

Supporting Information (SI) for

**An efficient photo-switch system combining
dimethyldihydropyrene pyridinium core and ruthenium(II) bis-
terpyridine entities**

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1. Crystal data

Table S1. Crystal Data and Structure Refinement for 2_c^{2+}

Formula	$C_{40.67} H_{36.50} B_1 F_4 N_{4.33} O_{0.25}$
Fw (g mol^{-1})	676.72
Crystal system	triclinic
Space group	P -1
a (Å)	9.4076(19)
b (Å)	13.294(3)
c (Å)	16.108(3)
α (deg.)	112.22(3)
β (deg.)	97.06(3)
γ (deg.)	96.57(3)
V (Å ³) / Z	1822.1(6)/2
D_x (g cm^{-3})	1.233
μ (cm^{-1})	0.087
Crystal dim. (mm)	0.33 x 0.42 x 0.48
T (K)	200.0
θ range for coll. (deg.)	2.54 - 25.00
nb. of rflns. coll.	27321
Data/restraints/parameters	6289/164/622
$R(I)$ ^a all/ $R[I > 2\sigma(I)]$	0.0937/0.1298
Goodness of fit S	1.115
$\Delta\rho_{\text{min}}/\Delta\rho_{\text{max}}$ (e Å^{-3})	-0.447/0.919

$$^a R = \sum ||I_o| - |I_c|| / \sum |I_o|.$$

2. Additional NMR data

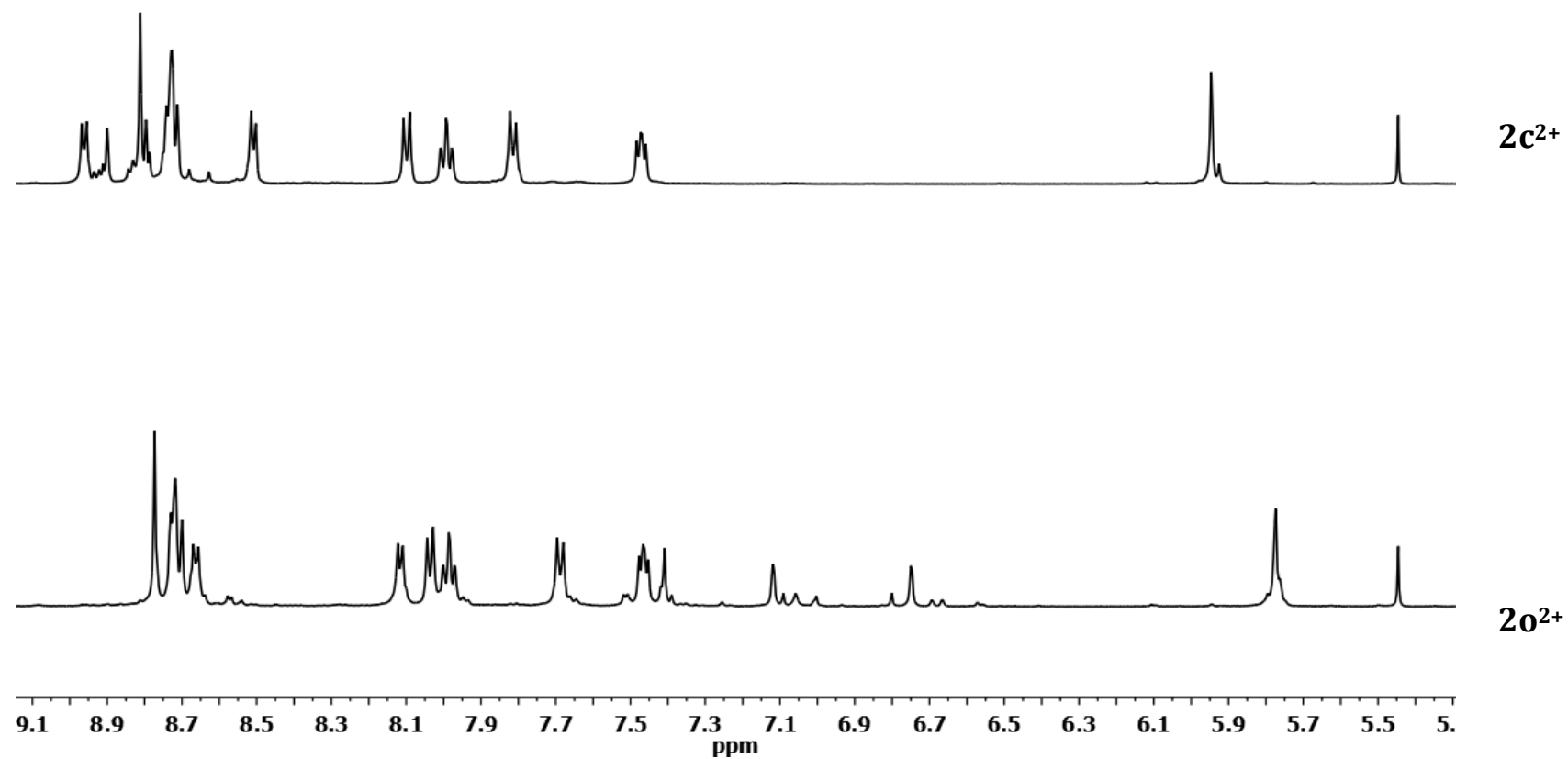


Figure S1: ^1H NMR spectrum for 2c^{2+} and 2o^{2+}

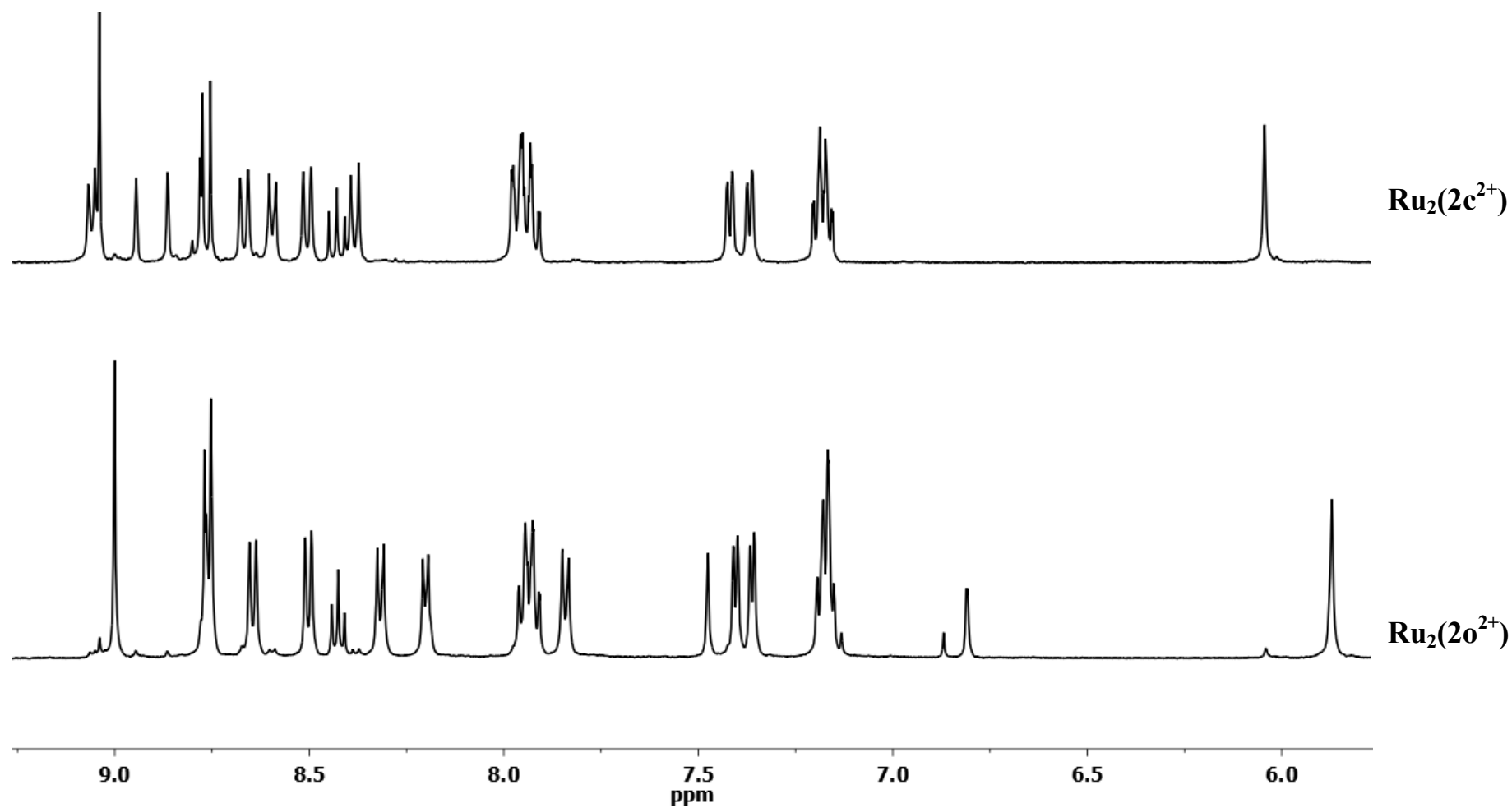
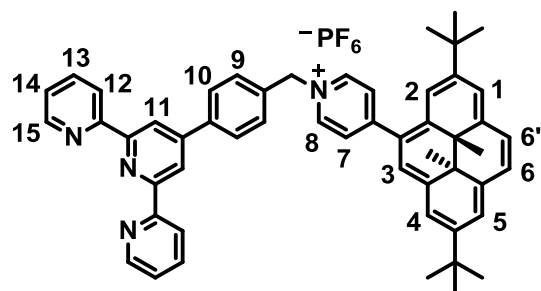


Figure S2 : ^1H NMR spectrum for $\text{Ru}_2(2\text{c}^{2+})$ and $\text{Ru}_2(2\text{o}^{2+})$

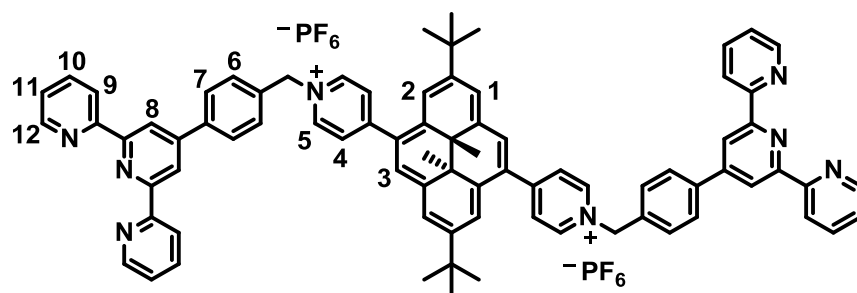
2,7-di-tert-butyl-4-(N-(4'-(4-methylphenyl)-2,2':6',2''-terpyridin-yl)pyridin-4-yl)-trans-10b,10c-dimethyl-10b,10c-dihydropyrene hexafluorophosphate (1c⁺)



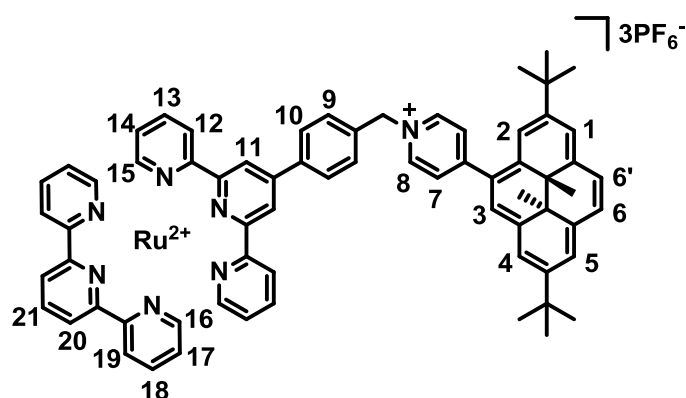
¹H NMR (500 MHz, 298 K, CD₃CN): δ (ppm) 8.91 (2H, d, *J* = 5 Hz, H₈); 8.80-8.60 (13H, m, H₁ + H₂ + H₃ + H₄ + H₅ + H₆ + H_{6'} + H₁₁ + H₁₂ + H₁₅); 8.51 (2H, d, *J* = 5 Hz, H₇); 8.09 (2H, d, *J* = 10 Hz, H₉); 7.99 (2H, t, *J* = 5 Hz, H₁₃); 7.80 (2H, d, *J* = 5 Hz, H₁₀); 7.47 (2H, dd, *J* = 5 Hz, H₁₄); 5.91 (2H, s, CH₂); 1.55 (9H, s, H_{tBu}); 1.53 (9H, s, H_{tBu}); -3.88 (3H, s, H_{Me}); -3.91 (3H, s, H_{Me}).

¹H NMR [CPD form] (500 MHz, 298 K, CD₃CN): δ (ppm) 8.76 (2H, s, H₁₁), 8.71 (4H, m, H₁₂ + H₁₅), 8.62 (2H, d, *J* = 6.5 Hz, H₈), 8.09 (2H, d, *J* = 6.5 Hz, H₇), 8.02 (2H, d, *J* = 8.0 Hz, H₁₀), 7.97 (2H, td, *J*_l = 5 Hz, H₁₃), 7.67 (2H, d, *J* = 8.0 Hz, H₉), 7.46 (2H, dd, *J*_l = 5 Hz, H₁₄), 7.34 (1H, s, H₃), 6.95 (1H, s, H₄), 6.94 (1H, s, H₁), 6.90 (1H, s, H₅), 6.61 (1H, s, H₂), 6.55 – 6.37 (2H, m, H₆ + H_{6'}), 5.75 (2H, s, H_{CH2}), 1.48 (3H, s, H_{Me}), 1.39 (3H, s, H_{Me}), 1.24 (9H, s, H_{tBu}), 1.21 (9H, s, H_{tBu}).

2,7-di-tert-butyl-4,9-di-(N-(4'-(4-methylphenyl)-2,2':6',2''-terpyridin-yl)pyridin-4-yl)-trans-10b,10c-dimethyl-10b,10c-dihydropyrene hexafluorophosphate (2c²⁺)



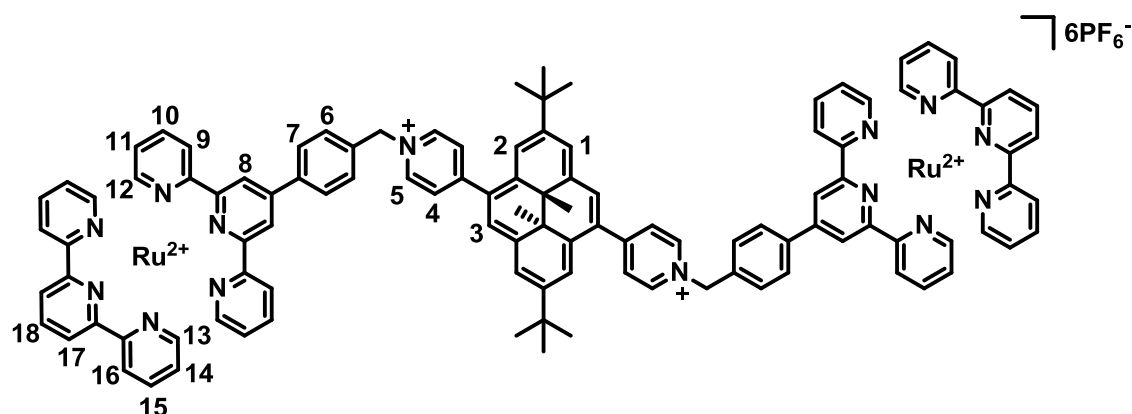
¹H NMR [CPD form] (500 MHz, 298 K, CD₃CN): δ (ppm) 8.77 (4H, s); 8.77 (4H, s, H₈), 8.75 – 8.69 (8H, m, H₉ + H₁₂), 8.66 (4H, d, *J* = 7 Hz, H₅), 8.11 (4H, d, *J* = 7 Hz, H₄), 8.04 (4H, d, *J* = 8 Hz, H₇), 7.98 (4H, td, *J* = 8 Hz, H₁₀), 7.69 (4H, d, *J* = 8 Hz, H₆), 7.47 (4H, dd, *J* = 8 Hz, H₁₁), 7.41 (2H, s, H₃), 7.12 (2H, s, H₂), 6.75 (2H, s, H₁), 5.77 (4H, s, H_{CH2}), 1.48 (6H, s, HMe), 1.20 (18H, s, H_{tBu}).



¹H NMR (500 MHz, 298 K, CD₃CN): δ (ppm) 9.03 (2H, s, H₁₁), 8.99 (2H, d, *J* = 5 Hz, H₈), 8.84 (1H, s, H₃), 8.82 (1H, s, H₂), 8.80 (2H, s, H₄ + H₅), 8.76 (2H, d, *J* = 8 Hz, H₂₀), 8.69 (1H, s, H₁), 8.67-8.64 (4H, m, H₆ + H₆ + H₁₂), 8.59 (2H, d, *J* = 5 Hz, H₇), 8.50 (2H, d, *J* = 8 Hz, H₁₉), 8.43 (1H, t, *J* = 8 Hz, H₂₁), 8.36 (2H, d, *J*₁ = 10, H₁₀), 7.98-7.90 (6H, m, H₉ + H₁₃ + H₁₈), 7.42 (2H, d, *J* = 5 Hz, H₁₅), 7.36 (2H, d, *J* = 5 Hz, H₁₆), 7.21-7.17 (4H, m, H₁₄ + H₁₇), 6.00 (2H, s, H_{CH2}), 1.71 (9H, s, H_{tBu}), 1.68 (9H, s, H_{tBu}), -3.80 (3H, s, H_{Me}), -3.85 (3H, s, H_{Me}).

^1H NMR [CPD form] (500 MHz, 298 K, CD_3CN): δ (ppm) 8.99 (2H, s, H_{11}), 8.76 (2H, d, $J = 10$ Hz, H_{20}), 8.69 (2H, d, $J = 5$ Hz, H_8), 8.64 (2H, d, $J = 10$ Hz, H_{12}), 8.50 (2H, d, $J = 10$ Hz, H_{19}), 8.42 (1H, t, $J = 10$ Hz, H_{21}), 8.30 (2H, d, $J = 10$ Hz, H_{10}), 8.17 (2H, d, $J = 5$ Hz, H_7), 7.96-7.91 (4H, m, $\text{H}_{13} + \text{H}_{18}$), 7.81 (2H, d, $J = 5$ Hz, H_9), 7.41 – 7.37 (3H, m, $\text{H}_{15} + \text{H}_3$), 7.5 (2H, d, $J = 5$ Hz, H_{16}), 7.24 – 7.11 (4H, m, $\text{H}_{14} + \text{H}_{17}$), 6.97 (2H, s, $\text{H}_4 + \text{H}_5$), 6.92 (1H, s, H_2), 6.66 (1H, s, H_1), 6.52 (1H, d, $J = 10$ Hz, H_6), 6.48 (1H, d, $J = 10$ Hz, H_6), 5.84 (2H, s, H_{CH_2}), 1.51 (3H, s, H_{Me}), 1.42 (3H, s, H_{Me}), 1.26 (9H, s, H_{tBu}), 1.23 (9H, s, H_{tBu}).

$[\text{Ru}_2(2\text{c}^{2+})][6\text{PF}_6^-]$

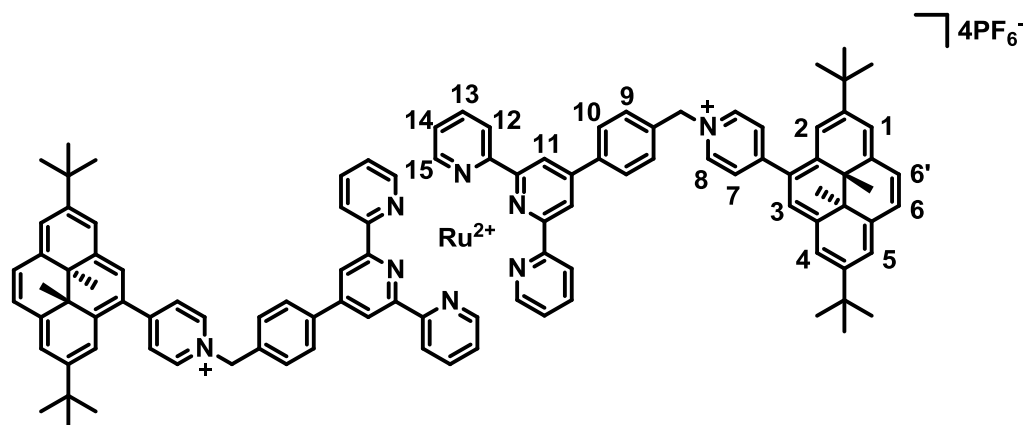


^1H NMR (400 MHz, 298 K, CD_3CN): δ (ppm) 9.10 – 9.01 (8H, m, $\text{H}_5 + \text{H}_8$), 8.95 (2H, s, H_3), 8.86 (2H, s, H_2), 8.78 (2H, s, H_1), 8.76 (4H, d, $J = 8$ Hz, H_{17}), 8.66 (4H, d, $J = 8$ Hz, H_9), 8.60 (4H, d, $J = 8$ Hz, H_5), 8.51 (4H, d, $J = 8$ Hz, H_{16}), 8.43 (2H, t, $J = 8$ Hz, H_{18}), 8.38 (4H, d, $J = 8$ Hz, H_7), 8.02 – 7.88 (12H, m, $\text{H}_6 + \text{H}_{10} + \text{H}_{15}$), 7.42 (4H, d, $J = 8$ Hz, H_{12}), 7.37 (4H, d, $J = 8$ Hz, H_{13}), 7.21-7.15 (8H, m, $\text{H}_{11} + \text{H}_{14}$), 6.04 (4H, s, H_{CH_2}), 1.69 (18H, s, H_{tBu}), -3.57 (6H, s, H_{Me}).

