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Electronic peculiarities of the excited states of $[RuN_5C]^+$ vs. $[RuN_6]^{2+}$ polypyridine complexes: insight from theory

Isabelle M. Dixon*, Fabienne Alary and Jean-Louis Heully

Table S1 : Optimized bond lengths (Å) computed with solvent effects for the singly oxidized species.

	$\mathbf{[RuN_6]^{3+}}$	$\mathbf{[RuN_5C]^{2+}}$
Ru-N1	2.059	2.049
Ru-N2	2.043	2.027
Ru-N3*	2.179	2.163
Ru-N4	2.059	2.142
Ru-N5	2.044	2.036
Ru-N6*	2.179	-
Ru-C	-	2.016

Table S2: NBO analysis of complexes $\mathbf{[RuN_6]^{2+}}$ and $\mathbf{[RuN_5C]^{+}}$ and their singly oxidized derivatives

		$\mathbf{[RuN_6]^{2+}}$	$\mathbf{[RuN_6]^{3+}}$	$\mathbf{[RuN_5C]^{+}}$	$\mathbf{[RuN_5C]^{2+}}$
Natural charges	Ru	+0.56	+0.93	+0.45	+0.75
	N1	-0.36	-0.38	-0.31	-0.33
	N2	-0.38	-0.41	-0.34	-0.40
	N3*	-0.38	-0.37	-0.36	-0.37
	N4	-0.36	-0.38	-0.41	-0.42
	N5	-0.38	-0.41	-0.35	-0.38
	N6*	-0.38	-0.37	-	-
	C	-	-	-0.05	-0.03
Wiberg bond indices	Ru-N1	0.44	0.44	0.49	0.44
	Ru-N2	0.42	0.40	0.48	0.43
	Ru-N3*	0.29	0.34	0.29	0.32
	Ru-N4	0.44	0.44	0.27	0.29
	Ru-N5	0.42	0.40	0.47	0.42
	Ru-N6*	0.29	0.34	-	-
	Ru-C	-	-	0.68	0.70
WBI/atom	Ru	3.03	2.85	3.48	3.07
	C	-	-	3.92	3.91