Occ.134	a	---	Virt.145	a	0.19013	X
Occ.134	a	---	Virt.146	a	-0.20264	X
Occ.135	a	---	Virt.138	a	0.47821	X
Occ.135	a	---	Virt.139	a	-0.16093	X
Occ.135	a	---	Virt.140	a	-0.08342	X
Occ.135	a	---	Virt.143	a	-0.18888	X
Occ.135	a	---	Virt.144	a	0.31114	X
Occ.135	a	---	Virt.145	a	-0.43994	X
Occ.136	a	---	Virt.138	a	-0.05481	X
Occ.136	a	---	Virt.143	a	-0.21603	X
Occ.136	a	---	Virt.144	a	-0.11606	X
Occ.136	a	---	Virt.145	a	0.11465	X
Occ.136	a	---	Virt.147	a	-0.10925	X
-----						
Root 19	singlet	a	0.160140237	a.u.	( 4.3576394	eV)
-----						
Transition Moments	X	0.07770	Y	0.04138	Z	-0.05793
Oscillator Strength						0.00119
Occ.134	a	---	Virt.143	a	0.13487	X

Occ.135	a	---	Virt.137	a	-0.24956	X
Occ.135	a	---	Virt.139	a	-0.06248	X
Occ.135	a	---	Virt.140	a	0.94159	X
Occ.135	a	---	Virt.145	a	-0.09850	X
Occ.136	a	---	Virt.146	a	0.06359	X
-----						
Root 20	singlet	a	0.160402488	a.u.	( 4.3647756	eV)
-----						
Transition Moments	X	0.05805	Y	0.01143	Z	-0.00920
Oscillator Strength						0.00038
Occ.134	a	---	Virt.137	a	0.25615	X
Occ.134	a	---	Virt.140	a	-0.92570	X
Occ.134	a	---	Virt.144	a	0.05636	X
Occ.135	a	---	Virt.138	a	0.08976	X
Occ.135	a	---	Virt.143	a	0.10739	X
Occ.135	a	---	Virt.144	a	0.13786	X
Occ.135	a	---	Virt.145	a	-0.13095	X
Occ.136	a	---	Virt.143	a	-0.08820	X
-----						
Root 21	singlet	a	0.160927390	a.u.	( 4.3790590	eV)
-----						
Transition Moments	X	0.78027	Y	0.72688	Z	-0.07481
Oscillator Strength						0.12260
Occ.134	a	---	Virt.138	a	-0.28446	X
Occ.134	a	---	Virt.139	a	0.25986	X
Occ.134	a	---	Virt.141	a	-0.18269	X
Occ.134	a	---	Virt.142	a	-0.08088	X
Occ.134	a	---	Virt.143	a	-0.31926	X
Occ.134	a	---	Virt.144	a	-0.26477	X
Occ.134	a	---	Virt.145	a	0.16716	X
Occ.134	a	---	Virt.146	a	-0.14831	X
Occ.134	a	---	Virt.147	a	0.25903	X
Occ.135	a	---	Virt.137	a	0.14562	X
Occ.135	a	---	Virt.138	a	0.20931	X
Occ.135	a	---	Virt.139	a	0.25473	X
Occ.135	a	---	Virt.142	a	0.10113	X
Occ.135	a	---	Virt.145	a	-0.11136	X
Occ.135	a	---	Virt.146	a	-0.27437	X
Occ.135	a	---	Virt.147	a	-0.13828	X
Occ.136	a	---	Virt.144	a	-0.27832	X
Occ.136	a	---	Virt.145	a	-0.27041	X
Occ.136	a	---	Virt.146	a	0.31966	X
Occ.136	a	---	Virt.147	a	0.06127	X
-----						
Root 22	singlet	a	0.161343078	a.u.	( 4.3903704	eV)
-----						
Transition Moments	X	0.61807	Y	-0.71171	Z	-0.02560
Oscillator Strength						0.09564
Occ.134	a	---	Virt.137	a	-0.15212	X
Occ.134	a	---	Virt.138	a	0.24294	X
Occ.134	a	---	Virt.139	a	0.36915	X
Occ.134	a	---	Virt.140	a	-0.06838	X
Occ.134	a	---	Virt.141	a	0.05098	X
Occ.134	a	---	Virt.142	a	-0.09994	X
Occ.134	a	---	Virt.144	a	-0.29911	X
Occ.134	a	---	Virt.145	a	-0.30868	X
Occ.134	a	---	Virt.146	a	-0.21885	X
Occ.134	a	---	Virt.147	a	-0.14593	X
Occ.135	a	---	Virt.138	a	0.12616	X
Occ.135	a	---	Virt.139	a	-0.18345	X
Occ.135	a	---	Virt.143	a	-0.40812	X
Occ.135	a	---	Virt.144	a	0.10033	X
Occ.135	a	---	Virt.145	a	0.07127	X
Occ.135	a	---	Virt.146	a	0.13484	X
Occ.135	a	---	Virt.147	a	-0.26639	X
Occ.136	a	---	Virt.138	a	-0.06065	X
Occ.136	a	---	Virt.143	a	0.13477	X
Occ.136	a	---	Virt.144	a	-0.16551	X
Occ.136	a	---	Virt.145	a	0.19338	X
Occ.136	a	---	Virt.146	a	0.06131	X
Occ.136	a	---	Virt.147	a	-0.29780	X
-----						
Root 23	singlet	a	0.162155143	a.u.	( 4.4124678	eV)
-----						