^1H NMR [CPD form] (500 MHz, 298 K, CD_3CN): δ (ppm) 9.00 (4H, s, H_8), 8.76 (8H, m, $\text{H}_{17} + \text{H}_5$), 8.65 (4H, d, $J = 8$ Hz, H_9), 8.50 (4H, d, $J = 8$ Hz, H_{16}), 8.43 (2H, t, $J = 8$ Hz, H_{18}), 8.32 (4H, d, $J = 8$ Hz, H_7), 8.18 (4H, d, $J = 8$ Hz, H_4), 7.96-7.91 (8H, m, $\text{H}_{10} + \text{H}_{15}$), 7.84 (4H, d, $J = 8$ Hz, H_6), 7.48 (2H, s, H_3), 7.41 (4H, d, $J = 5$ Hz, H_{12}), 7.37 (4H, d, $J = 5$ Hz, H_{13}),

7.20 – 7.15 (10H, m, $H_{11} + H_{14} + H_2$), 6.81 (2H, s, H_1), 5.87 (4H, s, H_{CH_2}), 1.5 (6H, s, H_{Me}),
1.26 (18H, s, H_{tBu})

[Ru(1c**⁺)₂][4PF₆[−]]**



¹H NMR (500 MHz, 298K, CD₃CN) : δ (ppm) 9.05 (4H, s, H_{11}), 8.99 (4H, d, J = 6.85 Hz, H_8), 8.84 (2H, s, H_3), 8.82 (2H, s, H_2), 8.80 (4H, s, $H_4 + H_5$), 8.69-8.62 (10H, m, $H_1 + H_6 + H_6' + H_{10}$), 8.58 (4H, d, J = 6.85 Hz, H_7), 8.37 (4H, d, J = 8.4 Hz, H_{12}), 7.98-7.94 (8H, m, $H_9 + H_{13}$), 7.45 (4H, d, J = 5.55 Hz, H_{15}), 7.21-7.18 (4H, m, H_{14}), 6.00 (4H, s, H_{CH_2}), 1.70 (18H, s, H_{tBu}), 1.68 (18H, s, H_{tBu}), -3.80 (6H, s, H_{Me}), -3.85 (6H, s, H_{Me}).

¹H NMR [CPD form] (500 MHz, 298K, CD₃CN) : δ (ppm) 9.01 (4H, s, H_{11}), 8.70 (4H, d, J = 6.75 Hz, H_8), 8.65 (4H, d, J = 8 Hz, H_{12}), 8.31 (4H, d, J = 8.25 Hz, H_{10}), 8.17 (4H, d, J = 7 Hz, H_7), 7.96 (4H, t, J = 8 Hz, H_{13}), 7.82 (4H, d, J = 8.3 Hz, H_9), 7.43 (4H, d, J = 5.5 Hz, H_{15}), 7.39 (2H, s, H_3), 7.20 – 7.18 (4H, m, H_{14}), 6.98-6.97 (4H, m, $H_4 + H_5$), 6.92 (2H, s, H_2), 6.66 (2H, s, H_1), 6.52 (2H, d, J = 11 Hz, $H_{6'}$), 6.48 (2H, d, J = 11 Hz, H_6), 5.84 (4H, s, H_{CH_2}), 1.51 (6H, s, H_{Me}), 1.42 (6H, s, H_{Me}), 1.26 (18H, s, H_{tBu}), 1.23 (18H, s, H_{tBu}).

Table S2. B3LYP/6-311G(d,p) Cartesian coordinates and energy for S₀ **2c²⁺**_{model} in the same conformation as the X-ray structure.

N	1.583391330249	5.960207116502	2.997504783673	N	2.319943985140	-15.776573039760	-0.124743899836
C	0.969536178961	3.469621013522	1.871097737561	C	0.967628657056	-15.810776008168	-2.110506035583
C	2.222757498029	4.844841232170	3.421354873193	C	0.133978255395	-13.781999172626	5.114965543825
H	2.969241377396	4.983610357809	4.192312842180	C	-2.115759953391	-13.002725813998	4.911970291987
C	1.899408141858	7.286187123074	3.676506608024	H	-2.684487958371	-12.551588121423	2.882689792139
H	1.363129723493	7.269981219479	4.627248903463	C	2.992548391647	-16.821232859472	-0.605493337972
H	2.969515946327	7.254059754441	3.882887190660	H	0.135696861748	-15.400159088439	-2.670445265802
C	0.065332900743	1.226142217511	-2.826832072036	C	1.674836221599	-16.905798902034	-2.597275663277
H	0.012155066388	0.996801270577	-3.885818216891	C	-1.082166279506	-13.462933493335	5.719358957074
C	0.477203865495	2.489275400167	-2.418370046799	H	0.965954409069	-14.145038807614	5.711890720186
C	0.392111747776	1.907670846266	-0.047221151188	H	-3.083636276129	-12.758654185805	5.335011087177
C	0.474520318526	1.090086652885	2.262582281502	C	2.712533896804	-17.424432762710	-1.831854614127
H	0.530179437143	1.314063769359	3.322749076263	H	3.7963398542001	-17.197176505293	0.021152269945
C	0.625061991816	2.140472629522	1.335275234281	H	1.411858534187	-17.350747768765	-3.550101486714
C	0.676870913753	2.806205431928	-1.066149807876	H	-1.210933576628	-13.581869393822	6.788322759098
H	1.122105478692	3.765852143919	-0.835123968278	H	3.289738875028	-18.277258621079	-2.167728366232
C	1.938929363051	3.610075262585	2.886413433772				
H	2.493977736902	2.752648507816	3.242508486446				
C	-1.815709087020	0.814437292129	-0.133083269346				
H	-2.183580526395	1.617497816037	-0.773311649707				
H	-1.988501386440	1.093689988216	0.906542984172				
H	-2.392527289475	-0.085249849542	-0.352036774339				
C	-0.289389836680	0.583536986804	-0.418139389995				
C	0.644464536283	5.866296693500	2.030903878278				
H	0.162494534994	6.790651505050	1.744947362077				
C	0.326597889414	4.652268640977	1.460117045218				
H	-0.454821686456	4.626747276190	0.713604428730				
C	-0.202169755167	0.223947738974	1.892990489734				
N	-1.583391330249	5.960207116502	2.997504783673				
C	0.969536178961	3.469621013522	1.871097737561				
C	2.222757498029	4.844841232170	3.421354873193				
H	2.969241377396	4.983610357809	4.192312842180				
C	1.899408141858	7.286187123074	3.676506608024				
H	1.363129723493	7.269981219479	4.627248903463				
H	2.969515946327	7.254059754441	3.882887190660				
C	0.065332900743	1.226142217511	-2.826832072036				
H	0.012155066388	0.996801270577	-3.885818216891				
C	0.477203865495	2.489275400167	-2.418370046799				
C	0.392111747776	1.907670846266	-0.047221151188				
C	0.474520318526	1.090086652885	2.262582281502				
H	0.530179437143	1.314063769359	3.322749076263				
C	0.625061991816	2.140472629522	1.335275234281				
C	0.676870913753	2.806205431928	-1.066149807876				
H	1.122105478692	3.765852143919	-0.835123968278				
C	1.938929363051	3.610075262585	2.886413433772				
H	2.493977736902	2.752648507816	3.242508486446				
C	-1.815709087020	0.814437292129	-0.133083269346				
H	-2.183580526395	1.617497816037	-0.773311649707				
H	-1.988501386440	1.093689988216	0.906542984172				
H	-2.392527289475	-0.085249849542	-0.352036774339				
C	-0.289389836680	0.583536986804	-0.418139389995				
C	0.644464536283	5.866296693500	2.030903878278				
H	0.162494534994	6.790651505050	1.744947362077				
C	0.326597889414	4.652268640977	1.460117045218				
H	-0.454821686456	4.626747276190	0.713604428730				
C	-0.202169755167	0.223947738974	1.892990489734				
N	-1.583391330249	5.960207116502	2.997504783673				
C	0.969536178961	3.469621013522	1.871097737561				
C	2.222757498029	4.844841232170	3.421354873193				
H	2.969241377396	4.983610357809	4.192312842180				
C	1.899408141858	7.286187123074	3.676506608024				
H	1.363129723493	7.269981219479	4.627248903463				
H	2.969515946327	7.254059754441	3.882887190660				
C	0.065332900743	1.226142217511	-2.826832072036				
H	0.012155066388	0.996801270577	-3.885818216891				
C	0.477203865495	2.489275400167	-2.418370046799				
C	0.392111747776	1.907670846266	-0.047221151188				
C	0.474520318526	1.090086652885	2.262582281502				
H	0.530179437143	1.314063769359	3.322749076263				
C	0.625061991816	2.140472629522	1.335275234281				
C	0.676870913753	2.806205431928	-1.066149807876				
H	1.122105478692	3.765852143919	-0.835123968278				
C	1.938929363051	3.610075262585	2.886413433772				
H	2.493977736902	2.752648507816	3.242508486446				
C	-1.815709087020	0.814437292129	-0.133083269346				
H	-2.183580526395	1.617497816037	-0.773311649707				
H	-1.988501386440	1.093689988216	0.906542984172				
H	-2.392527289475	-0.085249849542	-0.352036774339				
C	-0.289389836680	0.583536986804	-0.418139389995				
C	0.644464536283	5.866296693500	2.030903878278				
H	0.162494534994	6.790651505050	1.744947362077				
C	0.326597889414	4.652268640977	1.460117045218				
H	0.454821686456	4.626747276190	0.713604428730				
C	0.202169755167	-0.223947738974	1.892990489734				
H	2.392527289475	0.085249849542	0.352036774339				
H	0.717083277909	3.233975741206	-3.168091030686				
H	-0.717083277909	-3.233975741206	3.168091030686				
C	1.535160653443	8.493553885006	2.865931551646				
C	0.333266635505	9.170699902741	3.099640001932				
C	2.399161892447	8.974943355535	1.874758547758				
C	-0.005282373358	10.289717036102	2.347984300486				
H	-0.342592472415	8.826672722970	3.876491032352				
C	2.060073314453	10.094573518676	1.127387543970				
H	3.352607746904	8.486411785893	1.699533827063				
C	0.848629520762	10.771469514173	1.344480566382				
H	-0.949174807425	10.787958283737	2.531342227955				
H	2.755261791663	10.470323564741	0.386781275945				
C	-1.535160653443	-8.493553885006	-2.865931551646				
C	-2.399161892447	-8.974943355535	-1.874758547758				
C	-0.333266635505	-9.170699902741	-3.099640001932				
C	-2.060073314453	-10.094573518677	-1.127387543970				
H	-3.352607746904	-8.486411785893	-1.699533827063				
C	0.005282373358	-10.289717036102	-2.347984300486				
H	-0.342592472415	-8.826672722970	-3.876491032352				
C	-0.848629520762	-10.771469514173	-1.344480566382				
H	-2.755261791663	-10.470323564741	-0.386781275945				
H	0.949174807425	10.787958283737	-2.531342227955				
C	0.479294715440	11.959154695935	0.536464783175				
C	-0.206962510475	13.035867730849	1.102950447638				
C	0.774517202264	12.023947326107	-0.827938653064				
H	-0.587510378470	14.111029171857	0.290758238139				
H	-0.448682163873	13.045171545541	2.158416592321				
C	0.352399435719	13.135099829550	-1.567411077948				
H	1.271281752718	11.201351899815	-1.327614369375				
N	-0.324089934038	14.147535143945	-0.1018740296782				
C	-1.323761001934	15.277288361753	0.866730887976				
C	0.636411206355	13.228065658605	-3.032121825816				
N	-2.319943985140	15.776573039760	0.124743899836				
C	-0.967628657056	15.810776008168	2.110506035583				
N	-0.360590731220	13.673572265273	-3.806550910785				
C	1.891015264643	12.878597647847	-3.544451103187				
C	-2.992548391647	16.821232859472	0.605493337972				
C	-1.674836221599	16.905798902034	2.597275663277				
H	-0.135696861748	15.400159088439	2.670445265802				
C	-0.133978255395	13.781999172626	-5.114965543825				
H	2.684487958371	12.551588121423	-2.882689792139				
C	2.115759953391	13.002725813998	-4.911970291987				
C	-2.712533896804	17.424432762710	1.831854614127				
H	-3.7963398542001	17.197176505293	-0.021152269945				
H	-1.411858534187	17.350747768765	3.550101486714				
C	1.082166279506	13.462933493335	-5.719358957074				
H	-0.965954409069	14.145038807614	-5.711890720186				
H	3.083636276129	12.758654185805	-5.335011087177				
H	3.289738875028	18.277258621079	2.167728366232				
H	1.210933576628	13.581869393822	-6.788322759098				
C	-0.479294715440	-11.959154695935	-0.536464783175				
C	-0.774517202264	-12.023947326107	0.827938653064				
C	0.206962510475	-13.035867730849	-1.102950447638				

Table S2 (continued). B3LYP/6-311G(d,p) Cartesian coordinates and energy for S_0 $2c^{2+}$,_{model} lowest energy structure.

N	-1.368469592479	2.875966728169	6.071969028295	N	-2.706352285624	2.235087237613	-14.324596501050
C	-0.761806956026	1.612905347273	3.646122234018	C	-3.594507060512	0.055481404722	-13.843791709053
C	-0.370100921180	1.967975806796	6.013079393887	C	2.934722203460	2.855853628969	-16.346386612345
H	0.152980240856	1.775498264982	6.939460101270	C	4.137568919400	0.791054763287	-16.364909283012
C	-1.682581236279	3.617034910195	7.361648722552	H	3.245225371281	-0.730682748193	-15.127926944672
H	-1.118950622665	4.551129864265	7.322084835902	C	-3.937213217119	2.627402086799	-14.650319542022
H	-2.745261862036	3.854112392140	7.303481802029	H	-3.414555666994	-0.971177004093	-13.547170061910
C	-0.161073148440	2.692843251814	-1.490672534016	C	-4.873729501859	0.477232605253	-14.192605911080
H	-0.004672953080	3.178163328167	-2.448203760333	C	4.011463689167	2.100962971150	-16.812114701686
C	-0.356910834075	3.467103262861	-0.353070541714	H	2.802239269814	3.883685852472	-16.672340192276
C	-0.435807371852	1.526373741609	1.128779031085	H	4.949818351722	0.162150953142	-16.711002462875
C	-0.258848662104	-0.503269612116	2.492676154704	C	-5.053890657972	1.792544451961	-14.604197240065
H	-0.411357367784	-0.992281518265	3.449075805074	H	-4.037115235800	3.661908043014	-14.966742856507
C	-0.464845317824	0.887651233282	2.397990062138	H	-5.709456536417	-0.212323211231	-14.156565606287
C	-0.447248929814	2.899593964318	0.927103378996	H	4.721646021293	2.530395952411	-17.508206115342
H	-0.466303456184	3.572718050727	1.775185764697	H	-6.029619797993	2.165727889937	-14.890664417536
C	-0.054709704548	1.333086051494	4.831489494468				
H	0.764357436998	0.626523653142	4.830902997494				
C	-1.965628621888	0.196472492637	-0.274546216879				
H	-2.566903113552	1.088355591122	-0.456699230612				
H	-2.344881501369	-0.300622381800	0.618634367757				
C	-2.088958599500	-0.475197547328	-1.125262679591				
C	-0.461692618280	0.612527111863	-0.103767744374				
C	-2.075620583420	3.168159119964	4.954737174250				
H	-2.875798855053	3.887354742315	-5.068614386054				
C	-1.797751482546	2.563839504464	3.750469606611				
H	-2.417548399978	2.804227447458	-2.898051103182				
C	-0.081240741998	1.301988269081	-1.404644904298				
N	1.368469592479	2.875966728169	-6.071969028295				
C	0.761806956026	1.612905347273	-3.646122234018				
C	0.370100921180	1.967975806796	-6.013079393887				
H	0.152980240856	1.775498264982	-6.939460101270				
C	-1.682581236279	3.617034910195	-7.361648722552				
H	-1.118950622665	4.551129864265	-7.322084835902				
H	-2.745261862036	3.854112392140	-7.303481802029				
C	0.161073148440	2.692843251814	1.490672534016				
H	0.004672953080	3.178163328167	2.448203760333				
C	0.356910834075	3.467103262861	0.353070541714				
C	0.435807371852	1.526373741609	-1.128779031085				
C	0.258848662104	0.503269612116	-2.492676154704				
H	0.411357367784	0.992281518265	-3.449075805074				
C	0.464845317824	-0.887651233282	-2.397990062138				
C	0.447248929814	-2.899593964318	-0.927103378996				
H	0.466303456184	-3.572718050727	-1.775185764697				
C	0.054709704548	-1.333086051494	-4.831489494468				
H	-0.764357436998	-0.626523653142	-4.830902997494				
C	1.965628621888	-0.196472492637	0.274546216879				
H	2.566903113552	-1.088355591122	0.456699230612				
H	2.344881501369	0.300622381800	-0.618634367757				
C	0.461692618280	-0.612527111863	0.103767744374				
C	2.075620583420	3.168159119964	-4.954737174250				
H	2.875798855053	-3.887354742315	-5.068614386054				
C	1.797751482546	-2.563839504464	-3.750469606611				
H	2.417548399978	-2.804227447458	-2.898051103182				
C	0.081240741998	-1.301988269081	1.404644904298				
H	2.088958599500	0.475197547328	1.125262679591				
H	-0.372566370172	4.546609142085	-0.445999223304				
H	0.372566370172	-4.546609142085	0.445999223304				
C	-1.359831621309	2.837191641468	8.602121999210				
C	-0.220144598758	3.137590268219	9.355178396837				
C	-2.203460322709	1.806883411518	9.035174038507				
C	0.076658434683	2.416216096033	10.506520439386				
H	0.429148269713	3.954451574935	9.055827459096				
C	-1.901957098381	1.084786386060	10.181022380419				
H	-3.102343706070	1.566128271534	8.476004571454				
C	-0.753775617295	1.371985400298	10.938156310477				
H	0.947417879610	2.683823292571	11.092233869708				
H	-2.55504996442	0.278219370340	10.489696802727				
C	1.359831621309	2.837191641468	-8.602121999210				
C	2.203460322709	-1.806883411518	-9.035174038507				
C	0.220144598758	-3.137590268219	-9.355178396837				
C	1.901957098381	-1.084786386060	-10.181022380419				
H	3.102343706070	-1.566128271534	-8.476004571454				
C	-0.076658434683	-2.416216096033	-10.506520439386				
H	-0.429148269713	-3.954451574935	-9.055827459096				
C	0.753775617295	-1.371985400298	-10.938156310477				
H	2.55504996442	-0.278219370340	-10.489696802727				
H	-0.947417879610	-2.683823292571	-11.092233869708				
C	-0.431521687558	0.587821267681	12.155247141072				
C	0.886209801434	0.236212231414	12.459162474283				
C	-1.436593486905	0.144393314951	13.018048474492				
C	1.140747261919	-0.558459238228	13.583417831871				
H	1.700733322882	0.520827173409	11.804457782950				
C	-1.092959887833	-0.641828805782	14.124362072782				
H	-2.473512745980	0.399803570118	12.838535111109				
N	0.168213415063	-0.995608869848	14.387921935361				
C	2.536787682230	-0.968186357794	13.926382287572				
C	-2.144974676326	-1.130663943210	15.066990129747				
N	2.706352285624	-2.235087237613	14.324596501050				
C	3.594507060512	-0.055481404722	13.843791709053				
N	-2.018094668811	-2.391672507884	15.498266836241				
C	-3.190973238193	-0.294778312464	15.473966176722				
C	3.937213217119	-2.627402086799	14.650319542022				
C	4.873729501859	-0.477232605253	14.192605911080				
H	3.414555666994	0.971177004093	13.547170061910				
C	-2.934722203460	-2.855853628969	16.346386612345				
H	3.245225371281	0.730682748193	15.127926944672				
C	-4.137568919400	-0.791054763287	16.364909283011				
C	5.053890657972	-1.792544451961	14.604197240065				
H	4.037115235800	-3.661908043014	14.966742856507				
H	5.709456536417	0.212323211231	14.156565606287				
C	-4.011463689167	-2.100962971150	16.812114701686				
H	-2.802239269814	-3.883685852472	16.672340192276				
H	-4.949818351722	-0.162150953142	16.711002462875				
H	6.029619797993	-2.165727889937	14.890664417536				
H	-4.721646021293	-2.530395952411	17.508206115342				
C	0.431521687558	-0.587821267681	-12.155247141072				
C	1.436593486905	-0.144393314951	-13.018048474492				
C	-0.886209801434	-0.236212231414	-12.459162474283				
C	1.092959887833	0.641828805782	-14.124362072782				
H	2.473512745980	-0.399803570118	-12.838535111109				
C	-1.140747261919	0.558459238228	-13.583417831871				
H	-1.700733322882	-0.520827173409	-11.804457782950				
N	-0.168213415063	0.995608869848	-14.387921935361				
C	2.144974676326	1.130663943210	-15.066990129747				
C	-2.536787682230	0.968186357794	-13.926382287572				
N	2.018094668811	2.391672507884	-15.498266836241				
C	3.190973238193	0.294778312464	-15.473966176722				

B3LYP energy:

E(S₀) = -3214.429573 a.u.

