

Supporting Information

Exploring the Photophysics and Excited State Reactivity of $[\text{Ru}(4,4'\text{-BTFMB})_2(\text{L})]^{2+}$ Complexes ($\text{L}=\text{bpy}$, phen , TAP) as Photodynamic Therapy Agents: A Theoretical Investigation

Sandy Veríssimo Moraes Quintão,^{*,†} Aline S. Bozzi,^{*,†} and Willian R. Rocha^{*,†,‡}

[†]*Laboratório de Estudos Computacionais em Sistemas Moleculares, eCsMo^{lab},
Departamento de Química, ICEx, Universidade Federal de Minas Gerais 31270-901,
Pampulha, Belo Horizonte, MG, Brazil*

[‡]*Corresponding author*

E-mail: sandyvmq@ufmg.br; alinebozzi@qui.grad.ufmg.br; wrocha@ufmg.br

Benchmark

In order to determine the most suitable functional for the system, the absorption spectra for **C1** have been carried out using several functionals using def2-TZVP basis set in implicit methanol. The results were compared with the experimental data, which showed two MLCT transitions at 470.0 nm and 438.5 nm, and one IL transition at 296.0 nm (Table S1). The computed absorption peaks shown here are those that have the highest oscillator strength for each corresponding band in the spectrum. As it can be seen, TPSSh and B3LYP were the functionals that best reproduced the experimental data and, since the spectra were very

similar (Figures S1-S2), B3LYP was chosen because it is widely used in other studies of ruthenium with polypyridyl complexes.¹⁻⁵

Table S1: Main electronic absorption transitions, in nanometers, obtained by using several functionals in methanol, on B3LYP/def2-TZVP optimized geometry, and experimental values for **C1**.

Exp ⁶	B3LYP	CAM-B3LYP	PBE0	wB97X-D3BJ	M062X	TPSSh
470.0	453.7	380.8	433.3	345.1	357.5 348.7	470.9
438.5	424.5	357.5	405.9	325.9	333.0	443.0
	280.6	258.7	273.5	252.5	249.3	281.2
296.0	278.6	255.9	271.9	243.6	248.4	272.5
	270.7		262.9		247.4	271.5