Transition Moments X -0.02600 Y 0.07111 Z -0.02514  
Oscillator Strength 0.00069

Occ.133	a	---	Virt.137	a	-0.05323	X
Occ.134	a	---	Virt.138	a	0.15297	X
Occ.134	a	---	Virt.139	a	-0.07782	X
Occ.134	a	---	Virt.140	a	0.08330	X
Occ.134	a	---	Virt.141	a	-0.42407	X
Occ.134	a	---	Virt.142	a	-0.15642	X
Occ.134	a	---	Virt.143	a	-0.38615	X
Occ.134	a	---	Virt.144	a	0.18814	X
Occ.134	a	---	Virt.145	a	-0.21180	X
Occ.134	a	---	Virt.147	a	-0.06810	X
Occ.135	a	---	Virt.138	a	-0.07829	X
Occ.135	a	---	Virt.139	a	-0.18006	X
Occ.135	a	---	Virt.140	a	0.08975	X
Occ.135	a	---	Virt.141	a	-0.11773	X
Occ.135	a	---	Virt.142	a	0.54504	X
Occ.135	a	---	Virt.143	a	0.19539	X
Occ.135	a	---	Virt.144	a	0.24105	X
Occ.135	a	---	Virt.145	a	0.17943	X
Occ.135	a	---	Virt.146	a	0.06781	X
Occ.136	a	---	Virt.142	a	0.10335	X

-----  
Root 24 singlet a 0.162521932 a.u. ( 4.4224487 eV)  
-----

Transition Moments X -0.24914 Y 0.23280 Z -0.05846  
Oscillator Strength 0.01297

Occ.134	a	---	Virt.139	a	0.07684	X
Occ.134	a	---	Virt.140	a	0.08751	X
Occ.134	a	---	Virt.141	a	0.20921	X
Occ.134	a	---	Virt.142	a	-0.50274	X
Occ.134	a	---	Virt.143	a	0.22202	X
Occ.134	a	---	Virt.144	a	-0.19771	X
Occ.134	a	---	Virt.145	a	-0.14774	X
Occ.135	a	---	Virt.138	a	0.12435	X
Occ.135	a	---	Virt.141	a	-0.52101	X
Occ.135	a	---	Virt.142	a	-0.08122	X
Occ.135	a	---	Virt.143	a	0.39577	X
Occ.135	a	---	Virt.144	a	0.20396	X
Occ.135	a	---	Virt.145	a	-0.21511	X
Occ.136	a	---	Virt.141	a	0.08655	X
Occ.136	a	---	Virt.144	a	0.06839	X
Occ.136	a	---	Virt.145	a	-0.05857	X
Occ.136	a	---	Virt.147	a	0.05066	X

-----  
Root 25 singlet a 0.162981987 a.u. ( 4.4349674 eV)  
-----

Transition Moments X 0.35263 Y -0.27962 Z 0.02231  
Oscillator Strength 0.02206

Occ.134	a	---	Virt.140	a	-0.06291	X
Occ.134	a	---	Virt.141	a	-0.27306	X
Occ.134	a	---	Virt.142	a	0.29854	X
Occ.134	a	---	Virt.143	a	-0.17423	X
Occ.134	a	---	Virt.146	a	0.16717	X
Occ.134	a	---	Virt.147	a	0.05193	X
Occ.135	a	---	Virt.140	a	0.05585	X
Occ.135	a	---	Virt.141	a	-0.72775	X
Occ.135	a	---	Virt.142	a	-0.27725	X
Occ.135	a	---	Virt.143	a	-0.27276	X
Occ.135	a	---	Virt.144	a	-0.07348	X
Occ.135	a	---	Virt.147	a	0.09073	X
Occ.136	a	---	Virt.143	a	0.11235	X
Occ.136	a	---	Virt.144	a	-0.10259	X
Occ.136	a	---	Virt.145	a	0.08433	X
Occ.136	a	---	Virt.146	a	-0.05615	X
Occ.136	a	---	Virt.147	a	0.13301	X