CAM-B3LYP energy:

E(S₀) = -3212.623421 a.u.

Table S2 (continued). B3LYP/6-311G(d,p) Cartesian coordinates and energy for S_0 Z_{o}^{2+} ,_{model}.

N	-1.971969614907	2.363269156863	6.033875203926	N	-3.478669220807	0.893499743452	-14.426652975029
C	-0.908306435395	1.360211402108	3.642206056009	C	-3.550039797542	-1.455700299632	-13.929701899853
C	-0.711277598604	1.876375237775	6.003084817447	C	1.621520973128	3.443282001752	-16.376076533356
H	-0.170136081764	1.900295093324	6.938733461054	C	3.473562385858	1.933455825749	-16.345086069905
C	-2.552437255079	2.960906640599	7.304518472999	H	3.149875284303	0.207066721334	-15.097256983612
H	-2.353964555367	4.033405531929	7.257883227018	C	-4.762314448341	0.823791916980	-14.776596428494
H	-3.629124064848	2.807226517778	7.226922289665	H	-3.025261669941	-2.350529027726	-13.616189006827
C	-0.876270576718	2.428909628370	-1.504145736796	C	-4.888827065635	-1.515130770330	-14.303998112194
H	-0.770219812549	2.815739585163	-2.511895400993	C	2.903482817302	3.110909643803	-16.814523348606
C	-0.809107625630	3.297748288764	-0.420698346361	H	1.142359329410	4.355644627485	-16.719935185063
C	-0.875335145412	1.384240980750	1.081318704942	H	4.461405733443	1.627115793260	-16.669706122022
C	0.541551358614	-0.197435437197	2.428573933955	C	-5.513386296026	-0.351089142705	-14.736255113973
H	0.809803599353	-0.573555991794	3.412235778037	H	-5.214596910220	1.754108698695	-15.108632915188
C	-0.393215960514	0.802956849490	2.382086043330	H	-5.428176469547	-2.454950000060	-14.271382854249
C	-0.703484494702	2.760759792696	0.858231875041	H	3.430347387097	3.755940975764	-17.507103602949
H	-0.454628126209	3.411262417498	1.689670874541	H	-6.552349206265	-0.348374648017	-15.042721555043
C	-0.163821330965	1.385315045052	4.839500580251				
H	0.861528092013	1.043096011555	4.867940656406				
C	-1.922348679549	-0.771629710750	0.212986941380				
H	-3.001411298479	-0.591247721188	0.140566989513				
H	-1.732642515372	-1.199315824385	1.195064631320				
H	-1.678116727731	-1.509610611236	-0.548184043454				
C	-1.236331493886	0.551280242311	0.002051602683				
C	-2.710838658877	2.377789769247	-4.899271604169				
H	-3.711261826973	2.780915944613	-4.983670116767				
C	-2.210532025124	1.899037461431	3.711503927651				
H	-2.840650521110	1.928891730370	2.833005955869				
C	-0.992054297629	1.042021877343	-1.306126925094				
N	1.971969614907	-2.363269156863	-6.033875203926				
C	0.908306435395	-1.360211402108	-3.642206056009				
C	0.711277598604	-1.876375237775	-6.003084817447				
H	0.170136081764	-1.900295093324	-6.938733461054				
C	2.552437255079	-2.960906640599	-7.304518472999				
H	2.353964555367	-4.033405531929	-7.257883227018				
H	3.629124064848	-2.807226517778	-7.226922289665				
C	0.876270576718	-2.428909628370	1.504145736796				
H	0.770219812549	-2.815739585163	2.511895400993				
C	0.809107625630	-3.297748288764	0.420698346361				
C	0.875335145412	-1.384240980750	-1.081318704942				
C	-0.541551358614	0.197435437197	-2.428573933955				
H	-0.809803599353	0.573555991794	-3.412235778037				
C	0.393215960514	-0.802956849490	-2.382086043330				
C	0.703484494702	-2.760759792696	-0.858231875041				
H	0.454628126209	-3.411262417498	-1.689670874541				
C	0.163821330965	-1.385315045052	-4.839500580251				
H	-0.861528092013	-1.043096011555	-4.867940656406				
C	1.922348679549	0.771629710750	-0.212986941380				
H	3.001411298479	0.591247721188	-0.140566989513				
H	1.732642515372	1.199315824385	-1.195064631320				
C	1.236331493886	-0.551280242311	-0.002051602683				
C	2.710838658877	-2.377789769247	-4.899271604169				
H	3.711261826973	-2.780915944613	-4.983670116767				
C	2.210532025124	-1.899037461431	-3.711503927651				
H	2.840650521110	-1.928891730370	-2.833005955869				
C	0.992054297629	-1.042021877343	1.306126925094				
H	1.678116727731	1.509610611236	0.548184043454				
H	-0.732928539720	4.366323102967	-0.577804259950				
H	0.732928539720	-4.366323102967	0.577804259950				
C	-2.000142696736	2.358464850207	8.563034970657				
C	-1.058741200697	3.052056935285	9.330396289936				
C	-2.430890339247	1.099274639293	8.998492627041				
C	-0.549625041747	2.944418489116	10.498327804200				
H	-0.736530184262	4.043899891026	9.028919850947				
C	-1.917245306366	0.542664323636	10.161086808444				
H	-3.172644760314	0.548921295706	8.427938449686				
C	-0.963242479086	1.227022696633	10.932797840449				
H	0.156049580603	3.059931765634	11.094271312291				
H	-2.247392955495	-0.440851424803	10.472020418641				
C	2.000142696736	-2.358464850207	-8.563034970657				
C	2.430890339247	-1.099274639293	-8.998492627041				
C	1.058741200697	-3.052056935285	-9.330396289936				
C	1.917245306366	-0.542664323636	-10.161086808444				
H	3.172644760314	-0.548921295706	-8.427938449686				
C	0.549625041747	-2.944418489116	-10.498327804200				
H	0.736530184262	-4.043899891026	-9.028919850947				
C	0.963242479086	-1.227022696633	-10.932797840449				
H	2.247392955495	0.440851424803	-10.472020418641				
H	-0.156049580603	-3.059931765634	-11.094271312291				
C	-0.409599387752	0.620037526748	12.167766581993				
C	0.940961203827	0.759807148692	12.497632022868				
C	-1.210648507059	-0.141203385783	13.022198631235				
C	1.437047804079	0.116978286872	13.638211034489				
H	1.615514658528	1.307519949392	11.851025526059				
C	-0.633971969727	-0.744159524484	14.146465441528				
H	-2.267109315842	-0.270394583592	12.822466081918				
N	0.665418780413	-0.627440382754	14.434824572844				
C	2.880915757969	0.229082907625	14.008509636696				
C	-1.464624683398	-1.562931851467	15.081285271631				
N	3.478669220807	-0.893499743452	14.426652975029				
C	3.550039797542	1.455700299632	13.929701899853				
N	-0.910723867494	-2.694525444304	15.533989390534				
C	-2.745205130522	-1.144539889534	15.460087280301				
C	4.762314448341	-0.823791916980	14.776596428494				
C	4.888827065635	1.515130770330	14.303998112194				
H	3.025261669941	2.350529027726	13.616189006827				
C	-1.621520973128	-3.443282001752	16.376076533356				
H	-3.149875284303	0.207066721334	15.097256983612				
C	-3.473562385858	-1.933455825749	16.345086069905				
C	5.513386296026	0.351089142705	14.736255113973				
H	5.214596910220	-1.754108698695	15.108632915188				
H	5.428176469547	2.454950000060	14.271382854249				
C	-2.903482817302	-3.110909643803	16.814523348606				
H	-1.142359329410	-4.355644627485	16.719935185063				
H	-4.461405733443	-1.627115793260	16.669706122022				
H	6.552349206265	0.348374648017	15.042721555043				
H	-3.430347387097	-3.755940975764	17.507103602949				
C	0.409599387752	-0.620037526748	-12.167766581993				
C	1.210648507059	0.141203385783	-13.022198631235				
C	-0.940961203827	-0.759807148692	-12.497632022868				
C	0.633971969727	0.744159524484	-14.146465441528				
H	2.267109315842	0.270394583592	-12.822466081918				
C	-1.437047804079	-0.116978286872	-13.638211034489				
H	-1.615514658528	-1.307519949392	-11.851025526059				
N	-0.665418780413	0.627440382754	-14.434824572844				
C	1.464624683398	1.562931851467	-15.081285271631				
C	-2.880915757969	-0.229082907625	-14.008509636696				
N	0.910723867494	2.694525444304	-15.533989390534				
C	2.745205130522	1.144539889534	-15.460087280301				

B3LYP energy:

E(S_0) = -3214.402171 a.u.

Table S2 (continued). UB3LYP/6-311G(d,p) Cartesian coordinates and energies for S_0 transition state between $2c^{2+}_{\text{model}}$ and $2o^{2+}_{\text{model}}$.

N	-2.294935379883	2.171938422129	6.046257396821	N	-3.516512196915	0.412559598248	-14.428603947632
C	-1.129815714928	1.284734117242	3.650309730211	C	-3.302360628359	-1.929140860476	-13.937433575725
C	-0.981265920467	1.848201585972	6.007144076238	C	1.235928144432	3.564448789779	-16.373214547947
H	-0.438953073974	1.952087694364	6.936535315364	C	3.259164195435	2.293293726631	-16.341568910788
C	-2.933483468341	2.706343781238	7.313854657611	H	3.148476860861	0.538769425685	-15.096027927254
H	-2.854795026859	3.794323486597	7.266096087164	C	-4.782284971578	0.188492686374	-14.778896892512
H	-3.987413500519	2.436067387335	7.241088133770	H	-2.672915136606	-2.754459051349	-13.625927491907
C	-1.467941435213	2.185489890799	-1.537994075487	C	-4.624102713663	-2.149599672372	-14.312027798957
H	-1.567078208964	2.589662949831	-2.539890026042	C	2.549405282852	3.392408353010	-16.810578038726
C	-1.686097593951	3.007635030808	-0.438058956572	H	0.648777220830	4.411522938378	-16.716702441506
C	-1.039618049408	1.220142164207	1.090404264226	H	4.277483973399	2.110835294870	-16.665297909854
C	0.472701919382	-0.164144774583	2.494699189781	C	-5.385329822339	-1.068871447919	-14.741565602145
H	0.749351153940	-0.539140919740	3.474874878840	H	-5.344117437836	1.057897485700	-15.108749293788
C	-0.539382324927	0.770706088269	2.415554164729	H	-5.045458437455	-3.147985893843	-14.281744087220
C	-1.386446435642	2.538840049653	0.857424722883	H	2.993822388884	4.097955732606	-17.501969384977
H	-1.407303467121	3.243983117829	1.680849632977	H	-6.416993498414	-1.191457670075	-15.048197633401
C	-0.386811528462	1.416043602932	4.845224760165				
H	0.673442256167	1.204539408651	4.866609387080				
C	-1.721158768874	-1.044034297168	0.150261577010				
H	-2.797451202396	-0.850798909695	0.104045144151				
H	-1.505822811062	-1.506554453919	1.112709802159				
H	-1.481553261844	-1.753069933346	-0.641396146054				
C	-0.991884584255	0.283640879740	-0.030141766399				
C	-3.039221943574	2.074821414810	4.917203590531				
H	-4.083912038366	2.340665378983	5.008442246623				
C	-2.493494768025	1.650107997262	3.730377292922				
H	-3.137377644439	1.574456481019	2.865249352386				
C	-1.041156688876	0.862994037706	1.372306780369				
N	2.294935379883	-2.171938422129	-6.046257396821				
C	1.129815714928	-1.284734117242	-3.650309730211				
C	0.981265920467	-1.848201585972	-6.007144076238				
H	0.438953073974	-1.952087694364	-6.936535315364				
C	2.933483468341	-2.706343781238	-7.313854657611				
H	2.854795026859	-3.794323486597	-7.266096087164				
H	3.987413500519	-2.436067387335	-7.241088133770				
C	1.467941435213	-2.185489890799	1.537994075487				
H	1.567078208964	-2.589662949831	2.539890026042				
C	1.686097593951	-3.007635030808	0.438058956572				
C	1.039618049408	-1.220142164207	-1.090404264226				
C	-0.472701919382	0.164144774583	-2.494699189781				
H	-0.749351153940	0.539140919740	-3.474874878840				
C	0.539382324927	-0.770706088269	-2.415554164729				
C	1.386446435642	-2.538840049653	-0.857424722883				
H	1.407303467121	-3.243983117829	-1.680849632977				
C	0.386811528462	-1.416043602932	-4.845224760165				
H	-0.673442256167	-1.204539408651	-4.866609387080				
C	1.721158768874	1.044034297168	-0.150261577010				
H	2.797451202396	0.850798909695	-0.104045144151				
H	1.505822811062	1.506554453919	-1.112709802159				
C	0.991884584255	-0.283640879740	0.030141766399				
C	3.039221943574	-2.074821414810	-4.917203590531				
H	4.083912038366	-2.340665378983	-5.008442246623				
C	2.493494768025	-1.650107997262	-3.730377292922				
H	3.137377644439	-1.574456481019	-2.865249352386				
C	1.041156688876	-0.862994037706	1.372306780369				
H	1.481553261844	1.753069933346	0.641396146054				
H	-2.000881889199	4.033725462222	-0.579914501740				
H	2.000881889199	-4.033725462222	0.579914501740				
C	-2.315012811475	2.171301124044	8.572926783941				
C	-1.463721926058	2.970288461091	9.342650059962				
C	-2.592170257894	0.868627671669	9.004985721507				
C	-0.891817225612	2.474503561486	10.509528145812				
H	-1.261881485104	3.994110919857	9.043515898854				
C	-2.015830959302	0.374215098070	10.166344284813				
H	-3.262214385245	0.234847385719	8.432291521623				
C	-1.150553468518	1.165566153762	10.940254129222				
H	-0.258764222709	3.118762244442	11.107130187292				
H	-2.225859356991	-0.642695343887	10.474240812301				
C	2.315012811475	-2.171301124044	-8.572926783941				
C	2.592170257894	-0.868627671669	-9.004985721507				
C	1.463721926058	-2.970288461091	-9.342650059962				
C	2.015830959302	-0.374215098070	-10.166344284813				
H	3.262214385245	-0.234847385719	-8.432291521623				
C	0.891817225612	-2.474503561486	-10.509528145812				
H	1.261881485104	-3.994110919857	-9.043515898854				
C	1.150553468518	-1.165566153762	-10.940254129222				
H	2.225859356991	0.642695343887	-10.474240812301				
H	0.258764222709	-3.118762244442	-11.107130187292				
C	-0.527286105053	0.625673609743	12.173298282924				
C	0.796681033189	0.926295769884	12.503594122900				
C	-1.230065497204	-0.229299944190	13.025542429301				
C	1.367115255733	0.345008503595	13.642388758334				
H	1.399854813179	1.553368237810	11.858565658840				
C	-0.584361472848	-0.761600219687	14.147966653053				
H	-2.263270179067	-0.484465580614	12.825384152736				
N	0.691465012357	-0.489503072904	14.436874370721				
C	2.786858435844	0.630238127939	14.013172765349				
C	-1.309509406188	-1.677524679788	15.080453514134				
N	3.516512196915	-0.412559598248	14.428603947632				
C	3.302360628359	1.929140860476	13.937433575725				
N	-0.621544402460	-2.733244818633	15.532626079046				
C	-2.632178879077	-1.419946509156	15.458253697386				
C	4.782284971578	-0.188492686374	14.778896892512				
C	4.624102713663	2.149599672372	14.312027798957				
H	2.672915136606	2.754459051349	13.625927491907				
C	-1.235928144432	-3.564448789779	16.373214547947				
H	-3.148476860861	-0.538769425685	15.096027927254				
C	-3.259164195435	-2.293293726631	16.341568910788				
C	5.385329822339	1.068871447919	14.741565602145				
H	5.344117437836	-1.057897485700	15.108749293788				
H	5.045458437455	3.147985893843	14.281744087220				
C	-2.549405282852	-3.392408353010	16.810578038726				
H	-0.648777220830	-4.411522938378	16.716702441506				
H	-4.277483973399	-2.110835294870	16.665297909854				
H	6.416993498414	1.191457670075	15.048197633401				
H	-2.993822388884	-4.097955732606	17.501969384977				
C	0.527286105053	-0.625673609743	-12.173298282924				
C	1.230065497204	0.229299944190	-13.025542429301				
C	-0.796681033189	-0.926295769884	-12.503594122900				
C	0.584361472848	0.761600219687	-14.147966653053				
C	2.263270179067	0.484465580614	-12.825384152736				
H	-1.367115255733	-0.345008503595	-13.642388758334				
H	-1.399854813179	-1.553368237810	-11.858565658840				
N	-0.691465012357	0.489503072904	-14.436874370721				
C	1.309509406188	1.677524679788	15.080453514134				
C	-2.786858435844	-0.630238127939	-14.013172765349				
N	0.621544402460	2.733244818633	-15.532626079046				
C	2.632178879077	1.419946509156	-15.458253697386				

UB3LYP energies:

$E(S_0) = -3214.367433$ a.u.
 $\langle S^2 \rangle = 0.985282$

$E(T_1) = -3214.362943$ a.u.
 $\langle S^2 \rangle = 2.036754$

Table S2 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energy for S₁(CT-Z) 2c²⁺_{,model} (CPD*).