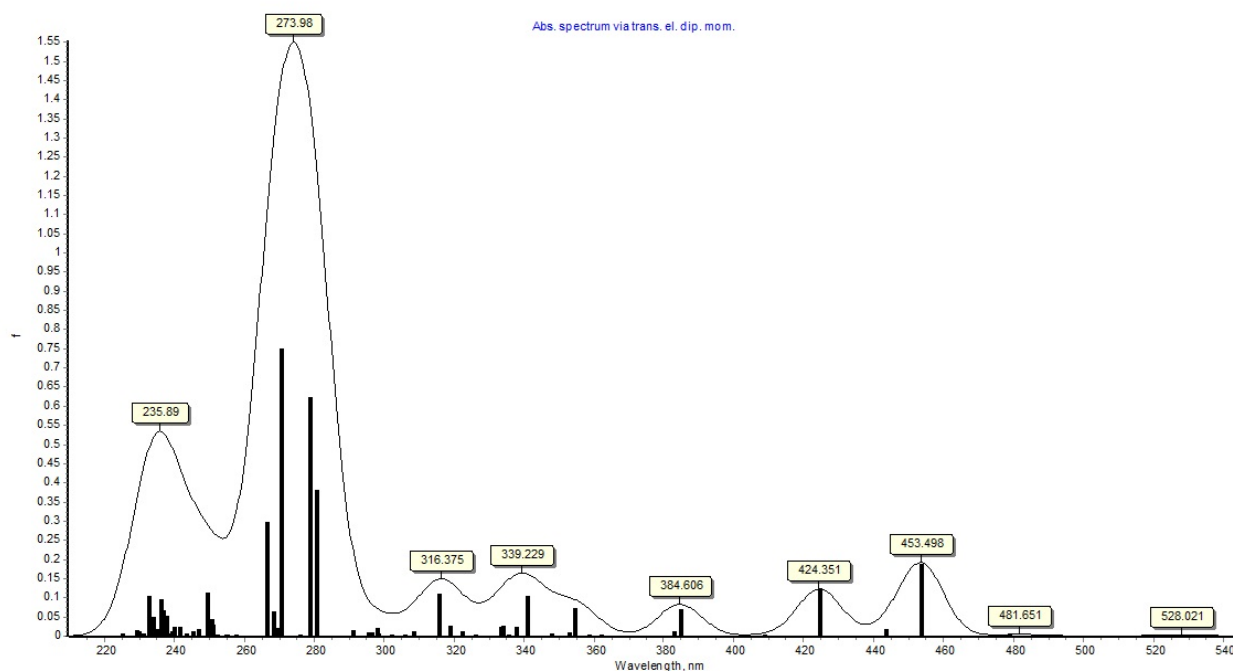


Figure S1: Computed Absorption Spectra of **C1** at B3LYP/def2-TZVP level of theory in methanol.

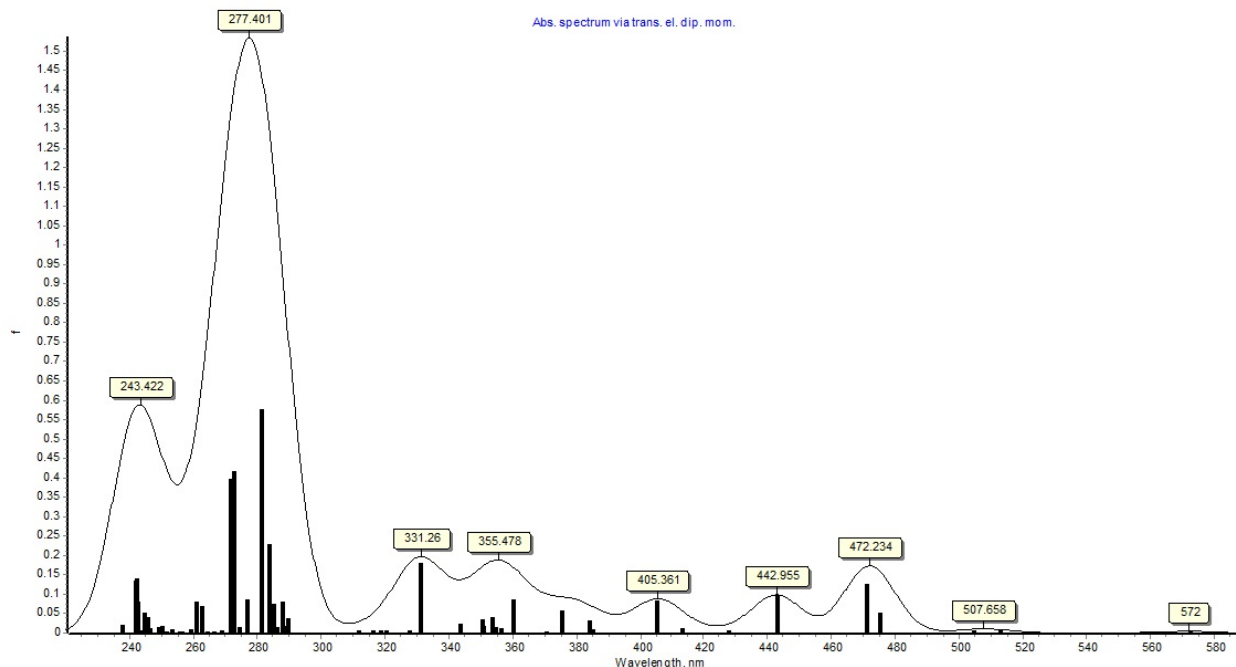


Figure S2: Computed Absorption Spectra of **C1** at TPSSH/def2-TZVP level of theory in methanol.

Cartesian Coordinates

All the Cartesian coordinates for the optimized geometries of S_0 , S_1 , T_1 and T_2 states of all complexes are shown below.