N	-1.182492442382	2.974067506021	6.041071717919	N	-2.674798483838	2.253290631112	-14.212150188194
C	-0.561892029210	1.692573284373	3.631604936331	C	-3.541390055374	0.047117403727	-13.902568032095
C	-0.152702966055	2.105206533845	5.979960660085	C	3.040266000598	2.945716989597	-16.032300162781
H	0.393301515826	1.950183662225	6.899817232947	C	4.205623527206	0.872440250704	-16.119076251716
C	-1.491188396596	3.719050308993	7.307185070143	H	3.262831138069	-0.685813378653	-14.974817961060
H	-0.901459474079	4.636835164911	7.291219946015	C	-3.890785633905	2.647193180224	-14.567257698932
H	-2.544306995350	3.990901402518	7.241183972917	H	-3.354866130549	-0.990870287831	-13.656707955845
C	-0.578386826915	2.573601423036	-1.573192805578	C	-4.806259982792	0.469286675589	-14.280646665835
C	-0.581614719842	3.005740114217	-2.566693573293	C	4.110650614744	2.197861740115	-16.506119306221
C	-0.638116528613	3.394128988629	-0.464008784674	H	2.931501515069	3.988744176266	-16.312887580213
C	-0.433133447418	1.532290136608	1.092203263561	H	5.016032412983	0.247647426032	-16.474613434903
C	0.144584171043	-0.368623508552	2.517166328876	C	-4.989199362176	1.798574982068	-14.620139602319
H	0.165857722979	-0.829753817035	3.498033407017	H	-3.993875189390	3.696438618674	-14.826067233870
C	-0.264009614671	0.961530653923	2.408183356702	H	-5.631120292381	-0.231868968690	-14.321471347740
C	-0.520694350585	2.882792126468	0.842000144112	H	4.842565757367	2.647123818614	-17.164830052400
H	-0.457289812505	3.589824167372	1.658107195896	H	-5.956586024417	2.174703529251	-14.927015094191
C	0.169426344395	1.464712418264	4.814936959078				
H	1.021911378640	0.800349986584	4.819479030291				
C	-1.970036207162	-0.065108763323	0.008565843825				
H	-2.722701099710	0.716944541480	-0.091990874485				
H	-2.116640707484	-0.574455453709	0.961293271009				
H	-2.112975788317	-0.783099555094	-0.798564304199				
C	-0.543305418025	0.561573681819	-0.065332824788				
C	-1.910555032246	3.217963888311	4.928936937729				
H	-2.736762107852	3.906823188004	5.040385355972				
C	-1.625689416892	2.612310771249	3.737442216429				
H	-2.265094807855	2.821579405199	2.892274132494				
C	-0.424024309426	1.195052760501	-1.422669974925				
N	1.182492442382	-2.974067506021	-6.041071717919				
C	0.561892029210	-1.692573284373	-3.631604936331				
C	0.152702966055	-2.105206533845	-5.979960660085				
H	-0.393301515826	-1.950183662225	-6.899817232947				
C	1.491188396596	-3.719050308993	-7.307185070143				
H	0.901459474079	-4.636835164911	-7.291219946015				
H	2.544306995350	-3.990901402518	-7.241183972917				
C	0.578386826915	-2.573601423036	1.573192805578				
H	0.581614719842	-3.005740114217	2.566693573293				
C	0.638116528613	-3.394128988629	0.464008784674				
C	0.433133447418	-1.532290136608	-1.092203263561				
C	-0.144584171043	0.368623508552	-2.517166328876				
H	-0.165857722979	0.829753817035	-3.498033407017				
C	0.264009614671	-0.961530653923	-2.408183356702				
C	0.520694350585	-2.882792126468	-0.842000144112				
H	0.457289812505	-3.589824167372	-1.658107195896				
C	-0.169426344395	-1.464712418264	-4.814936959078				
H	-1.021911378640	-0.800349986584	-4.819479030291				
C	1.970036207162	0.065108763323	-0.008565843825				
H	2.722701099710	0.716944541480	0.091990874485				
H	2.116640707484	0.574455453709	-0.961293271009				
C	0.543305418025	-0.561573681819	0.065332824788				
C	1.910555032246	-3.217963888311	-4.928936937729				
H	2.736762107852	-3.906823188004	-5.040385355972				
C	1.625689416892	-2.612310771249	-3.737442216429				
H	2.265094807855	-2.821579405199	-2.892274132494				
C	0.424024309426	-1.195052760501	1.422669974925				
H	2.112975788317	0.783099555094	0.798564304199				
H	-0.717543838446	4.465855814387	-0.598272642633				
H	0.717543838446	-4.465855814387	0.598272642633				
C	-1.212946402220	2.920801080370	8.545609620802				
C	-0.122483324252	3.225256911465	9.353649990007				
C	-2.048489146667	1.866127603822	8.908336921878				
C	0.136131397544	2.482416424938	10.495347047693				
H	0.522266699646	4.061134380267	9.103603564371				
C	-1.785493958336	1.122836700404	10.043705285223				
H	-2.912901252022	1.621220524170	8.299880706250				
C	-0.685730739015	1.415453250558	10.855315004193				
H	0.973900620731	2.748774786785	11.127122013745				
H	-2.432415206254	0.294342512540	10.302736612497				
C	1.212946402220	-2.920801080370	-8.545609620802				
C	2.048489146667	-1.866127603822	-8.908336921878				
C	0.122483324252	-3.225256911465	-9.353649990007				
C	1.785493958336	-1.122836700404	-10.043705285223				
H	2.912901252022	-1.621220524170	-8.299880706250				
C	-0.136131397544	-2.482416424938	-10.495347047693				
H	-0.522266699646	-4.061134380267	-9.103603564371				
C	0.685730739015	-1.415453250558	-10.855315004193				
H	2.432415206254	-0.294342512540	-10.302736612497				
H	-0.973900620731	-2.748774786785	-11.127122013745				
C	-0.401356024885	0.603589431530	12.062146566837				
C	0.900865955149	0.252429019735	12.399048512486				
C	-1.428352306773	0.138215878744	12.874692718942				
C	1.119072542763	-0.564003783725	13.506556835482				
H	1.736567896317	0.559280991120	11.783138530329				
C	-1.118657301633	-0.669461199108	13.966777830219				
H	-2.459843079603	0.392464887974	12.667387381318				
N	0.127920231524	-1.021690924985	14.263656752220				
C	2.502884315207	-0.974206519257	13.885597059791				
C	-2.198036967314	-1.183958060919	14.859477040801				
N	2.674798483838	-2.253290631112	14.212150188194				
C	3.541390055374	-0.047117403727	13.902568032095				
N	-2.101947111209	-2.458713997265	15.230951691523				
C	-3.234323628826	-0.353526315135	15.277328508256				
C	3.890785633905	-2.647193180224	14.567257698932				
C	4.806259982792	-0.469286675589	14.280646665835				
H	3.354866130549	0.990870287831	13.656707955845				
C	-3.040266000598	-2.945716989597	16.032300162781				
H	-3.262831138069	0.685813378653	14.974817961060				
C	-4.205623527206	-0.872440250704	16.119076251716				
C	4.989199362176	-1.798574982068	14.620139602318				
H	3.993875189390	-3.696438618674	14.826067233870				
H	5.631120292381	0.231868968690	14.321471347740				
C	-4.110650614744	-2.197861740115	16.506119306221				
H	-2.931501515069	-3.988744176266	16.312887580213				
H	-5.016032412983	-0.247647426032	16.474613434903				
H	5.956586024417	-2.174703529251	14.927015094191				
H	-4.842565757367	-2.647123818614	17.164830052400				
C	0.401356024885	-0.603589431530	-12.062146566837				
C	1.428352306773	-0.138215878744	-12.874692718942				
C	-0.900865955149	-0.252429019735	-12.399048512486				
C	1.118657301633	0.669461199108	-13.966777830219				
H	2.459843079603	-0.392464887974	-12.667387381318				
C	-1.119072542763	0.564003783725	-13.506556835482				
H	-1.736567896317	-0.559280991120	-11.783138530329				
N	-0.127920231524	1.021690924985	-14.263656752220				
C	2.198036967314	1.183958060919	-14.859477040801				
C	-2.502884315207	0.974206519257	-13.885597059791				
N	2.101947111209	2.458713997265	-15.230951691523				
C	3.234323628826	0.353526315135	-15.277328508256				

TD-CAM-B3LYP energy:

E(S₁) = -3212.558236 a.u.

Table S2 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energy for S₂(CT-LE) 2c²⁺,_{model}.

N	-1.278776512620	2.927324026458	6.025454684231	N	-2.687305496211	2.253676581195	-14.172351217444
C	-0.672681700929	1.646046555516	3.621790671103	C	-3.559322395577	0.055520149504	-13.823244726070
C	-0.269018895000	2.037058484200	5.970661170395	C	2.992709633791	2.899454206322	-16.111365238928
H	0.264465586678	1.865517697847	6.894940015873	C	4.147045676590	0.820047472558	-16.200357356680
C	-1.585920831366	3.673824716701	7.295222717747	H	3.220004202957	-0.722624502143	-15.022606798566
H	-1.006234557879	4.597550616072	7.266404143586	C	-3.907990851843	2.650778029745	-14.507165640227
H	-2.642783983794	3.931951314802	7.236119652333	H	-3.373511658356	-0.981007355904	-13.570733371928
C	-0.370326218970	2.647425537013	-1.529947119117	C	-4.829210098708	0.480907329313	-14.180405644411
H	-0.307213287684	3.097791718330	-2.514385795910	C	4.050346666260	2.142036327957	-16.598507123185
C	-0.504294387340	3.446531619414	-0.418848074386	H	2.883088697397	3.940168130265	-16.400040554293
C	-0.455645232090	1.521792354982	1.094954513370	H	4.947627831134	0.188130426500	-16.565420030152
C	-0.071129757632	-0.450911383435	2.503029878492	C	-5.011747975472	1.807720120456	-14.529612864233
H	-0.159255031984	-0.926234272325	3.473248213462	H	-4.010596809748	3.697928508823	-14.774461048130
C	-0.375311842078	0.919431019407	2.388082234459	H	-5.658462824940	-0.216021057182	-14.197791092379
C	-0.485003888306	2.883900614968	0.876458901292	H	4.771274501867	2.581474602485	-17.275694856473
H	-0.442759950239	3.565056633603	1.716863329509	H	-5.983032173198	2.186109460245	-14.820994539630
C	0.046549435272	1.393322697112	4.803016888559				
H	0.879422999964	0.704158247443	4.805630310743				
C	-1.966770851719	0.012274904479	-0.158943791134				
H	-2.669296935087	0.831217054562	-0.316784751543				
H	-2.234547016636	-0.499156154911	0.765514911282				
H	-2.075265900082	-0.692168293661	-0.983685651970				
C	-0.519471439398	0.574114679003	-0.092772352690				
C	-1.996645981283	3.191709618460	4.913494819664				
H	-2.807391829532	3.898952354246	5.024147498204				
C	-1.719588282209	2.581218812837	3.720277180394				
H	-2.350524745027	2.797972547490	2.870521332524				
C	-0.247815396198	1.247756223955	-1.414787779250				
N	1.278776512620	-2.927324026458	-6.025454684231				
C	0.672681700929	-1.646046555516	-3.621790671103				
C	0.269018895000	-2.037058484200	-5.970661170395				
H	-0.264465586678	-1.865517697847	-6.894940015873				
C	1.585920831366	-3.673824716701	-7.295222717747				
H	1.006234557879	-4.597550616072	-7.266404143586				
H	2.642783983794	-3.931951314802	-7.236119652333				
C	0.370326218970	-2.647425537013	-1.529947119117				
H	0.307213287684	-3.097791718330	-2.514385795910				
C	0.504294387340	-3.446531619414	0.418848074386				
C	0.455645232090	-1.521792354982	-1.094954513370				
C	0.071129757632	0.450911383435	-2.503029878492				
H	0.159255031984	0.926234272325	-3.473248213462				
C	0.375311842078	0.919431019407	-2.388082234459				
C	0.485003888306	-2.883900614968	-0.876458901292				
H	0.442759950239	-3.565056633603	-1.716863329509				
C	-0.046549435272	-1.393322697112	-4.803016888559				
H	-0.879422999964	-0.704158247443	-4.805630310743				
C	1.966770851719	-0.012274904479	0.158943791134				
H	2.669296935087	-0.831217054562	0.316784751543				
H	2.234547016636	0.499156154911	-0.765514911282				
C	0.519471439398	-0.574114679003	0.092772352690				
C	1.996645981283	-3.191709618460	-4.913494819664				
H	2.807391829532	-3.898952354246	-5.024147498204				
C	1.719588282209	-2.581218812837	-3.720277180394				
H	2.350524745027	-2.797972547490	-2.870521332524				
C	0.247815396198	-1.247756223955	1.414787779250				
H	2.075265900082	0.692168293661	0.983685651970				
H	-0.557371802889	4.521452292786	-0.528147005684				
H	0.557371802889	-4.521452292786	0.528147005684				
C	-1.286676739364	2.885865098385	8.534135134178				
C	-0.177373976339	3.191307873094	9.316291050373				
C	-2.121246610103	1.840122921780	8.924338042092				
C	0.100425564856	2.457677804326	10.459178319811				
H	0.466804358802	4.021074888563	9.045218172498				
C	-1.838866963850	1.105919159273	10.060994268687				
H	-3.000291770896	1.595509598996	8.337086783062				
C	-0.720478258182	1.399259151137	10.846541658732				
H	0.952479054979	2.724942283235	11.071112719596				
H	-2.485495196829	0.284284552228	10.341602152108				
C	1.286676739364	-2.885865098385	-8.534135134179				
C	2.121246610103	-1.840122921780	-8.924338042092				
C	0.177373976339	-3.191307873094	-9.316291050373				
C	1.838866963850	-1.105919159273	-10.060994268687				
H	3.000291770896	-1.595509598996	-8.337086783062				
C	-0.100425564856	-2.457677804326	-10.459178319811				
H	-0.466804358802	-4.021074888563	-9.045218172498				
C	0.720478258182	-1.399259151137	-10.846541658732				
H	2.485495196829	0.284284552228	-10.341602152108				
H	-0.952479054979	-2.724942283235	-11.071112719596				
C	-0.416213499741	0.597796022066	12.055330281626				
C	0.890785994358	0.243443208623	12.369698039568				
C	-1.429315302874	0.145714625978	12.892451112404				
C	1.126884707173	-0.563216097363	13.480727064719				
H	1.715678157446	0.539772055356	11.734365470046				
C	-1.101957642973	-0.652706900986	13.986236859371				
H	-2.463484368878	0.403126831695	12.703206521656				
N	0.148592760061	-1.008194248728	14.261742933526				
C	2.515818419154	-0.977008646936	13.836338820997				
C	-2.165877692374	-1.153121181163	14.905080588463				
N	2.687305496211	-2.253676581195	14.172351217444				
C	3.559322395577	-0.055520149504	13.823244726070				
N	-2.068066637311	-2.424583296250	15.287173405231				
C	-3.190098408819	-0.313837292276	15.334732278063				
C	3.907990851843	-2.650778029745	14.507165640227				
C	4.829210098708	-0.480907329313	14.180405644411				
H	3.373511658356	0.981007355904	13.570733371928				
C	-2.992709633791	-2.899454206322	16.111365238928				
H	-3.220004202957	0.722624502143	15.022606798566				
C	-4.147045676590	-0.820047472558	16.200357356680				
C	5.011747975472	-1.807720120456	14.529612864233				
H	4.010596809748	-3.697928508823	14.774461048130				
H	5.658462824940	0.216021057182	14.197791092379				
C	-4.050346666260	-2.142036327957	16.598507123185				
H	-2.883088697397	-3.940168130265	16.400040554293				
H	-4.947627831134	-0.188130426500	16.565420030152				
H	5.983032173198	-2.186109460245	14.820994539630				
H	-4.771274501867	-2.581474602485	17.275694856473				
C	0.416213499741	-0.597796022066	-12.055330281626				
C	1.429315302874	-0.145714625978	-12.892451112404				
C	-0.890785994358	-0.243443208623	-12.369698039568				
C	1.101957642973	0.652706900986	-13.986236859371				
H	-2.463484368878	-0.403126831695	-12.703206521656				
C	-1.126884707173	0.563216097363	-13.480727064719				
H	-1.715678157446	-0.539772055356	-11.734365470046				
N	-0.148592760061	1.008194248728	-14.261742933526				
C	2.165877692374	1.153121181163	-14.905080588463				
C	-2.515818419154	0.977008646936	-13.836338820997				
N	-2.068066637311	2.424583296250	-15.287173405231				
C	3.190098408819	0.313837292276	-15.334732278063				

TD-CAM-B3LYP energy:

E(S₂) = -3212.545156 a.u.

Table S2 (continued). B3LYP Cartesian coordinates and energy for S_0 $\text{Ru}_2(2\text{c}^{2+})_{\text{model}}$.

N	0.097967364429	2.360201632890	6.450707281034	H	1.074012609976	0.592236018380	22.628594727280
C	0.046333838521	1.224730002674	3.876828597720	N	-0.602085709151	-2.266062975916	17.709115786205
C	0.866901527721	1.280530315766	6.165109703821	C	-1.236298760165	-4.094919607393	19.1375500353068
H	1.503236437534	0.922213053686	6.963039579285	H	-0.622428625442	-3.248239909416	21.769632760593
C	0.271067724062	3.125465426485	7.735853408091	C	1.432471068560	2.551425497325	17.892355003720
H	1.194356182863	3.697882801052	7.627813673090	C	2.077714605202	3.627959334726	19.929392140707
H	-0.552508559502	3.839450168018	7.760147130279	H	1.754278030227	2.443132632879	21.688438733089
C	0.016059711353	2.857135980174	-1.153063184077	H	0.229136000944	-1.598946853180	23.404524797957
H	0.091796136761	3.436819380228	-2.066778630752	C	-1.008447754974	-2.988916807280	16.651894488577
C	0.124490621781	3.497724313395	0.074268974199	C	-1.653401863144	-4.831642004364	18.035183804959
C	-0.026785727691	1.413760546553	1.343280621942	H	-1.318529479071	-4.515401081140	20.130637317037
C	0.059469853370	-0.780125634816	2.436926014831	C	1.956523826925	3.659505403702	18.544404636695
H	-0.017375185357	-1.368691015231	3.345109702963	H	1.323089821516	2.540584010983	16.815752746106
C	0.042402546672	0.627274457042	2.531275236129	H	2.481904903512	4.473886863916	20.471533901622
C	0.147530874644	2.788290471415	1.286395213671	C	-1.536727301466	-4.267359046544	16.769451777636
H	0.368771076702	3.347214707175	2.186909057347	H	-0.902252515690	-2.517436688294	15.683566584907
C	0.850314277720	0.701613453566	4.915784842957	H	-2.061193723948	-5.826464293893	18.165086559701
H	1.507685982876	-0.137955634662	4.732954759203	H	2.260849687308	4.526134215562	17.971995462917
C	-1.934301510231	0.480546570324	0.088878960641	H	-1.848441181117	-4.803772331247	15.882693220256
H	-2.420041121119	1.457177672985	0.103393090076	C	-0.250974118304	-0.827212831133	-13.068480544949
H	-2.240647026421	-0.071878892728	0.977380409409	C	0.867011309308	-1.098686396002	-13.873523235895
H	-2.284623229890	-0.058541223812	-0.792461054809	C	-1.346295130336	-0.179278273203	-13.661396855905
C	-0.376835644759	0.674931427482	0.042151401235	C	0.864535447938	-0.744134109332	-15.220726459581
C	-0.727670690590	2.857425885741	5.494471517705	H	1.715712260927	-1.621516969246	-13.454364374985
H	-1.341443728540	3.701117439982	5.779653366985	C	-1.311978538209	0.161403988611	-15.012127569758
C	-0.773662340669	2.318212625468	4.230546718680	H	-2.214889742569	0.063232035049	-13.064463924807
H	-1.470212971641	2.740647997048	3.520064909311	N	-0.218240472198	-0.130536207061	-15.758740995756
C	-0.104886345258	1.467363048118	1.226982885846	C	1.943124568838	-0.988053579560	-16.201708777706
N	-0.097967364429	-2.360201632890	-6.450707281034	C	-2.381053504786	0.829255056535	-15.784408610169
C	-0.046333838521	-1.224730002674	-3.876828597720	Ru	-0.216361825781	0.318810819474	-17.705934048580
C	-0.866901527721	-1.280530315766	-6.165109703821	N	1.679128220214	-0.570651643833	-17.480934111065
H	-1.503236437534	-0.922213053686	-6.963039579285	C	3.153937850734	-1.599262117464	-15.884066134545
C	-0.271067724062	-3.125465426485	-7.735853408091	N	-2.111288506835	1.023074757677	-17.114880440875
H	-1.194356182863	-3.697882801052	-7.627813673090	C	-3.591209001850	1.243050100494	-15.232249934332
H	0.552508559502	-3.839450168018	-7.760147130279	N	-0.220043317429	0.759437768853	-19.669133585825
C	-0.016059711353	-2.857135980174	1.153063184077	C	2.614279775990	-0.763464056585	-18.426276410527
H	-0.091796136761	-3.436819380228	2.066778630752	C	4.113190767591	-1.793528117480	-16.871826519213
C	-0.124490621781	-3.497724313395	-0.074268974199	H	3.350133105505	-1.924395711478	-14.871181044240
C	0.026785727691	-1.413760546553	-1.343280621942	C	-3.041063646273	1.620212213998	-17.879325593821
C	-0.059469853370	0.780125634816	-2.436926014831	H	-3.790923350665	1.08650538742	-14.180696129428
H	0.017375185357	1.368691015231	-3.345109702963	C	-4.544915290368	1.860050610249	-16.034222194535
C	-0.042402546672	-0.627274457042	-2.531275236129	C	-0.690179892690	-0.158201101295	-20.546890456474
C	-0.147530874644	-2.788290471415	-1.286395213671	C	0.247560550715	1.964651792187	-20.072173716271
H	-0.368771076702	-3.347214707175	-2.186909057347	C	3.837722382088	-1.367550044535	-18.166245378559
C	-0.850314277720	-0.701613453566	-4.915784842957	H	2.264895095166	-0.419906555956	-19.421552339262
H	-1.507685982876	0.137955634662	-4.732954759203	H	5.056800121653	-2.268952735595	-16.634572918878
C	1.934301510231	-0.480546570324	-0.088878960641	C	-4.264317687306	2.051357805003	-17.382393459184
H	2.420041121119	-1.457177672985	-0.103393090076	H	-2.787827692175	1.752368251909	-18.922968719860
H	2.240647026421	0.071878892728	-0.977380409409	H	-5.488708396208	2.184535861471	-15.613913062273
C	0.376835644759	-0.674931427482	-0.042151401235	C	-1.149845584784	-1.405172533462	-19.903912933767
C	-0.727670690590	-2.857425885741	-5.494471517705	C	-0.702510655638	0.127441109689	-21.911956917360
H	1.341443728540	-3.701117439982	-5.779653366985	C	0.713522562265	2.815676859069	-18.959401150372
C	-0.773662340669	-2.318212625468	-4.230546718680	C	0.253198467079	2.290875302085	-21.428068283185
H	-1.470212971641	-2.740647997048	-3.520064909311	H	4.552970992241	-1.497606212746	-18.968174637589
C	-0.104886345258	-1.467363048118	1.226982885846	H	-4.975705058163	2.525858967441	-18.045977420142
H	2.284623229890	0.058541223812	0.792461054809	N	-1.034021037839	-1.443113553393	-18.539061141233
H	0.262802605813	4.572152667422	0.098163181247	C	-1.669064078093	-2.487579707854	-20.611093670551
H	-0.262802605813	-4.572152667422	-0.098163181247	C	-0.226503079684	1.361564064695	-22.347968695533
C	0.301485852853	2.334179637905	9.025910166280	H	-1.074012609976	-0.592236018380	-22.628594727280
C	1.455121244582	2.356220288541	9.815499345450	N	0.602085709151	2.266062975916	-17.709115786205
C	-0.850312787694	1.272606503339	9.544071758125	C	1.236298760165	4.094919607393	-19.1375500353068
C	1.449234853415	1.830518475536	11.104904212672	H	0.622428625442	3.248239909416	-21.769632760593
H	2.356420869805	2.834989658151	9.447855078568	C	-1.432471068560	-2.551425497325	-17.892355003720
C	-0.856498102016	1.201363941939	10.830714547602	C	-2.077714605202	-3.627959334726	-19.929392140707
H	-1.761836850690	1.690175418422	8.956876584206	H	-1.754278030227	-2.443132632879	-21.688438733089
C	0.285676634722	1.269193293739	11.646886532886	H	-0.229136000944	1.598946853180	-23.404524797956
H	2.344489773391	1.918522498598	11.708738757983	C	1.008447754974	2.988916807280	-16.651894488577
H	-1.763595064996	0.741701225491	11.205222926680	C	1.653401863144	4.831642004364	-18.035183804959
C	-0.301485852853	-2.334179637905	-9.025910166280	H	1.318529479071	-4.515401081140	-20.130637317037
C	0.850312787694	-1.272606503339	-9.544071758125	C	-1.956523826925	-3.659505403702	-18.544404636694
C	-1.455121244582	-2.356220288541	-9.815499345450	H	-1.323089821516	-2.540584010983	-16.815752746106
C	0.856498102016	-1.201363941939	-10.830714547602	H	-2.481904903512	-4.473886863916	-20.471533901622
H	1.761836850690	-1.690175418422	-8.956876584206	C	1.536727301466	4.267359046544	-16.769451777636
H	-1.449234853415	-1.830518475536	-11.104904212671	H	0.902252515690	2.517436688294	-15.683566584907
H	-2.356420869805	-2.834989658151	-9.447855078568	H	2.061193723948	5.826464293893	-18.165086559701
C	-0.285676634722	-1.269193293739	-11.646886532886	H	-2.260849687308	4.526134215562	-17.971995462917
H	1.763595064996	-0.741701225491	-11.205222926680	H	1.848441181117	4.803772331247	-15.882693220256
H	-2.344489773391	-1.918522498598	-11.708738757983				
C	0.250974118304	0.827212831133	13.068480544949				
1.346295130336	0.179278273203	13.661396855905					
-0.867011309308	1.098686396002	13.873523235895					
1.311978538209	-0.161403988611	15.012127569758					
H	2.214889742569	-0.063232035049	13.064463924807				
C	-0.864535447938	0.744134109332	15.220726459581				
H	-1.715712260927	1.621516969246	13.454364374985				
N	0.218240472198	0.130536207061	15.758740995756				
C	2.381053504786	-0.829255056535	15.784408610169				
C	-1.943124568838	0.988053579560	16.201708777706				
Ru	0.216361825781	-0.318810819474	17.705934048580				
N	2.111288506835	-1.023074757677	17.114880440875				
C	3.591209001850	-1.243050100494	15.232249934332				
N	-1.679128220214	0.570651643833	17.480934111065				
C	-3.153937850734	1.599262117464	15.884066134545				
N	0.220043317429	-0.759437768853	19.669133585825				
C	3.041063646273	-1.620212213998	17.879325593821				
C	4.544915290368	-1.860050610249	16.034222194535				
H	3.790923350665	-1.08650538742	14.180696129428				
C	-2.614279775990	0.763464056585	18.426276410527				
H	-3.350133105505	1.924395711478	14.871181044240				
C	-4.113190767591	1.793528117480	16.871826519213				
C	0.690179892690	0.158201101295	20.546890456474				
C	-0.247560550715	-1.964651792187	20.072173716271				
C	4.264317687306	-2.051357805003	17.382393459184				
H	-3.837722382088	1.367550044535	18.166245378559</				