[Ru(4,4'-BTFMB)₂(bpy)]²⁺	
S₀	
Ru -0.828429000 -0.511960000 -0.191697000	H 1.291529000 2.402665000 -3.916224000
N -0.385271000 1.200497000 -1.275462000	N -1.854378000 0.938307000 0.885027000
C 0.392462000 1.243110000 -2.366153000	C -1.769673000 2.199589000 0.391438000
C -0.932640000 2.349307000 -0.804959000	C -2.596324000 0.710913000 1.977700000
C -0.700323000 3.563953000 -1.440512000	C -3.283484000 1.719212000 2.629791000
C 0.658955000 2.421351000 -3.040176000	C -2.438045000 3.253521000 1.004239000
H 0.802056000 0.303388000 -2.703995000	H -2.631314000 -0.307252000 2.334505000
H -1.141044000 4.471530000 -1.056800000	H -3.868708000 1.483919000 3.507356000
	H -2.363812000 4.252096000 0.601253000
	N -2.607436000 -0.937504000 -1.159625000

C -3.105519000 -0.254713000 -2.199470000	C 2.441954000 0.570043000 2.457125000
C -3.313248000 -1.979062000 -0.652140000	H 0.384992000 1.104361000 2.169603000
C -4.539678000 -2.346779000 -1.191000000	H 4.044615000 -1.683839000 0.520317000
C -4.319469000 -0.569167000 -2.781474000	H 2.579746000 1.236194000 3.297145000
H -2.509048000 0.562279000 -2.574402000	C -5.044415000 -1.634954000 -2.266171000
H -5.092067000 -3.177822000 -0.780718000	C -2.560037000 -4.361424000 2.165806000
H -4.677150000 0.010275000 -3.619861000	C -3.203490000 3.013475000 2.134085000
N -1.499755000 -2.147689000 0.889163000	C 0.102603000 3.602971000 -2.569110000
C -2.684201000 -2.669272000 0.478961000	C 3.474428000 -0.232034000 1.984359000
C -0.854189000 -2.721610000 1.912734000	C 2.105826000 -3.567337000 -2.512028000
C -1.348849000 -3.827870000 2.579583000	H -3.728985000 3.825492000 2.617936000
C -3.235714000 -3.778276000 1.105442000	H 0.289863000 4.542223000 -3.071445000
H 0.082268000 -2.275923000 2.209319000	C 4.823309000 -0.176268000 2.655949000
H -0.789437000 -4.251883000 3.400026000	C 3.038086000 -4.552993000 -3.170241000
H -4.177234000 -4.185656000 0.770345000	C -6.392501000 -1.991686000 -2.839676000
N 0.366546000 -1.812235000 -1.270238000	C -3.173110000 -5.541053000 2.877296000
C 1.641232000 -1.937780000 -0.824433000	F -3.753423000 -6.396829000 2.013827000
C -0.036337000 -2.546109000 -2.317024000	F -2.267631000 -6.235851000 3.584914000
C 0.800179000 -3.433505000 -2.966779000	F -4.131201000 -5.141251000 3.742191000
C 2.532122000 -2.815554000 -1.430975000	F -6.481573000 -1.680164000 -4.144865000
H -1.056602000 -2.410248000 -2.640924000	F -6.660562000 -3.304620000 -2.718668000
H 0.429876000 -3.999853000 -3.808858000	F -7.382842000 -1.326178000 -2.204237000
H 3.543479000 -2.910122000 -1.067954000	F 2.853691000 -5.800119000 -2.683300000
N 0.981038000 -0.311899000 0.789447000	F 2.835831000 -4.615685000 -4.499368000
C 1.213406000 0.502323000 1.830201000	F 4.330805000 -4.240252000 -2.972060000
C 1.988867000 -1.086764000 0.317864000	F 5.691391000 -1.063772000 2.143107000
C 3.250485000 -1.062723000 0.902333000	F 4.722348000 -0.430219000 3.977058000

F 5.380665000 1.046762000 2.533379000

S₁

Ru -0.880535000 -0.472784000 -0.154151000

N -0.342081000 1.213355000 -1.216216000

C 0.495851000 1.208728000 -2.261105000

C -0.870364000 2.382775000 -0.774941000

C -0.561120000 3.581032000 -1.404646000

C 0.834349000 2.371460000 -2.928707000

H 0.888129000 0.250001000 -2.563192000

H -0.982673000 4.508480000 -1.048349000

H 1.508717000 2.323969000 -3.771486000

N -1.915078000 1.009871000 0.870056000

C -1.754284000 2.268184000 0.388652000

C -2.709452000 0.795755000 1.926861000

C -3.372435000 1.828589000 2.564025000

C -2.400732000 3.343117000 0.984589000

H -2.801723000 -0.224489000 2.267657000

H -3.998742000 1.613201000 3.417648000

H -2.270005000 4.341469000 0.596042000

N -2.687798000 -0.893537000 -1.090363000

C -3.215074000 -0.170304000 -2.084016000

C -3.328396000 -2.001256000 -0.645501000

C -4.524568000 -2.410070000 -1.218945000

C -4.401364000 -0.525452000 -2.699175000

H -2.664613000 0.702044000 -2.401680000

H -5.029535000 -3.295177000 -0.864990000

H -4.787361000 0.079905000 -3.505975000

N -1.518308000 -2.144711000 0.898201000

C -2.671589000 -2.704016000 0.461128000

C -0.839619000 -2.710167000 1.902249000

C -1.281028000 -3.862705000 2.525649000

C -3.165188000 -3.865510000 1.040467000

H 0.073032000 -2.224564000 2.210758000

H -0.703456000 -4.288638000 3.332729000

H -4.080016000 -4.311421000 0.682791000

N 0.271164000 -1.812415000 -1.228502000

C 1.573145000 -1.926035000 -0.770833000

C -0.155326000 -2.586540000 -2.243419000

C 0.650728000 -3.492858000 -2.878339000

C 2.438906000 -2.853613000 -1.388156000

H -1.180386000 -2.452229000 -2.555680000

H 0.266104000 -4.083032000 -3.695997000

H 3.453855000 -2.956089000 -1.037426000

N 0.933623000 -0.260613000 0.808945000

C 1.199703000 0.594719000 1.812795000

C 1.932807000 -1.081051000 0.312815000

C 3.216330000 -1.025852000 0.894984000

C 2.429439000 0.681529000 2.409153000

H 0.381456000 1.214257000 2.149168000

H 4.002238000 -1.662973000 0.521014000

H 2.593448000 1.374085000 3.220523000

C -5.057098000 -1.665630000 -2.258233000

C -2.457984000 -4.446316000 2.079733000

C -3.215550000 3.121765000 2.083862000	C -0.897932000 2.416471000 -0.780698000
C 0.297389000 3.575280000 -2.493032000	C -0.616384000 3.619831000 -1.413722000
C 3.458802000 -0.164066000 1.928901000	C 0.772994000 2.434048000 -2.964203000
C 1.987094000 -3.622148000 -2.425167000	H 0.867183000 0.312441000 -2.599854000
H -3.722604000 3.950978000 2.557994000	H -1.045894000 4.540775000 -1.049375000
H 0.545304000 4.502073000 -2.992145000	H 1.433806000 2.399054000 -3.818523000
C 4.811066000 -0.084051000 2.571300000	N -1.891255000 1.030490000 0.886203000
C 2.881570000 -4.616511000 -3.102327000	C -1.766229000 2.288046000 0.395096000
C -6.371095000 -2.073596000 -2.883700000	C -2.660376000 0.806672000 1.958420000
C -2.982226000 -5.693556000 2.753938000	C -3.337786000 1.828920000 2.599633000
F -3.764632000 -6.417844000 1.938025000	C -2.427482000 3.353244000 0.993779000
F -1.981931000 -6.488599000 3.169355000	H -2.722694000 -0.213307000 2.308230000
F -3.718785000 -5.376395000 3.838932000	H -3.944731000 1.605269000 3.465399000
F -6.422123000 -1.748861000 -4.186217000	H -2.326050000 4.351755000 0.596310000
F -6.584409000 -3.395729000 -2.784001000	N -2.675773000 -0.864629000 -1.102669000
F -7.403014000 -1.453523000 -2.275498000	C -3.215665000 -0.137080000 -2.086144000
F 2.379189000 -5.872039000 -3.022893000	C -3.305141000 -1.979631000 -0.662914000
F 3.015698000 -4.346714000 -4.423174000	C -4.505040000 -2.390332000 -1.227980000
F 4.120636000 -4.655283000 -2.581747000	C -4.404896000 -0.494575000 -2.695207000
F 5.689708000 -0.966969000 2.065808000	H -2.674835000 0.741992000 -2.402519000
F 4.741178000 -0.313032000 3.904191000	H -5.003168000 -3.280283000 -0.875830000
F 5.359146000 1.146345000 2.426787000	H -4.800974000 0.114897000 -3.494333000
	N -1.483299000 -2.129384000 0.869960000
T₁	C -2.630907000 -2.694629000 0.426792000
Ru -0.853234000 -0.438882000 -0.169828000	C -0.794378000 -2.704887000 1.861754000
N -0.355774000 1.256296000 -1.232620000	C -1.216503000 -3.877005000 2.461874000
C 0.464367000 1.265544000 -2.292427000	C -3.105006000 -3.875456000 0.982819000