Table S2 (continued). B3LYP Cartesian coordinates and energy for S_0 $\text{Ru}_2(2\text{c}^{2+})_{\text{model}}$.

N	-0.111956631267	2.296482196373	6.390979337116	H	0.666051737645	0.761212159566	22.606656823035
C	0.092022956498	1.129217904782	3.837005935986	N	-0.619189221978	-2.280972721396	17.679803067550
C	0.738460530659	1.261825563855	6.177289891585	C	-1.099574280039	-4.153970690763	19.111010814658
H	1.331332335928	0.948258215334	7.025820886057	H	-0.627266354268	-3.233118265137	21.747493425824
C	-0.086339435810	3.086307541181	7.673750373982	C	0.928705057872	2.714235526630	17.861616945758
H	0.758975413089	3.772549590327	7.592826869257	C	1.423442180960	3.862415144841	19.901673696239
H	-0.996343603691	3.686624838865	7.660849866153	H	1.181693455488	2.663190230332	21.664125118159
C	0.165903689775	2.743294056692	-1.168661072209	H	0.024162083839	-1.497099177404	23.384663051950
C	0.345358634007	3.179913986714	-2.145100452414	C	-0.931912109142	-3.046866813928	16.621051590150
C	0.703222294508	3.344787368273	-0.036412766679	C	-1.420342116867	-4.935135997927	18.007052485149
C	-0.080792691158	1.467316061318	1.301833416908	H	-1.159876388918	-4.574132613136	20.105857816587
C	0.591686464592	-0.732455057429	2.313825383781	C	1.328190498918	3.872680134594	18.514330232093
H	0.743447560518	-1.320075761023	3.215590708517	H	0.843081794457	2.685594005141	16.783177919315
C	0.195570894136	0.5711133725105	2.481116652548	H	1.731690146677	4.747488796772	20.444359622230
C	0.666721440514	2.649880073838	1.168302068475	C	-1.334634638553	-4.370173450657	16.739139357342
H	1.248564232142	3.014897800749	2.007698003231	H	-0.853400921309	-2.573287480074	15.651111489706
C	0.853899682853	0.6727252028759	4.939016493578	H	-1.731045512994	-5.964369379133	18.137372027033
H	1.583283478137	-0.117551689431	4.824360585948	H	1.557877686342	4.761153330470	17.940594242810
C	-2.043072311603	0.110378314430	0.401993830069	H	-1.574773188665	-4.940246232974	15.851109536799
H	-2.930525478307	0.749167166260	0.482322755850	C	-0.018716192877	-0.844666963571	-13.029266972529
H	-1.988224104918	-0.480250834783	1.313901295031	C	1.135984993726	-1.012577165828	-13.810383158099
H	-2.215157155144	-0.554759486046	-0.21474820737	C	-1.160175585850	-0.311908213974	-13.649136999659
C	-0.858753775987	0.118874402850	0.213316564235	C	1.125428907303	-0.671246087103	-15.160967302832
C	-0.877513855123	2.746564452131	5.363689658066	H	2.023201477154	-1.446379202897	-13.369914304704
H	-1.543515807134	3.569779260694	5.584426296929	C	-1.132682619090	0.019289391034	-15.002426158296
C	-0.793241503062	2.196121522439	4.107802882668	H	-2.059801805797	-0.150329106278	-13.071048136582
H	-1.418793564656	2.602683188657	3.324687717759	N	-0.001207983714	-0.170626301088	-15.725348133893
C	-0.531843541823	1.525818178363	-1.072797291025	C	2.241804271875	-0.816673712709	-16.118947165856
N	0.111956631267	-2.296482196373	-6.390979337116	C	-2.246318840061	0.573201439322	-15.801374772774
C	-0.092022956498	-1.129217904782	-3.837005935986	Ru	-0.004048285302	0.262875532097	-17.676074688037
C	-0.738460530659	-1.261825563855	-6.177289891585	N	1.964400116553	-0.435562523902	-17.406641712798
H	-1.331332335928	-0.948258215334	-7.025820886057	C	3.499203456878	-1.306239175595	-15.772744699687
C	0.086339435810	-3.086307541181	-7.673750373982	N	-1.970410293787	0.781959565486	-17.128328360755
H	-0.758975413089	-3.772549590327	-7.592826869257	C	-3.501874052530	0.807839180727	-15.726401727083
H	0.996343603691	-3.686624838865	-7.660849866153	N	-0.010997255545	0.687939140438	-19.642588333140
C	-0.165903689775	-2.743294056692	1.168661072209	C	2.932566276138	-0.543656064439	-18.332038169589
C	-0.345358634007	-3.179913986714	2.145100452414	C	4.492216301900	-1.414026567416	-16.740140044451
C	-0.703222294508	-3.344787368273	0.036412766679	H	3.705439009151	-1.604125931351	-14.753500009716
C	0.080792691158	-1.467316061318	-1.301833416908	C	-2.938779991748	1.279002521926	-17.916161048209
C	-0.591686464592	0.732455057429	-2.313825383781	H	-3.706218633031	0.703717388374	-14.227368213047
H	-0.743447560518	1.320075761023	-3.215590708517	C	-4.495207624015	1.385092481007	-16.102376002909
C	-0.195570894136	-0.5711133725105	-2.481116652548	C	-0.370246612570	-0.277431601510	-20.521531086100
C	-0.666721440514	-2.649880073838	-1.168302068475	C	0.344293684081	1.930556549891	-20.046710563985
H	-1.248564232142	-3.014897800749	-2.007698003231	C	4.202985021095	-1.025312845125	-18.043250997957
C	-0.853899682853	-0.6727252028759	-4.939016493578	H	2.671508236565	-0.232269348131	-19.334881968080
H	-1.583283478137	0.117551689431	-4.824360585948	H	5.472193677356	-1.794874027592	-16.480684434825
C	2.043072311603	-0.110378314430	-0.401993830069	C	-4.207941882336	1.592200404942	-17.446803533501
H	2.930525478307	-0.749167166260	-0.482322755850	H	-2.679112305885	1.426914022831	-18.956101722681
H	1.988224104918	0.480250834783	-1.313901295031	H	-5.474365937121	1.618939131288	-15.703301188746
C	0.858753775987	0.118874402850	-0.213316564235	C	-0.718442123546	-1.559211585676	-19.876998605120
C	0.877513855123	-2.746564452131	-5.363689658066	C	-0.382080308305	-0.003634083485	-21.889036538066
H	1.543515807134	-3.569779260694	-5.584426296929	C	0.701402774323	2.830701180599	-18.932306249219
C	0.793241503062	-2.196121522439	-4.107802882668	C	0.346416588960	2.246507921215	-21.405044576062
H	-1.418793564656	-2.602683188657	-3.324687717759	H	4.943321941161	-1.091286299410	-18.830103685026
C	0.531843541823	-1.525818178363	1.072797291025	H	-4.949005076789	1.989441575920	-18.128417469694
H	2.215157155144	0.554759486046	0.441748280737	N	-0.627522018318	-1.576514714269	-18.509856848067
H	1.231794915423	4.286469197810	-0.113660141273	C	-1.114556895884	-2.691995135274	-20.584979217485
H	-1.231794915423	-4.286469197810	0.113660141273	C	-0.020432419926	1.268320951529	-22.326212784196
C	-0.000920028308	2.314720472901	8.972691132452	H	-0.666051737645	-0.761212159566	-22.606656823035
C	1.128544436354	2.459620673216	9.784271852905	N	0.619189221978	-2.280972721396	-17.679803067550
C	-1.096107846391	1.599614290434	9.475161886455	C	1.099574280039	-4.153970690763	-19.111010814658
C	1.149768021076	1.946459077014	11.078524895793	H	0.627266354268	-3.233118265137	-21.747493425824
H	1.984014519139	3.024313598334	9.429255841340	C	-0.928705057872	2.714235526630	-17.861616945758
C	-1.075376830896	1.086392328011	10.766980711025	C	-1.423442180960	-3.862415144841	-19.901673696239
H	-1.987366808899	1.466727234490	8.870955775813	H	-1.181693455488	-2.663190230332	-21.664125118159
C	0.037687382247	1.275488631957	11.603886138453	H	-0.024162083839	-1.497099177404	-23.384663051950
H	2.019057101424	2.129449270267	11.698773664502	C	0.931912109142	3.046866813928	-16.621051590150
H	-1.939389243929	0.541747096998	11.129210458169	C	1.420342116867	4.935135997927	-18.007052485149
C	0.000920028308	-2.314720472901	-8.972691132452	H	1.159876388918	4.574132613136	-20.105857816587
C	1.096107846391	-1.599614290434	-9.475161886455	C	-1.328190498918	-3.872680134594	-18.514330232093
C	-1.128544436354	-2.459620673216	-9.784271852905	H	-0.843081794457	2.685594005141	-16.783177919315
C	1.075376830896	-1.086392328011	-10.766980711025	H	-1.731690146677	4.747488796772	-20.444359622230
H	1.987366808899	-1.466727234490	-8.870955775813	C	1.334634638553	4.370173450657	-16.739139357342
C	-1.149768021076	-1.946459077014	-11.078524895793	H	0.853400921309	-2.573287480074	-15.651111489706
H	-1.984014519139	-3.024313598334	-9.429255841340	H	1.731045512994	5.964369379133	-18.137372027033
C	-0.037687382247	-1.275488631957	-11.603886138453	H	-1.557877686342	-4.761153330470	-17.940594242810
H	1.939389243929	-0.541747096998	11.129210458169	H	1.574773188665	4.940246232974	-15.851109536799
H	-2.019057101424	-2.129449270267	-11.698773664501				
C	0.018716192877	0.844666963571	13.029266972529				
C	1.160175585850	0.311908213974	13.649136999659				
C	-1.135984993726	0.1012577165828	13.810383158099				
C	1.132682619090	-0.019289391034	15.002426158296				
H	2.059801805797	0.150329106278	13.071048136582				
C	-1.125428907303	0.671246087103	15.160967302832				
H	-0.023201477154	1.446379202897	13.369914304704				
N	0.001207983714	0.170626301088	15.725348133893				
C	2.246318840061	-0.573201439322	15.801374772774				
C	-2.241804271875	0.816673712709	16.118947165856				
Ru	0.004048285302	-0.262875532097	17.676074688037				
N	1.970410293787	-0.781959565486	17.128328360755				
C	3.501874052530	-0.807839180727	15.726401727083				
N	-1.964400116553	0.435562523902	17.406641712798				
C	-3.499203456878	1.306239175595	15.772744699687				
N	0.010997255545	-0.687939140438	19.642588333140				
C	2.938779991748	-1.279002521926	17.916161048209				
C	4.495207624015	-1.385092481007	16.102376002909				
H	3.706218633031	-0.703717388374	14.227368213047				
C	-2.932566276138	0.543656064439	18.332038169589				
H	-3.705439009151	1.604125931351	14.753500009716				
C	-4.492216301900	1.414026567416	16.740140044451				
C	0.370246612570	-0.277431601510	20.521531086100				
C	-0.344293684081	1.930556549891	20.046710563985				
C	4.207941882336	-1.592200404942	17.446803533501				
H	2.679112305885	-1.426914022831	18.956101				

Table S2 (continued). UB3LYP Cartesian coordinates and energies for S₀ transition state between Ru₂(2c²⁺)_{model} and Ru₂(2o²⁺)_{model}.

N	-2.293052055805	0.100345736298	6.444312067242	C	3.879077218067	-1.299924528219	-18.554803148858
C	-1.136766275557	0.214866112763	3.873093339978	H	2.678735736540	-0.843799456266	-16.824948320923
C	-1.233299274406	0.916117812532	6.202622832267	C	-4.191064824660	0.976007946787	-19.163230136760
H	-0.897668436635	1.520848985037	7.034142731995	C	-4.417498648520	1.198391076901	-16.791082861473
C	-3.077753001881	0.195803409371	7.727726114404	H	-2.613958135320	0.748937851650	-15.700379855664
H	-3.685917893194	1.099447856309	7.645264677870	H	0.977685512869	4.920551448648	-18.855943796222
H	-3.759045742845	-0.655323255120	7.709464287644	H	-1.916712332627	-5.030824736907	-18.194505789192
C	-2.823412259832	-0.001777349760	-1.127556820858	C	-1.276215868312	-0.075875771995	-22.375169489673
C	-3.359452523335	0.056590012751	-2.068785993220	H	0.766032267644	-0.681379097362	-22.652722730901
C	-3.448917328267	0.398123039030	0.046155385215	H	-3.254578182083	0.531720204891	-21.799154802930
C	-1.406445129887	0.026236760418	1.328909280220	C	3.874155991400	-1.390038652142	-19.942515718525
C	0.773704577764	0.592499255081	2.374603718208	H	2.675101550629	-1.164196983854	-21.707184282340
H	1.386122655804	0.691122115517	3.265267777716	H	4.770188715322	-1.515200869574	-17.979573942099
C	-0.565862512032	0.288745593070	2.531606353163	C	-4.981019786187	1.277391314687	-18.060069525787
C	-2.706358549712	0.488990053686	1.242427321510	H	-4.610024119670	1.031404461683	-20.158871455751
H	-3.171990464786	0.956008911025	2.102903974382	H	-4.994319883359	1.424006183440	-15.903602879628
C	-0.649741746871	0.985136129341	4.960914006900	H	-1.502264817402	-0.080272569816	-23.434199736681
H	0.160856108222	1.688046300082	4.82468159329	H	4.766229091140	-1.679596421638	-20.484029306122
C	-0.077554025998	-1.910273673269	0.346058405637	H	-6.015898830233	1.568089692437	-18.191819323971
H	-0.843123281383	-2.680784027074	0.479763502911	C	-0.831713908297	0.081686217831	13.077349455781
H	0.560218697524	-1.917063516452	1.229041899543	C	-1.106988620659	-1.053776312299	13.856149491717
H	0.519451839787	-2.190389402321	-0.521072558755	C	-0.91939335259	1.165970186037	13.698554580498
C	-0.781802577060	-0.571820261107	0.149744410049	C	-0.764315698268	-1.078602697754	15.206191604747
C	-2.766037581652	-0.680923224360	5.436284173597	H	-1.623624274597	-1.894650766569	13.41410408425
H	-3.600446801391	-1.324871132376	5.678982752530	C	0.138637949216	1.103409949164	15.050841275740
C	-2.22232381772	-0.642693253030	4.177002263675	H	0.052502249198	2.047627724291	13.121852476015
H	-2.641579962918	-1.291251506423	3.420470245653	N	-0.157049901856	-0.006369284631	15.771716779295
C	-1.479567553358	-0.398700077075	-1.125697807013	C	-1.015397519739	-2.177471415361	16.162578936502
N	2.293233329498	0.099745315437	-6.443648546059	C	0.799860727983	2.156346804811	15.850522859751
C	1.144007744458	-0.043943361406	-3.871224987272	Ru	0.278812189993	-0.049604583281	17.72177011430
C	1.246720683248	-0.733128314126	-6.204149211173	N	-0.608636774584	-1.939981137645	17.450383933057
H	0.918455239150	-1.333263634217	-7.038244618202	C	-1.623851260264	-3.381425524418	15.814967606946
C	3.077732436443	0.030380189663	-7.723970358297	N	0.985964070575	1.857880949953	17.175945816221
H	3.740287607837	-0.833054964584	-7.634290819837	C	1.215465552143	3.378726280709	15.327396736451
C	3.705495361290	0.922074042038	-7.727851129614	N	0.706656783120	-0.087829352231	19.687198249163
C	2.832418491143	0.162086036625	1.128286836747	N	2.225834655432	-0.868396439938	17.719923141235
H	3.368793615450	0.102895967431	2.069274621398	N	-1.488458859265	0.750264134290	18.560434205350
C	3.457906523253	-0.235443771075	-0.046165268683	C	-0.809230850208	-2.894391976034	18.374633566110
C	1.414461814937	0.135983497595	-1.327257133729	C	-1.826171554581	-4.360832368842	16.781086274700
C	-0.764723650160	-0.433221061203	-2.373111620651	H	-1.940734032068	-3.556499440598	14.795620984552
H	-1.376715814675	-0.532938125221	-3.264005772695	C	1.577708613874	2.771257351187	17.964003899329
C	0.573837028304	-0.126097950924	-2.529817929249	H	1.064846406064	3.601126195040	14.279540662992
C	2.714943664897	-0.325250135049	-1.242352200849	C	1.826551116284	4.315330377272	16.153668365266
C	3.180634193597	-0.790013565591	-2.104605213218	C	1.909201723464	-0.564190779692	20.087960966416
C	0.665909811186	-0.815823567392	-4.961518753674	C	-0.216667025832	0.363627529067	20.568823722511
H	-0.135486489704	-1.529619227738	-4.826914430862	C	2.767327910890	-1.006626548093	18.971078603901
C	0.085755079512	2.071159641257	-0.342886537023	C	2.955190624401	-1.252879302528	16.658997658182
H	0.851315536666	2.841481355974	-0.477782170030	C	-1.459383857562	0.837132426539	19.927647682741
H	-0.553381773190	2.077970775622	-1.224909098487	C	-2.592492653024	1.162560471021	17.915097793645
C	0.789936166870	0.732509368283	-0.147502838236	C	-1.411029587040	-4.112146270257	18.084422277696
C	2.758619086348	0.881185807317	-5.431895338512	H	-0.473954085670	-2.665590278801	19.377657351673
C	3.582955228776	1.538472037437	-5.673370669167	C	-2.299579068786	-5.299281963171	16.520481765490
C	2.219174881033	0.827708308411	-4.171624103175	C	2.010406479440	4.005484380459	17.496466742899
H	2.631831896258	1.476899282207	-3.411939736577	H	1.704091222129	2.495330090472	19.002598136386
C	1.488219587857	0.558179590099	1.127413151296	H	2.152326531120	5.268456857734	15.756030443348
H	-0.509869917864	2.351602437203	0.525052797192	C	2.226557526315	-0.598887415633	21.445557177999
H	-4.481602966303	0.722693508027	0.028383441012	C	0.060083830498	0.346737761103	21.935674129867
H	4.490955007253	-0.558901739583	-0.029276400951	C	4.045219031263	-1.533702813309	19.146264991721
C	-2.302431403040	0.208290288759	9.023295994247	C	4.232626758229	-1.784223955642	16.773546453377
C	-2.351750178077	1.340920110614	9.841564995089	H	2.489829668593	-1.126135774266	15.690182622225
C	-1.680672864071	-0.945482008871	9.518351385991	C	-2.546303699709	1.341546962339	20.638623928410
C	-1.836731273325	1.312092973816	11.135028474427	C	-3.704724272202	1.672967442484	18.075885363028
H	-2.843499793069	2.242528636900	9.492202601141	H	-2.574583703582	1.075889316794	16.836524310705
C	-1.167306856751	-0.975819980942	10.809942791377	H	-1.547742012203	-4.843744032940	18.870332696857
H	-1.622161891776	-1.840641688474	8.908207676243	H	2.480289332416	4.702635501182	18.178195088812
C	-1.261207959349	0.144593346954	11.652953483107	C	1.291311513211	-0.138749275146	22.369435564978
H	-1.944674026327	2.190253310767	11.760450947298	H	3.181636653027	-0.975577265342	21.785374770056
H	-0.696971049515	-1.884541738972	11.166983323735	H	-0.664256992536	0.702951303618	22.655374078825
C	2.301853001942	-0.051400491957	-9.021349791365	C	4.7888808404579	-1.927785765467	18.040105614307
C	1.579648293536	1.041304467895	-9.518844629695	H	4.459272616509	-1.637140099065	20.140120191355
C	2.450385611899	-1.177472683080	-9.836590105054	H	4.774539085294	-2.077529783041	15.883857277901
C	1.063391102313	1.021575720233	-10.809572340347	C	-3.682177757910	1.764801138987	19.958312808751
H	1.442362439144	1.929516075737	-8.911182876805	H	-2.508808476275	1.403945286807	21.717792186378
C	1.935429420024	-1.97311612330	-11.130023547554	H	-4.567590832959	1.989517438902	17.994422586158
C	3.018512838901	-2.431761018470	-9.484372226991	H	1.521805063812	-0.158764630479	23.427327572884
C	1.256888773659	-0.087678526111	-11.650647164419	H	5.782630454804	-2.338727200259	18.167706859439
H	0.512195093584	1.883333816652	-11.167288148528	H	-4.531574497016	2.157638275777	20.503365632349
H	2.121893564272	-2.063983679818	-11.752869125123				
C	0.822675242524	-0.068365886158	-13.074783056835				
C	0.970330784797	1.091961845959	-13.851750495129				
C	0.307907132435	-1.215849810482	-13.699032575771				
C	0.628024074890	1.080896173226	-15.202095586560				
H	1.389845882054	1.984600338877	-13.408430697456				
C	-0.023254547399	-1.189135782558	-15.052191764653				
H	0.161221974626	-2.120196586296	-13.124427156270				
N	0.147363279597	-0.052056532770	-15.770953073936				
C	0.753172667726	2.203458490705	-16.155733982818				
C	-0.556078548735	-2.309824134286	-15.855655312108				
Ru	-0.282596270346	-0.056433889586	-17.722650996132				
N	0.378223693930	1.923965498895	-17.444791511414				
C	1.218324286709	3.468620492546	-15.804206072927				
N	-0.766344539666	-2.033776273912	-17.182320422816				
C	-0.832703099844	-3.572003501582	-15.335092032244				
N	-0.702742172788	-0.064761731192	-19.690063845930				
N	1.570202291185	-0.642331668456	-18.553733889481				
N	-2.312319899064	0.527808899400	-17.7291336105973				
C	0.468366607405	2.897738786472	-18.366226596853				
C	1.307730272506	4.467361938786	-16.76547898634				
H	1.511375802413	3.676402299321	-14.783880903119				
C	-1.243390776631	-3.008718259606	-17.974405937907				
H	-0.664858585423	-3.776332270581	-14.286172875035				
C	-1.326787479756	-4.571983029237	-16.165346013794				
C	0.271529464611	-0.402298142612	-20.567815836424				
C	-1.950993236158	0.2679135239					