H 0.111200000 -2.212224000 2.179856000	C 4.789056000 -0.100138000 2.602284000
H -0.630606000 -4.310463000 3.259221000	C 2.804404000 -4.757749000 -2.967372000
H -4.014085000 -4.327902000 0.618255000	C -6.367013000 -2.052234000 -2.875619000
N 0.283175000 -1.777013000 -1.243154000	C -2.889088000 -5.737684000 2.654797000
C 1.566183000 -1.942597000 -0.749636000	F -3.665041000 -6.455434000 1.826584000
C -0.147476000 -2.550898000 -2.257878000	F -1.875866000 -6.527504000 3.048979000
C 0.634753000 -3.505710000 -2.847101000	F -3.625525000 -5.454768000 3.749610000
C 2.406584000 -2.922043000 -1.319432000	F -6.425634000 -1.727875000 -4.178241000
H -1.154238000 -2.375425000 -2.605621000	F -6.577418000 -3.374992000 -2.774944000
H 0.248237000 -4.092959000 -3.665393000	F -7.397670000 -1.434360000 -2.262649000
H 3.403335000 -3.063521000 -0.933222000	F 2.240901000 -5.982877000 -2.838844000
N 0.929062000 -0.238264000 0.786308000	F 2.970422000 -4.555473000 -4.295569000
C 1.208892000 0.647297000 1.768588000	F 4.031474000 -4.830673000 -2.423424000
C 1.926257000 -1.094183000 0.326894000	F 5.664933000 -0.997917000 2.119581000
C 3.199211000 -1.056480000 0.929704000	F 4.694165000 -0.315374000 3.936258000
C 2.428762000 0.718686000 2.374295000	F 5.353847000 1.122493000 2.456362000
H 0.403348000 1.296910000 2.074549000	
H 3.973016000 -1.724063000 0.585714000	T₂
H 2.601254000 1.432068000 3.164939000	Ru -0.839463000 -0.472554000 -0.178349000
C -5.050777000 -1.641482000 -2.257433000	N -0.437846000 1.241203000 -1.257901000
C -2.385435000 -4.469101000 2.006427000	C 0.309760000 1.256820000 -2.371099000
C -3.219715000 3.121673000 2.107802000	C -0.944031000 2.397244000 -0.760815000
C 0.224426000 3.628727000 -2.516529000	C -0.700791000 3.605173000 -1.399992000
C 3.448068000 -0.169963000 1.938813000	C 0.590931000 2.432892000 -3.041654000
C 1.947963000 -3.693351000 -2.349872000	H 0.679198000 0.304147000 -2.718492000
H -3.738202000 3.942684000 2.584388000	H -1.109784000 4.522628000 -1.004821000
H 0.449424000 4.560494000 -3.017899000	H 1.199764000 2.404047000 -3.933977000

N -1.835995000 0.995070000 0.948689000	C 0.680895000 -3.472317000 -2.900833000
C -1.744145000 2.256434000 0.461395000	C 2.440262000 -2.886529000 -1.353250000
C -2.529891000 0.768992000 2.070667000	H -1.114378000 -2.358004000 -2.658875000
C -3.165517000 1.787565000 2.759962000	H 0.304352000 -4.053819000 -3.727765000
C -2.364392000 3.318174000 1.106977000	H 3.436103000 -3.026533000 -0.963718000
H -2.574558000 -0.250202000 2.423434000	N 0.947956000 -0.272248000 0.814933000
H -3.714885000 1.556388000 3.661458000	C 1.208932000 0.567944000 1.837063000
H -2.288029000 4.318405000 0.708151000	C 1.953340000 -1.080646000 0.315652000
N -2.623705000 -0.918460000 -1.185928000	C 3.230337000 -1.031574000 0.898150000
C -3.104786000 -0.247592000 -2.237066000	C 2.437037000 0.654015000 2.431737000
C -3.308308000 -1.980857000 -0.699364000	H 0.387567000 1.176595000 2.181899000
C -4.505304000 -2.385946000 -1.272848000	H 4.018432000 -1.660988000 0.516696000
C -4.289130000 -0.602592000 -2.859622000	H 2.597192000 1.336926000 3.251374000
H -2.526307000 0.590529000 -2.593351000	C -4.993825000 -1.689559000 -2.366793000
H -5.045374000 -3.232537000 -0.877745000	C -2.503983000 -4.385513000 2.084981000
H -4.636574000 -0.033597000 -3.709452000	C -3.083332000 3.082267000 2.268932000
N -1.546000000 -2.093271000 0.906147000	C 0.074849000 3.624140000 -2.549779000
C -2.684172000 -2.662078000 0.441168000	C 3.471132000 -0.178880000 1.944219000
C -0.894037000 -2.639707000 1.940063000	C 1.994196000 -3.654211000 -2.397544000
C -1.341570000 -3.793037000 2.557015000	H -3.571348000 3.900418000 2.781159000
C -3.188421000 -3.816824000 1.022478000	H 0.270511000 4.560334000 -3.055150000
H 0.001864000 -2.139449000 2.273438000	C 4.822227000 -0.097942000 2.587504000
H -0.784174000 -4.208517000 3.383823000	C 2.862052000 -4.704904000 -3.019103000
H -4.091822000 -4.271427000 0.646619000	C -6.308079000 -2.095307000 -2.990915000
N 0.307671000 -1.766042000 -1.273253000	C -3.040043000 -5.628946000 2.758063000
C 1.594032000 -1.925376000 -0.777523000	F -3.817252000 -6.352770000 1.937204000
C -0.109315000 -2.531667000 -2.307353000	F -2.046488000 -6.425900000 3.185480000

F -3.785165000 -5.303934000 3.834655000
 F -6.361211000 -1.774704000 -4.294176000
 F -6.522654000 -3.418033000 -2.887471000
 F -7.340509000 -1.474493000 -2.383252000
 F 2.312764000 -5.937932000 -2.897302000
 F 3.026021000 -4.495533000 -4.347015000
 F 4.090123000 -4.766912000 -2.475592000
 F 5.702137000 -0.977980000 2.079545000
 F 4.752206000 -0.330329000 3.919556000
 F 5.368253000 1.133820000 2.446655000

[Ru(4,4'-BTFMB)₂(phen)]²⁺

S₀

Ru -3.202029000 2.400363000 -1.607522000
 C -1.858946000 -0.335486000 -1.628254000
 N -2.308927000 0.683470000 -0.881149000
 C -2.175666000 0.623815000 0.466895000
 C -1.563585000 -0.461126000 1.083546000
 C -1.092876000 -1.500507000 0.303107000
 C -1.246501000 -1.444407000 -1.077059000
 N -3.290012000 2.730605000 0.431783000
 C -3.824347000 3.807211000 1.021590000
 C -3.818682000 3.983942000 2.394705000
 C -3.235818000 3.004390000 3.183898000
 C -2.677736000 1.887017000 2.583378000
 C -2.716368000 1.770701000 1.201641000
 C -0.444150000 -2.704745000 0.937095000