Table S2 (continued). TD-CAM-B3LYP Cartesian coordinates and energy for S₁(CT-Z) Ru₂(2c²⁺)_{model} (CPD*).

N	0.254160050870	2.324085332328	6.442016190994	H	0.959712569051	0.617788297594	22.552300680434
C	0.206972516568	1.192611059790	3.869313910283	N	-0.611848556966	-2.263443547920	17.629933107306
C	1.020014304235	1.245016250373	6.153343838678	C	-1.262608960068	-4.076567612988	19.049982616248
H	1.657977724841	0.887023771781	6.949916562182	H	-0.705543299865	-3.223789211104	21.681589466609
C	0.449924021728	3.092848084885	7.702495616402	C	1.399481945934	2.546626846190	17.829669436926
H	1.388070989385	3.640304309852	7.597779124092	C	2.000592213776	3.629352774139	19.863960279687
H	-0.350816513967	3.831522606994	7.727118212916	H	1.648014418778	2.454296558043	21.618980640442
C	-0.233910584900	2.841371630940	-1.130257476290	H	0.108510112122	-1.567392364072	23.319624144496
H	-0.267268171202	3.416680333702	-2.047694487567	C	-0.993814168883	-2.987849420502	16.574063991889
C	0.006767139442	3.478436058042	0.072119913581	C	-1.655493489096	-4.817738761569	17.947391426893
C	0.008049981636	1.396652849495	1.335052606534	H	-1.361515282043	-4.491510298279	20.043274356123
C	0.363524543898	-0.770737835153	2.405974971686	C	1.906479166219	3.655426772722	18.483234236147
H	0.412043196698	-1.378693955170	3.302253166362	H	1.310065564825	2.529654966243	16.751323682230
C	0.209619745680	0.610430429907	2.535464896513	H	2.392047891291	4.478185536751	20.410042096554
C	0.169506144858	2.761077992767	1.271387235618	C	-1.518259865698	-4.262853331897	16.686671548521
H	0.470481473202	3.314008191002	2.150807579610	H	-0.870755828834	-2.519717055102	15.606169987307
C	1.005245588645	0.668705887332	4.913856811131	H	-2.062142666109	-5.812852686186	18.0750545698975
H	1.669995277469	-0.165191610510	4.736749595673	H	2.219419694444	4.520241540884	17.913981674256
H	-1.930772016092	0.288394530172	0.283396016816	H	-1.811789910602	-4.805036178639	15.798035003708
H	-2.520909163297	1.198738891744	0.3888821357111	C	-0.322070472704	-0.813835902067	-13.020902114399
H	-2.065794365489	-0.233011322193	1.175829626851	C	0.808514409833	-1.083715983418	-13.795909773538
H	-2.305558582765	-0.263029267635	-0.578526116860	C	-1.402725141370	-0.171509725716	-13.629951956173
C	-0.425895532149	0.651553084238	0.087733987017	C	0.829152413522	-0.729889288139	-15.136953922102
C	-0.567639363002	2.819283442993	5.483790061469	H	1.648535377883	-1.603267228792	-13.356783338209
H	-1.183702346790	3.661115140814	5.768363872577	C	-1.338622507666	0.165349602051	-14.974251202476
H	-0.68157087196	2.289426988246	4.22646566722	H	-2.283593813938	0.065547466880	-13.049919898349
C	-1.300060762685	2.719799819083	3.516849555235	N	-0.236757246804	-0.123864941151	-15.689051530325
C	-0.342928956669	1.452992946414	-1.181803839946	C	1.928884473374	-0.972819896838	-16.099520100402
N	-0.254160050870	-2.324085332328	-6.442016190994	N	-2.395471733464	0.829776402669	-15.772249684137
C	-0.206972516568	-1.192611059790	-3.869313910283	Ru	-0.198991053266	0.318552201083	-17.637700711033
C	1.020014304235	-1.245016250373	-6.153343838678	N	1.690796541989	-0.562917540130	-17.375759911444
H	-1.657977724841	-0.887023771781	-6.949916562182	C	3.126466684904	-1.576876829540	-15.753303016889
C	-0.449924021728	-3.092848084885	-7.702495616402	N	-2.103396771323	0.108670702376	-17.088513737207
H	-1.388070989385	-3.640304309852	-7.597779124092	C	-3.608463633088	1.238470967569	-15.242489736281
H	-0.350816513967	-3.831522606994	-7.727118212916	N	-0.167180137516	0.749496518631	-19.598864463230
C	0.233910584900	-2.841371630940	1.130257476290	C	2.638590817402	-0.754381674751	-18.297595670467
H	0.267268171202	-3.416680333702	2.047694487567	C	4.102746562611	-1.771032156322	-16.718276194900
C	-0.006767139442	-3.478436058042	-0.072119913581	H	3.302399375309	-1.897991485470	-14.736132065596
C	-0.008049981636	-1.396652849495	-1.335052606534	C	-3.013958220712	1.607524352935	-17.868853081656
C	-0.363524543898	0.770737835153	-2.405974971686	H	-3.826355784190	1.084686083348	-14.194828665942
H	-0.412043196698	1.378693955170	-3.302253166362	C	-4.545824982353	1.848670343176	-16.061550229980
C	-0.209619745680	0.610430429907	-2.535464896513	C	-0.615197198389	-0.168533516358	-20.472071329291
C	-0.169506144858	2.761077992767	-1.271387235618	C	0.301319881858	1.945846543185	-19.992938308754
H	-0.470481473202	-3.314008191002	-2.150807579610	C	3.854297248944	-1.352276011117	-18.013224033853
C	-1.005245588645	-0.668705887332	-4.913856811131	H	2.407027457275	-0.414225240210	-19.298318923643
H	-1.669995277469	0.165191610510	-4.736749595673	H	5.042153384229	-2.243096204587	-16.460529668126
C	1.930772016092	-0.288394530172	-0.283396016816	C	-4.243350560097	2.035929415775	-17.398503670517
H	2.520909163297	-1.198738891744	-0.3888821357111	H	-2.740570491981	1.736554333725	-18.907783259673
H	2.065794365489	0.233011322193	-1.175829626851	H	-5.497541764092	2.171847828913	-15.659636962257
C	0.425895532149	-0.651553084238	-0.087733987017	C	-1.083919429277	-1.415747385414	-19.828589401491
C	0.567639363002	-2.819283442993	-5.483790061469	C	-0.604126619365	0.105865943133	-21.832445693617
H	1.183702346790	-3.661115140814	-5.768363872577	C	0.744067320410	2.803850754885	-18.871697129181
C	0.608157087196	-2.289426988246	-4.22646566722	C	0.332948304481	2.267498700598	-21.342471458551
C	1.300060762685	-2.719799819083	-3.516849555235	H	4.585712404182	-1.483257969932	-18.799424996066
C	0.342928956669	-1.452992946414	-1.181803839946	H	-4.943597410101	2.506314571477	-18.075712470362
H	2.305558582765	0.263029267635	-0.578526116860	N	-0.994296344770	-1.446686790174	-18.471165089007
H	0.132824639608	4.554023670797	0.087820445508	C	-1.583400502620	-2.494515125893	-20.540642127180
H	-0.132824639608	-4.554023670797	-0.087820445508	C	-0.125124311277	1.335072193292	-22.262441130010
C	0.455164649255	2.313203531459	8.996367119909	H	-0.959712569051	-0.617788297594	-22.552300680434
C	1.575925912314	2.371608132296	9.818100368694	N	0.611848556966	2.263443547920	-17.629933107306
C	-0.689423894073	1.675287369060	9.473822741786	C	1.262608960068	4.076567612988	-19.049982616248
C	1.543867167065	1.849514476934	11.103301980561	H	0.705543299865	3.223789211104	-21.681589466609
H	2.473968839583	2.873739600927	9.476544065072	C	-1.399481945934	-2.546626846190	-17.829669436926
C	-0.722434230801	1.153349164062	10.756308686773	C	-2.000592213776	-3.629352774139	-19.863960279687
H	-1.577712312388	1.609787265581	8.855331519778	H	-1.648014418778	-2.454296558043	-21.618980640442
C	0.386219424020	1.256519884655	11.602007113140	H	-0.108510112122	1.567392364072	-23.319624144496
H	2.415502584772	1.961103965904	11.736328650962	C	0.993814168883	2.987849420502	-16.574063991889
H	-1.626562519733	0.669134999232	11.104996167646	C	1.655493489096	4.817738761569	-17.947391426893
C	-0.455164649255	-2.313203531459	-8.996367119909	H	1.361515282043	-4.491510298279	-20.043274356123
C	0.689423894073	-1.675287369060	-9.473822741786	C	-1.906479166219	-3.655426772722	-18.483234236147
C	-1.575925912314	-2.371608132296	-9.818100368694	H	-1.310065564825	-2.529654966243	-16.751323682230
C	0.722434230801	-1.153349164062	-10.756308686773	H	-2.392047891291	-4.478185536751	-20.410042096554
H	1.577712312388	-1.609787265581	-8.855331519778	C	1.518259865698	4.262853331897	-16.686671548521
C	-1.543867167065	-1.849514476934	-11.103301980561	H	0.870755828834	-2.519717055102	-15.606169987307
H	-2.473968839583	-2.873739600927	-9.476544065072	H	2.062142666109	5.812852686186	-18.0750545698975
C	-0.386219424020	-1.256519884655	-11.602007113140	H	-2.219419694444	-4.520241540884	-17.913981674256
H	1.626562519733	-0.669134999232	-11.104996167646	H	1.811789910602	4.805036178639	-15.798035003708
H	-2.415502584772	-1.961103965904	-11.736328650962				
C	0.322070472704	0.813835902067	13.020902114399				
C	1.402725141370	0.171509725716	13.629951956173				
C	-0.808514409833	1.083715983418	13.795909773538				
C	1.338622507666	-0.165349602051	14.974251202476				
H	-2.283593813938	-0.065547466880	13.049919898349				
C	-0.829152413522	0.729889288139	15.136953922102				
H	-1.648535377883	1.603267228792	13.356783338209				
N	0.236757246804	0.123864941151	15.689051530325				
C	2.395471733464	-0.829776402669	15.772249684137				
C	-1.928884473374	0.972819896838	16.099520100403				
Ru	0.198991053266	-0.318552201083	17.637700711033				
N	2.103396771323	-0.108670702376	17.088513737208				
C	3.608463633088	-1.238470967569	15.242489736281				
N	-1.690796541989	0.562917540130	17.375759911444				
C	-3.126466684904	1.576876829540	15.753303016889				
N	0.167180137516	-0.749496518631	19.598864463230				
C	3.013958220712	-1.607524352965	17.868853081656				
C	4.545824982353	-1.848670343176	16.061550229980				
H	3.826355784190	-1.084686083348	14.194828665942				
C	-2.638590817402	0.754381674751	18.297595670467				
C	-3.302399375309	1.897991485470	14.736132065596				
H	-4.102746562611	1.771032156322	16.718276194900				
C	0.615197198389	0.168533516358	20.472071329291				
C	-0.301319881858	-1.945846543185	19.992938308755				
C	4.243350560097	-2.035929415775	17.398503670517				
H	2.740570491981	-1.736554333725	18.9				

Table S2 (continued). TD-CAM-B3LYP Cartesian coordinates and energy for S₂(CT-LE) Ru₂(2c²⁺)_{model}.