C -3.174387000 3.131769000 4.685075000
 F -1.260716000 -3.779390000 0.885687000
 F -0.138084000 -2.500251000 2.229103000
 F 0.693949000 -3.045815000 0.301621000
 F -3.950980000 4.124041000 5.146443000
 F -3.567667000 1.993667000 5.291784000
 F -1.913867000 3.380998000 5.102756000
 C -2.244095000 2.275286000 -4.502198000
 N -3.194968000 1.925145000 -3.625362000
 C -4.302884000 1.283682000 -4.074575000
 C -4.470960000 0.994484000 -5.422757000
 C -3.487179000 1.370064000 -6.321410000
 C -2.350614000 2.018565000 -5.857173000
 N -4.991503000 1.378998000 -1.793631000
 C -5.833174000 1.099519000 -0.789204000
 C -6.991524000 0.366216000 -0.971096000
 C -7.291514000 -0.092812000 -2.246068000
 C -6.432308000 0.196189000 -3.292993000
 C -5.283226000 0.934501000 -3.042124000
 C -3.683255000 1.116954000 -7.795591000
 C -8.512095000 -0.943713000 -2.493592000
 F -4.322584000 2.152124000 -8.385766000
 F -4.423730000 0.016995000 -8.024960000
 F -2.514859000 0.957528000 -8.440011000
 F -9.486386000 -0.705078000 -1.599283000
 F -9.028860000 -0.738471000 -3.719041000
 F -8.210481000 -2.259091000 -2.409177000

C -2.980147000 5.225582000 -2.242201000	H -2.405001000 8.520803000 -2.921737000
C -1.644041000 4.827636000 -1.953899000	H -5.949574000 3.833498000 -2.332097000
C -0.598014000 5.766511000 -2.016745000	H -4.855783000 7.906222000 -3.137349000
C -0.905278000 7.117926000 -2.374280000	H -6.604265000 6.133125000 -2.975646000
C -2.179848000 7.497290000 -2.651069000	H -0.071862000 2.075833000 -1.105057000
C -3.259386000 6.559184000 -2.592360000	H 1.872144000 3.603219000 -1.158844000
C -5.204575000 4.611392000 -2.415014000	H 1.532441000 6.001995000 -1.758077000
N -3.947732000 4.270301000 -2.152081000	
C -4.599567000 6.890772000 -2.863779000	S₁
C -5.565166000 5.914498000 -2.774432000	Ru -3.215629000 2.457733000 -1.632646000
N -1.440974000 3.520342000 -1.629822000	C -1.943466000 -0.317133000 -1.721207000
C -0.204641000 3.117999000 -1.355581000	N -2.355295000 0.709963000 -0.955783000
C 0.889645000 3.988609000 -1.391959000	C -2.234853000 0.639281000 0.422430000
C 0.700159000 5.310982000 -1.721712000	C -1.638906000 -0.500273000 1.001184000
H -1.988990000 -0.248131000 -2.695929000	C -1.204642000 -1.521344000 0.202169000
H -1.452818000 -0.492866000 2.155720000	C -1.363550000 -1.444457000 -1.203690000
H -0.896909000 -2.239026000 -1.720636000	N -3.280533000 2.777750000 0.405365000
H -4.274128000 4.543351000 0.373708000	C -3.742302000 3.883794000 1.016210000
H -4.265969000 4.869213000 2.821290000	C -3.732172000 4.040842000 2.376800000
H -2.224442000 1.115686000 3.187063000	C -3.200602000 2.987762000 3.160857000
H -1.376046000 2.775662000 -4.101799000	C -2.705362000 1.863837000 2.559038000
H -5.358213000 0.488003000 -5.769543000	C -2.734233000 1.748900000 1.153602000
H -1.557008000 2.324606000 -6.522888000	C -0.556015000 -2.739062000 0.787016000
H -5.568760000 1.477323000 0.186118000	C -3.174628000 3.142377000 4.652274000
H -7.635749000 0.166756000 -0.127523000	F -1.256986000 -3.862443000 0.502057000
H -6.652338000 -0.153051000 -4.289646000	F -0.433079000 -2.681303000 2.124930000
H -0.093861000 7.832813000 -2.420075000	F 0.686439000 -2.930480000 0.282620000