N	0.205746951248	2.348419039959	6.416403143189	H	1.000566431756	0.596438948214	22.519627289268
C	0.122076061997	1.211566201665	3.854464027881	N	-0.619425468646	-2.259479198900	17.598193958088
C	0.983828827586	1.282051908423	6.116786054782	C	-1.273525130516	-4.072580746221	19.016738224558
H	1.642535525209	0.936884663703	6.902100521229	H	-0.694741504871	-3.231614343048	21.647397222061
C	0.407954610113	3.115357326489	7.679069179654	C	1.423908497478	2.5370599591924	17.800379442831
H	1.346693639799	3.660415136891	7.568479264750	C	2.044323017493	3.609599763633	19.834284442426
H	-0.391239255290	3.855370033132	7.707563008121	H	1.694969803410	2.431330878726	21.587783787188
C	-0.224554442225	2.858091782493	-1.131632178345	H	0.139953317920	-1.585566959804	23.285469573830
H	-0.251182215516	3.430140469999	-2.052407994258	C	-1.012553289172	-2.978172441245	16.542507845167
C	-0.075241214320	3.504215413747	0.069410787454	C	-1.678011743967	-4.807794729851	17.914354454815
C	-0.069580144825	1.399112298929	1.330543885485	H	-1.369165481404	-4.489870691708	20.009366591611
C	0.228012613949	-0.781788733514	2.410501816061	C	1.941942034252	3.640596626826	18.454242649110
H	0.210847591694	-1.375845945267	3.317162225366	H	1.327819400982	2.524090523856	16.722552352841
C	0.111359793890	0.626781742540	2.516640585195	H	2.444508894279	4.454216104874	20.380580370264
C	0.059929004276	2.772824839298	1.271292061391	C	-1.544740088774	-4.250015146770	16.654482449646
H	0.324372728016	3.328278394905	2.161670999927	H	-0.892274195651	-2.507974028267	15.575266594245
C	0.951899509355	0.701826551598	4.877787244221	H	-2.090495880422	-5.800571668462	18.041503878741
H	1.621905957637	-0.124502516506	4.684182744928	H	2.256906024682	4.505199508811	17.885783891249
C	-1.948533394504	0.280192223537	0.171740026757	H	-1.847257808422	-4.787562714052	15.766042467879
H	-2.537841629865	1.196265278300	0.222224291128	C	-0.305114326869	-0.824845564846	-12.992718178176
H	-2.154309411152	-0.310225394293	1.064232608149	C	0.818770892662	-1.099866146407	-13.775631587184
H	-2.280871152909	-0.287596887818	-0.697494812658	C	-1.385683051628	-0.174263060448	-13.593041707777
C	-0.439972170288	0.636471556681	0.062490611181	C	0.833101626723	-0.742611079662	-15.115852203382
C	-0.648100269540	2.825377752896	5.479865047858	H	1.658381874836	-1.625786033123	-13.343360176528
H	-1.272016538269	3.657083629114	5.776996815399	C	-1.327981323377	0.165954422682	-14.936836159321
C	-0.710867500739	2.287577007648	4.224324050602	H	-2.261330209009	0.066895453162	-13.006817255023
H	-1.434482498438	2.691206670335	3.531052515893	N	-0.232483951056	-0.128257627995	-15.659443343496
C	-0.275597772820	1.446433828009	-1.203104312861	C	1.925185878721	-0.989717411467	-16.085991622488
N	-0.205746951248	2.348419039959	6.416403143189	C	-2.385506760682	0.839478488931	-15.726225959487
C	-0.122076061997	-1.211566201665	-3.854464027881	Ru	-0.203975683634	0.319809629997	-17.606790446531
C	0.983828827586	-1.282051908423	-6.116786054782	N	1.681733974557	-0.574397199552	-17.359462988335
H	-1.642535525209	-0.936884663703	-6.902100521229	C	3.121008187547	-1.602483316217	-15.749109980250
C	-0.407954610113	-3.115357326489	-7.679069179654	N	-2.100414033232	1.030366848224	-17.043735926236
H	-1.346693639799	-3.660415136891	-7.568479264750	C	-3.592489360004	1.254454850534	-15.187687310063
H	0.391239255290	-2.855370033132	-7.707563008121	N	-0.181348443990	0.756618663109	-19.566914358309
C	0.224554442225	-2.858091782493	1.131632178345	C	2.622505006511	-0.769066430697	-18.287792264332
H	0.251182215516	-3.430140469999	2.052407994259	C	4.089982986526	-1.799909851128	-16.720767916565
C	0.075241214320	-3.504215413747	-0.069410787454	H	3.301290592943	-1.927870006092	-14.734058130512
C	0.069580144825	-1.399112298929	-1.330543885485	C	-3.011996817002	1.627370307749	-17.816649628303
C	-0.228012613949	0.781788733514	-2.410501816060	H	-3.804853046925	1.099051225677	-14.139127820877
H	-0.210847591694	1.375845945267	-3.317162225366	C	-4.530964847334	1.873126224025	-15.999083920594
C	-0.111359793890	-0.626781742540	-2.516640585195	C	-0.640554730693	-0.155811089771	-20.440169641830
C	-0.059929004276	-2.772824839298	-1.271292061391	C	0.292503653889	1.951112845689	-19.960202233321
H	-0.324372728016	-3.328278394905	-2.161670999927	C	3.836121908212	-1.375581493845	-18.012847078665
C	-0.951899509355	-0.701826551598	-4.877787244221	H	2.386902917444	-0.424366174882	-19.286011645761
H	-1.621905957637	0.124502516506	-4.684182744928	H	5.027948260186	-2.278747887519	-16.470365771704
C	1.948533394504	-0.280192223537	-0.171740026757	C	-4.235629453152	2.062334720261	-17.337357748692
H	2.537841629865	-1.196265278300	-0.222224291128	H	-2.744287818641	1.757690278407	-18.856895126669
C	0.439972170288	-0.636471556681	-0.062490611181	H	-5.478029658804	2.201310945536	-15.590296727396
C	0.648100269540	-2.825377752896	-5.479865047857	C	-1.113338486076	-1.401993156754	-19.797674407258
H	1.272016538269	-3.657083629114	-5.776996815399	C	-0.635966148305	0.122690087239	-21.799746178669
C	0.710867500739	-2.287577007648	-4.224324050602	C	0.747662078903	2.802778120454	-18.839106310650
H	1.434482498438	-2.691206670335	-3.531052515892	C	0.318020669736	2.276714071657	-21.308919350939
C	0.275597772820	-1.446433828009	1.203104312861	H	4.561772398423	-1.508802187787	-18.804002716983
H	2.280871152909	0.287596887818	0.697494812658	H	-4.937024607669	2.539242054670	-18.008796410266
H	0.006962013126	4.582592984541	0.096965469283	N	-1.015632766440	-1.437742968231	-18.440935199352
H	-0.006962013126	-4.582592984541	-0.096965469283	C	-1.624036679182	-2.475327712609	-20.509989600553
C	0.418743678529	2.332488435285	8.970743837445	C	-0.151655606991	1.350104584883	-22.228912879695
C	1.545981283039	2.382297633104	9.784262178387	H	-1.000566431756	-0.596438948214	-22.519627289268
C	-0.726462393777	1.700834272518	9.455136084177	N	0.619425468646	2.259479198900	17.598193958088
C	1.519968176316	1.857356332967	11.068469327639	C	1.273525130516	4.072580746221	19.016738224558
H	2.444473924285	2.880252727629	9.437727073052	H	0.694741504871	3.231614343048	21.647397222061
C	-0.753144294235	1.175963996069	10.736481065204	C	-1.423908497478	-2.5370599591924	17.800379442831
H	-1.620060153903	1.642472089661	8.843568695892	C	-2.044323017493	-3.609599763633	19.834284442426
C	0.362290231384	1.270393187874	11.574343927291	H	-1.694969803410	2.431330878726	21.587783787188
H	2.396801789041	1.962253025983	11.695410535587	H	0.139953317920	-1.585566959804	23.285469573830
H	-1.657658065421	0.696520343043	11.090645383779	C	-1.012553289172	-2.978172441245	16.542507845167
C	-0.418743678529	-2.332488435285	-8.970743837445	C	-1.678011743967	-4.807794729851	17.914354454815
C	0.726462393777	-1.700834272518	-9.455136084177	H	1.369165481404	-4.489870691708	20.009366591611
C	-1.545981283039	-2.382297633104	-9.784262178387	C	1.941942034252	3.640596626826	18.454242649110
C	0.753144294235	-1.175963996069	-10.736481065204	H	1.327819400982	2.524090523856	16.722552352841
H	1.620060153903	-1.642472089661	-8.843568695892	H	2.444508894279	4.454216104874	20.380580370264
H	-1.519968176316	-1.857356332967	-11.068469327639	C	1.544740088774	4.250015146770	16.654482449646
C	-2.444473924285	-2.880252727629	-9.437727073052	H	0.892274195651	-2.507974028267	15.575266594245
C	-0.362290231384	1.270393187874	-11.574343927291	H	2.090495880422	-5.800571668462	18.041503878741
H	1.657658065421	-0.696520343043	-11.090645383779	H	-2.256906024682	4.505199508811	17.885783891249
H	-2.396801789041	-1.962253025983	-11.695410535587	H	1.847257808422	4.787562714052	-15.766042467879
C	0.305114326869	0.824845564846	12.992718178176				
C	1.385683051628	0.174263060448	13.593041707777				
C	-0.818770892662	1.099866146407	13.775631587184				
C	1.327981323377	-0.165954422682	14.936836159321				
H	2.261330209009	-0.066895453162	13.006817255023				
C	-0.833101626723	0.742611079662	15.115852203382				
H	-1.658381874836	1.625786033123	13.343360176528				
N	0.232483951056	0.128257627995	15.659443343496				
C	2.385506760682	-0.839478488931	15.726225959487				
C	-1.925185878721	0.989717411467	16.085991622488				
Ru	0.203975683634	-0.319809629997	17.606790446531				
N	2.100414033232	-1.030366848224	17.043735926236				
C	3.592489360004	-1.254454850534	15.187687310063				
N	-1.681733974557	0.574397199552	17.359462988335				
C	-3.121008187547	1.602483316217	15.749109980250				
N	0.181348443990	-0.756618663109	19.566914358309				
C	3.011996817002	-1.627370307749	17.816649628303				
C	4.530964847334	-1.873126224025	15.999083920594				
H	3.804853046925	-1.099051225677	14.139127820877				
C	-2.622505006511	0.769066430697	18.287792264332				
H	-3.301290592943	1.927870006092	14.734058130512				
C	-4.089982986526	1.799909851128	16.720767916565				
C	0.640554730693	0.155811089771	20.440169641830				
H	2.744287818641	-1.757690278407	18.856895126669				
C	5.478029658804	-2.201310945536	15.590296727396				
C	-3.836121908212	1.375581493845	18.012847078665				
H	-2.386902917444	0.424366174882	19.				

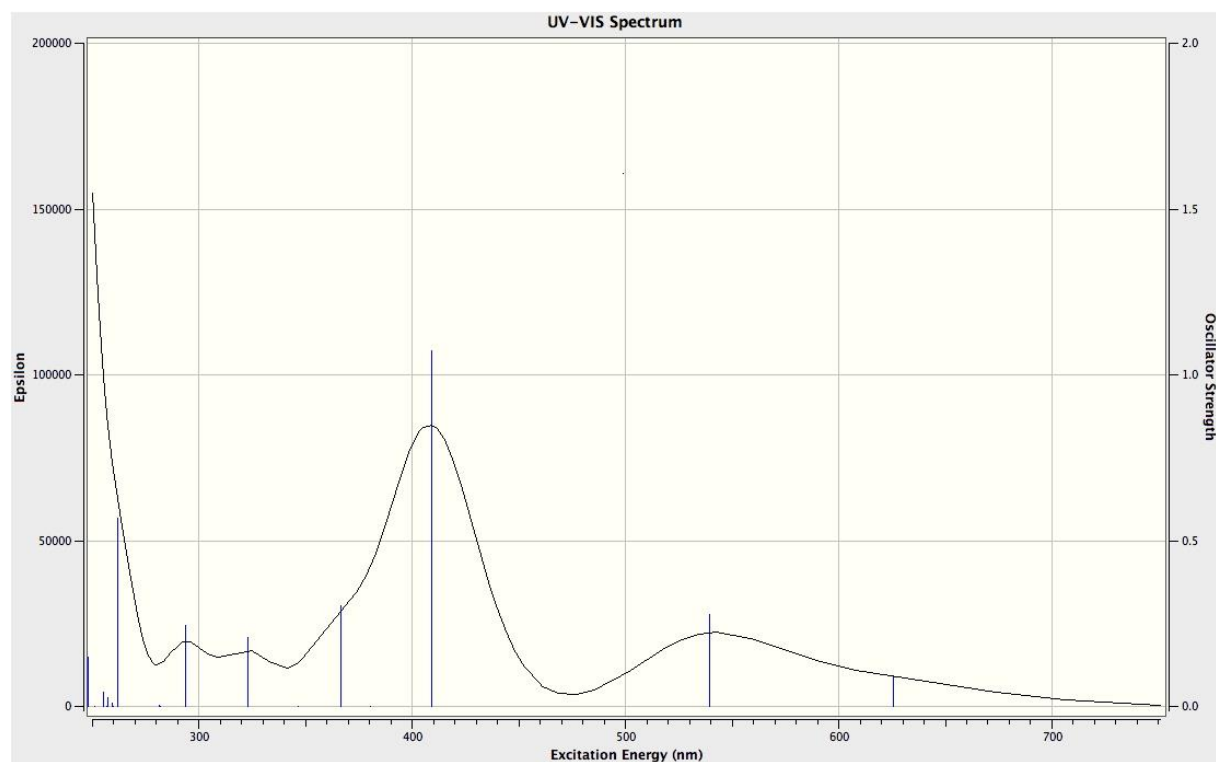


Figure S3. Computed absorption spectrum of $2c^{2+}_{\text{model}}$ at the TD-CAM-B3LYP/6-311G(d,p) level.

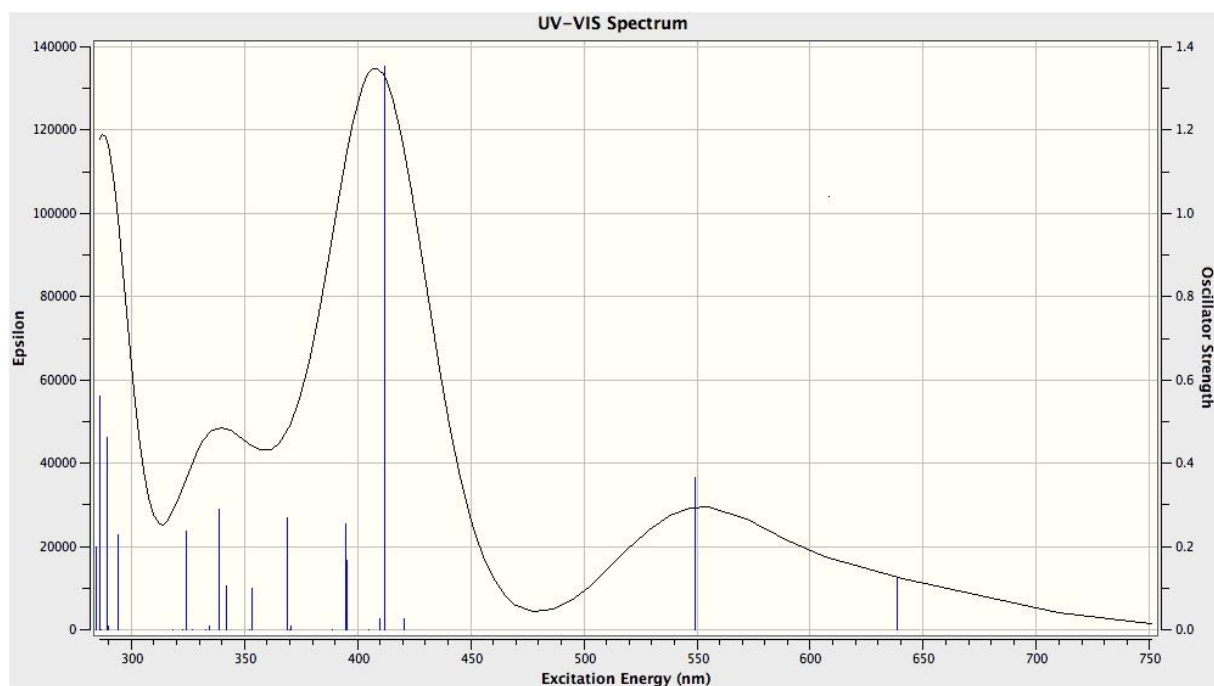


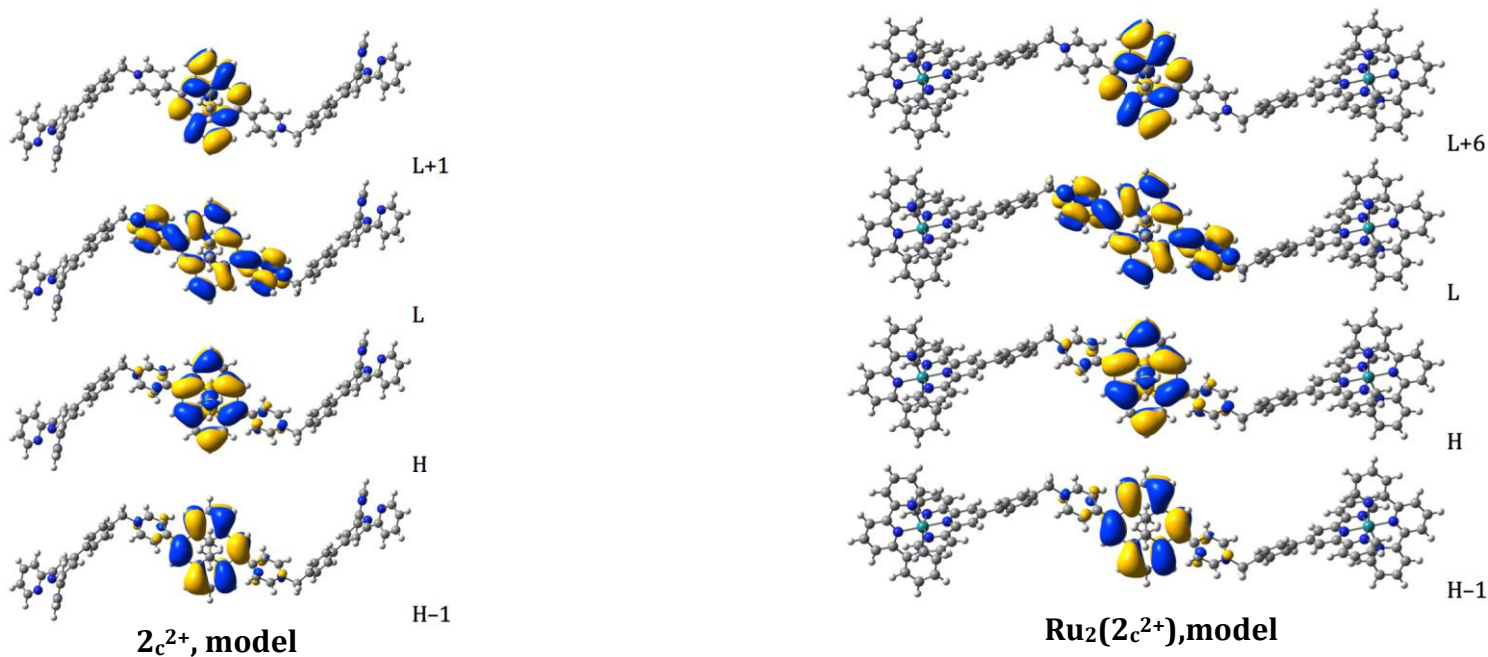
Figure S4. Computed absorption spectrum of $\text{Ru}_2(2\text{c}^{2+})_{\text{model}}$ at the TD-CAM-B3LYP level.

Note that the MLCT transition found just below 400 nm is blue-shifted compared to experiment and is due to a poor description with the CAM-B3LYP functional. This transition is located at 460 nm with the B3LYP functional, in much better agreement with experiment.

Table S3. UV/Vis absorption spectral data and TD-DFT results of $2c^{2+}$,_{model} and $Ru_2(2c^{2+})$,_{model}.

Compounds	State	Exp. λ_{max} /nm ($\epsilon/10^4 \text{ M}^{-1}\text{cm}^{-1}$)	Nature	Excitation Energy /eV	Calc. λ_{abs} /nm	Oscillator Strength (<i>f</i>)	Main transitions and amplitudes ^a
$2c^{2+}$, _{model}	S ₁ (¹ A _u)	686 (0.26)	(π, π^*)	1.983	625	0.089	0.54(H→L)+0.27(H-1→L)-0.25(H-1→L+1)
	S ₂ (¹ A _u)	537 (0.88)	(π, π^*)	2.298	540	0.279	0.44(H-1→L)+0.39(H→L+1)-0.37(H→L)
	S ₃ (¹ A _u)	427 (2.89)	(π, π^*)	3.032	409	1.075	0.52(H→L+1)-0.39(H-1→L)+0.24(H-1→L+1)
	S ₅ (¹ A _u)	322 (2.38)	(π, π^*)	3.382	367	0.305	0.54(H-1→L+1)+0.27(H-1→L)+0.25(H→L+3)
$Ru_2(2c^{2+})$, _{model}	S ₁ (¹ A _u)	689 (0.41)	(π, π^*)	1.942	638	0.126	0.57(H→L)+0.26(H-1→L)-0.24(H-1→L+6)
	S ₂ (¹ A _u)	541 (2.02)	(π, π^*)	2.258	549	0.365	0.47(H-1→L)+0.38(H→L+6)-0.35(H→L)
	S ₁₃ (¹ A _u)	483 (5.33)	MLCT	3.140, 2.698 ^b	395, 460 ^b	0.255, 0.446 ^b	0.31(H-5→L+2)+0.31(H-4→L+1)+0.28(H-5→L+4)+0.28(H-4→L+3), 0.40(H-5→L+2)+0.40(H-4→L+1) ^b
	S ₅ (¹ A _u)	430 (5.43)	(π, π^*)	3.009	412	1.354	0.53(H→L+6)-0.38(H-1→L)+0.21(H-1→L+6)
	S ₁₉ (¹ A _u)	330 (8.92)	(π, π^*)	3.362	369	0.268	0.53(H-1→L+6)+0.24(H-1→L)+0.29(H→L+11)

^a H and L represent the HOMO and LUMO, respectively. ^b Calculated with B3LYP. All other results are obtained with CAM-B3LYP.



4. Kinetic data

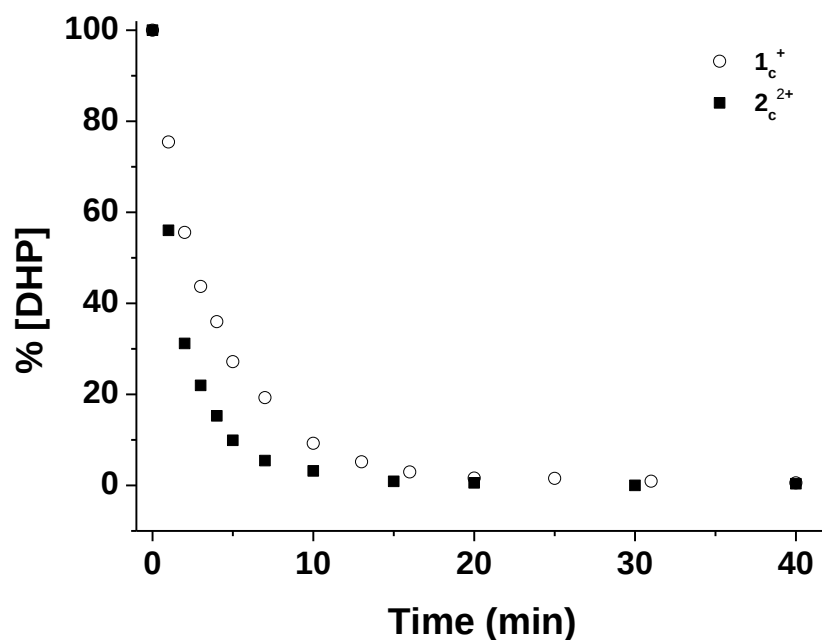


Figure S5. Rate of photo-opening of $1c^+$, $2c^{2+}$, as followed by UV/Vis spectroscopy. The amount of the closed form is determined by the absorbance at the maximum wavelengths

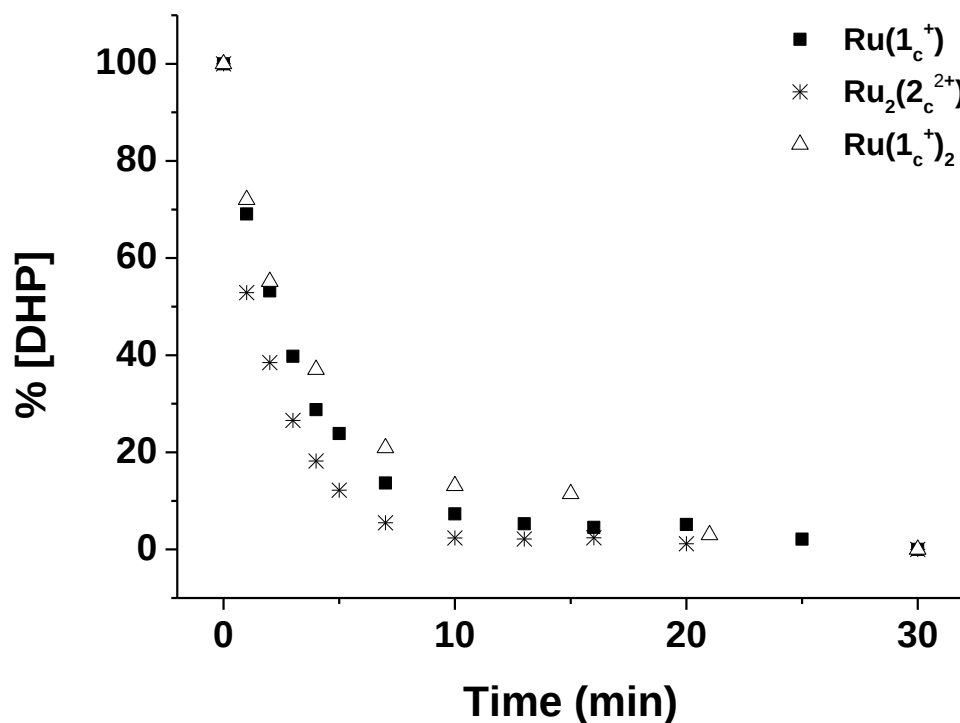


Figure S6. Rate of photo-opening of $Ru(1c^+)$, $Ru_2(2c^{2+})$, $Ru(1c^+)_2$, as followed by UV/Vis spectroscopy. The amount of the closed form is determined by the absorbance at the maximum wavelength

5. Fatigue resistance cycles

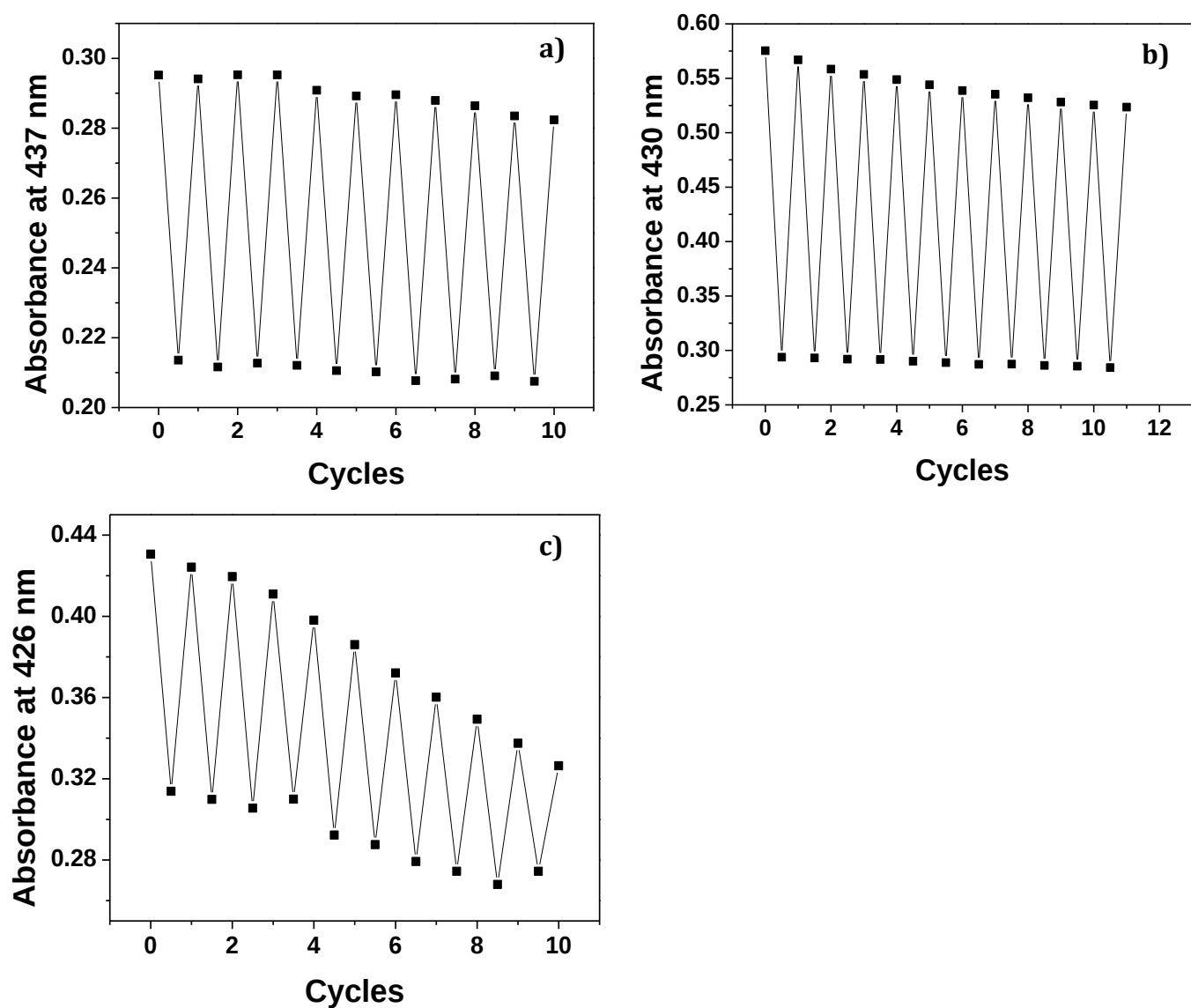


Figure S7 : Fatigue resistance cycles of compound **a) Ru(1c⁺)** , **b) Ru₂(2c²⁺)** and **c) Ru(1c⁺)₂** ($\lambda=630$ nm $t=5$ min and $\lambda=366$ nm $t=30$ s)

6. Additional Electrochemical data

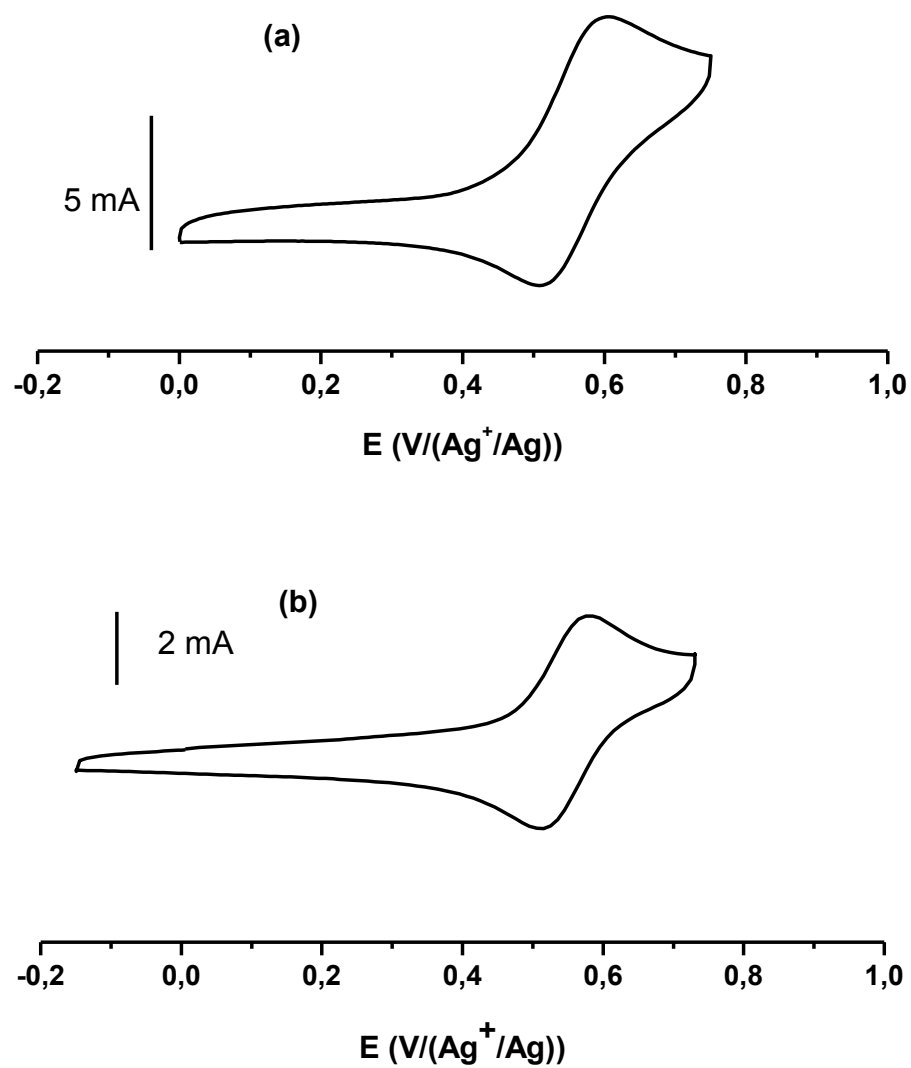


Figure S8. Partial cyclic voltammograms of (a) 2c^{2+} , and (b) $\text{Ru}_2(2\text{c}^{2+})$; 1mM in CH_3CN + 0.1 M TBAP; 0.1 V.s^{-1} ; WE : glassy carbon

7. High resolution –mass spectrometry



Fédération de Recherche Physique et Chimie du Vivant (FR2708 : CBM/ICOA)
Plate-forme de Spectrométrie de Masse Haute Résolution

HRMS

Analysis Info

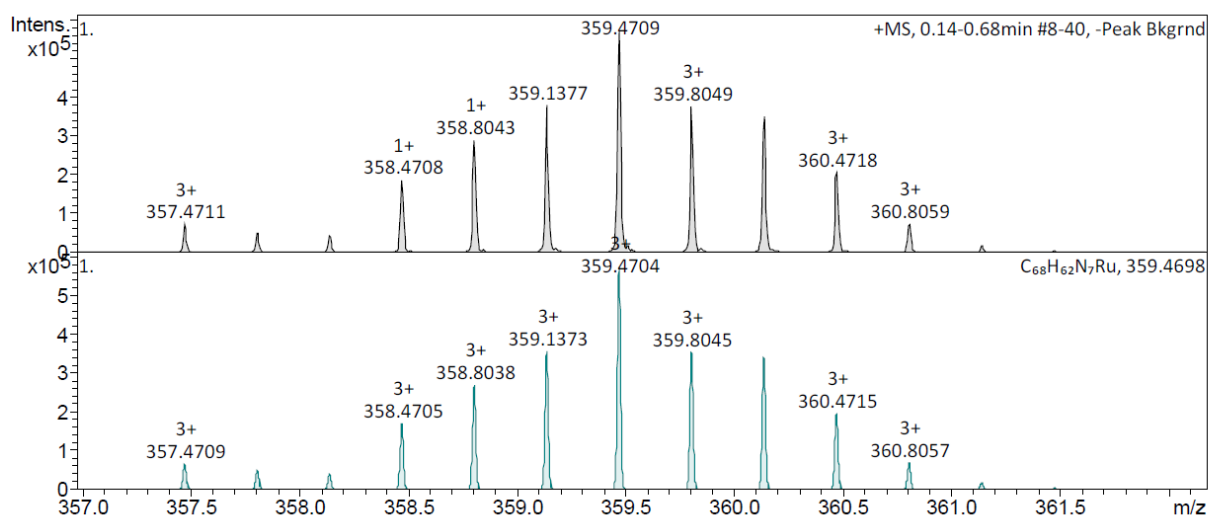
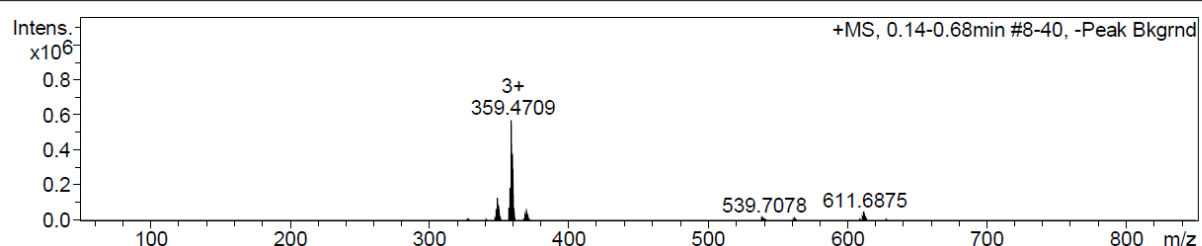
Sample Name **MJ48 Ru**
Analysis Name X012885CYC.d
Method Positif.m

Acquisition Date 05/03/2014 14:16:37

Laboratory
Instrument / Ser# maXis 255552.00086

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
359.470859	3+	1	C72H66NO2Ru	359.471354	1.4	19.7	41.0	odd
	3+	2	C68H62N7Ru	359.470408	-1.3	22.6	42.0	odd
539.707834	2+	1	C63H63N9O2Ru	539.707718	-0.2	90.0	37.5	odd
	2+	2	C68H63N7Ru	539.709799	3.6	90.8	41.5	odd

Figure S9 : HR mass spectra of compound Ru(1c⁺)



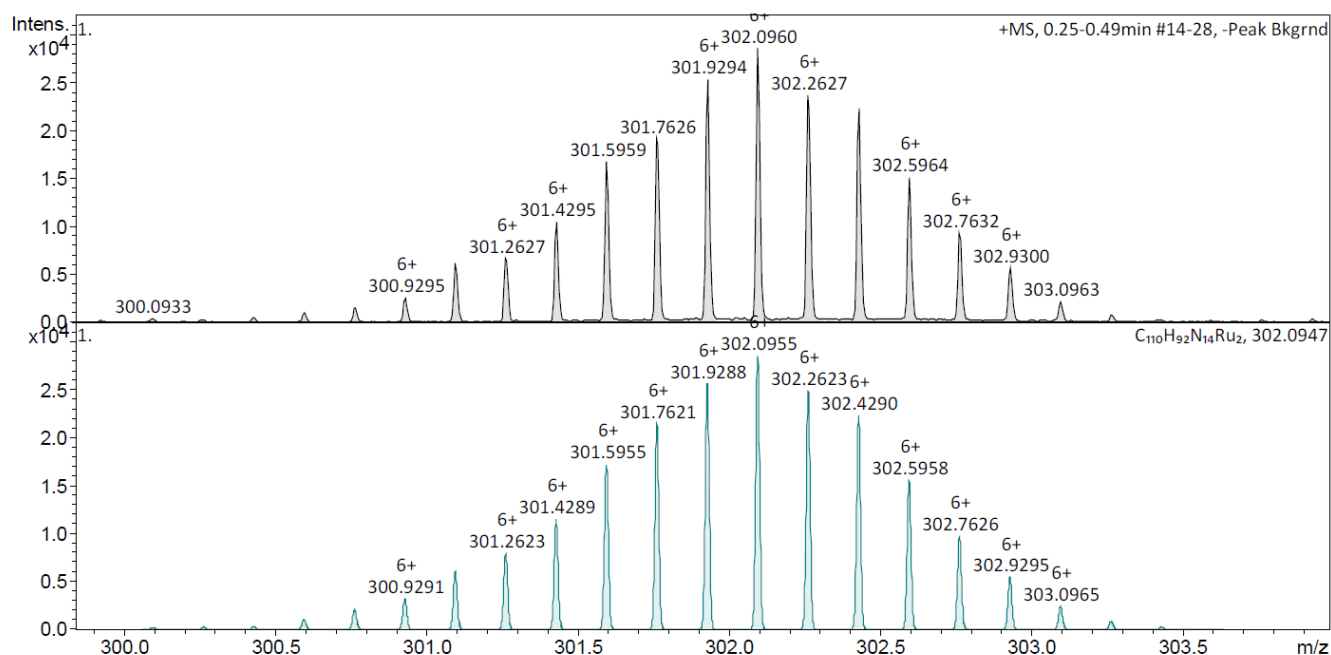
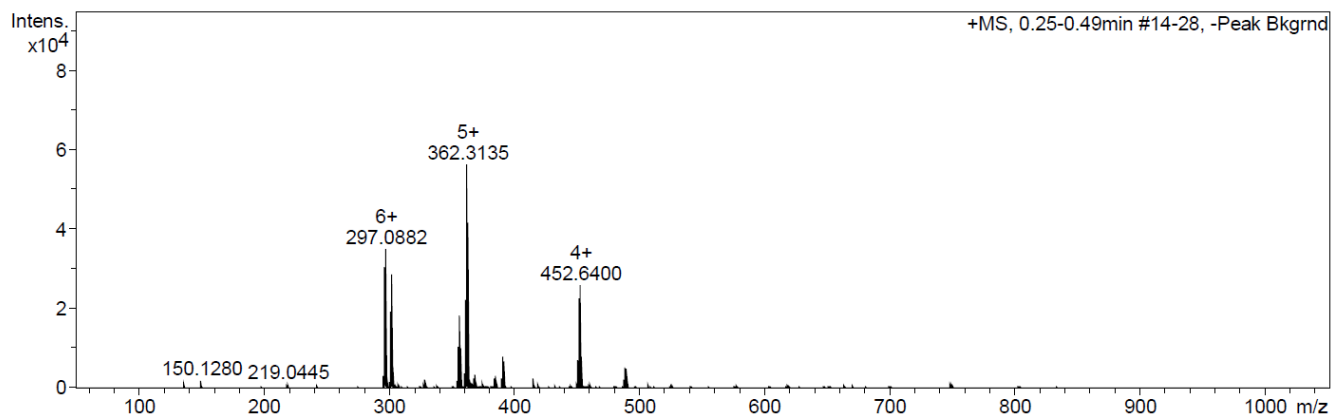
Analysis Info

Sample Name **MJ56**
Analysis Name X020290CYC.d

Acquisition Date 07/07/2015 12:50:29
Instrument / Ser# maXis 255552.00086
Method Positif.m

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Dry Gas	7.0 l/min



Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
297.088196	6+	1	C108H86N14Ru2	297.087643	-1.9	332.0	74.0	even
302.096007	6+	1	C110H92N14Ru2	302.095479	-1.7	332.6	73.0	even
356.304301	5+	1	C108H85N14Ru2	356.303716	-1.6	332.0	74.5	even
362.313531	5+	1	C110H91N14Ru2	362.313119	-1.1	332.6	73.5	even
391.507879	5+	1	C110H92F6N14PRu2	391.507521	-0.9	332.7	70.5	even
452.640044	4+	1	C110H90N14Ru2	452.639580	-3.5	385.2	74.0	even
489.132955	4+	1	C110H91F6N14PRu2	489.132582	-3.1	385.4	71.0	even

Figure S10 : HR mass spectra of compound Ru₂(2c²⁺)

ICMG – Plateau de Spectrometrie de Masse
Elemental Composition
HRMS – ESI/QToF – Waters Xevo G2-SQTof

Reference : SC230
 Dilution : 5 10e-5M ds ACN
 Compound : FOUND
 Error PPM/Target : 0,5340
 Formula : C106H102F24N8P4Ru

	pics simulation	pics mesurés	erreur
1	936,3293	936,3288	0,0005
2	936,8310	936,8310	0,0000
3	937,3312	937,3321	-0,0009
4	937,8292	937,8306	-0,0014
5	938,3292	938,3265	0,0027
6	938,8295	938,8303	-0,0008
7	939,3292	939,3292	0,0000
8	939,8301	939,8296	0,0005
9	940,3302	940,3264	0,0038
nb de pics	9		0,000489 Erreur Moyenne
			0,52 Erreur en PPM
			2 Charge calculée

M target	1872,6586
M	1872,6576
erreur en PPM	0,53

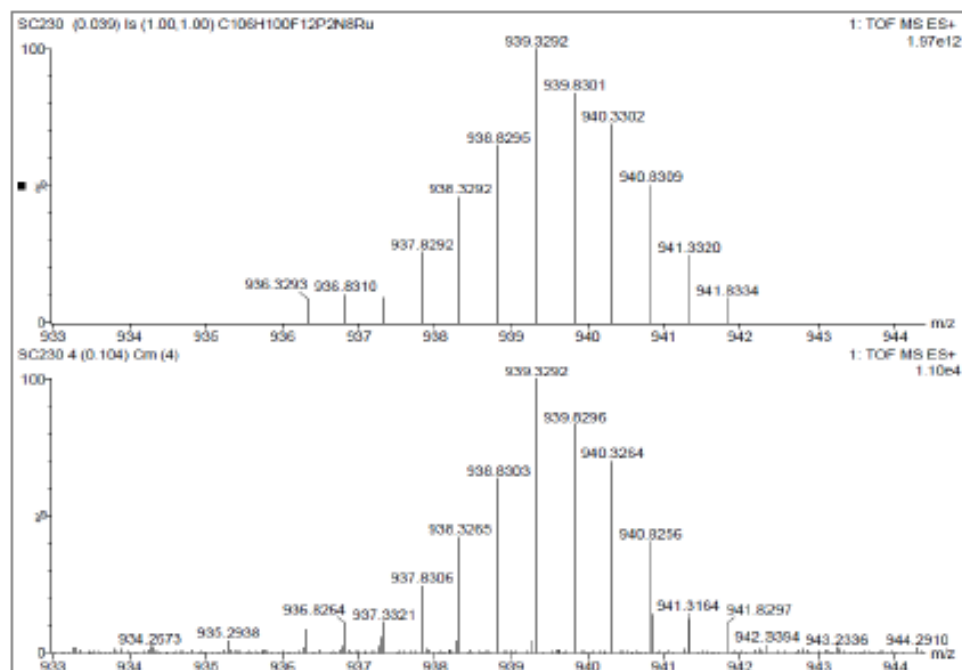


Figure S11 : HR mass spectra of compound Ru(1c⁺)₂