F -4.388513000 3.493358000 5.136365000	C -2.128180000 7.551224000 -2.596187000
F -2.802309000 2.020432000 5.293768000	C -3.217576000 6.623220000 -2.582520000
F -2.316588000 4.118748000 5.037189000	C -5.183891000 4.681349000 -2.505197000
C -2.329771000 2.389087000 -4.544602000	N -3.938735000 4.337359000 -2.198077000
N -3.251748000 1.994368000 -3.659991000	C -4.547003000 6.963350000 -2.893680000
C -4.309151000 1.253318000 -4.068891000	C -5.522277000 5.992642000 -2.853984000
C -4.448664000 0.885626000 -5.400544000	N -1.459870000 3.561981000 -1.588851000
C -3.486326000 1.290813000 -6.309834000	C -0.245029000 3.135870000 -1.262129000
C -2.409162000 2.054042000 -5.883498000	C 0.858649000 3.993810000 -1.260967000
N -4.973472000 1.376437000 -1.783352000	C 0.695356000 5.319966000 -1.593012000
C -5.777882000 1.104491000 -0.751146000	H -2.076144000 -0.207652000 -2.787496000
C -6.926853000 0.347241000 -0.897905000	H -1.522845000 -0.559950000 2.072003000
C -7.236344000 -0.144217000 -2.156471000	H -1.037515000 -2.238286000 -1.858148000
C -6.402010000 0.128930000 -3.228911000	H -4.144354000 4.655340000 0.376829000
C -5.266951000 0.897856000 -3.016945000	H -4.125779000 4.940972000 2.823484000
C -3.634263000 0.945640000 -7.773630000	H -2.295471000 1.062800000 3.153779000
C -8.454619000 -1.013920000 -2.366452000	H -1.506526000 2.976073000 -4.167236000
F -4.255222000 1.943767000 -8.436248000	H -5.291839000 0.295126000 -5.723190000
F -4.360356000 -0.168661000 -7.957840000	H -1.640307000 2.386434000 -6.565178000
F -2.441878000 0.757347000 -8.362488000	H -5.493904000 1.508443000 0.208147000
F -9.374872000 -0.830605000 -1.407411000	H -7.553441000 0.154419000 -0.040009000
F -9.044405000 -0.765726000 -3.549032000	H -6.633096000 -0.250561000 -4.212189000
F -8.115832000 -2.319910000 -2.355926000	H -0.047000000 7.863097000 -2.295060000
C -2.960851000 5.284785000 -2.237878000	H -2.335056000 8.579593000 -2.861994000
C -1.640918000 4.871766000 -1.914502000	H -5.934035000 3.904895000 -2.464349000
C -0.584086000 5.798231000 -1.931117000	H -4.789381000 7.983684000 -3.161464000
C -0.866189000 7.156143000 -2.283873000	H -6.551920000 6.222068000 -3.087686000

H -0.144196000 2.092016000 -1.004829000	N -3.249855000 1.978799000 -3.654849000
H 1.828123000 3.597761000 -0.995036000	C -4.308329000 1.247841000 -4.076758000
H 1.538003000 5.999228000 -1.595604000	C -4.438216000 0.885652000 -5.411227000
	C -3.463494000 1.285400000 -6.310060000
	C -2.385128000 2.039224000 -5.870478000
T₁	N -4.996270000 1.361902000 -1.794887000
Ru -3.233362000 2.439186000 -1.616863000	C -5.814714000 1.090178000 -0.773271000
C -1.992162000 -0.336038000 -1.712999000	C -6.965831000 0.339503000 -0.936553000
N -2.380086000 0.706232000 -0.950141000	C -7.262107000 -0.146213000 -2.200664000
C -2.229454000 0.642461000 0.428019000	C -6.413228000 0.126945000 -3.261937000
C -1.622274000 -0.490962000 1.005969000	C -5.277515000 0.890649000 -3.034264000
C -1.213989000 -1.522502000 0.209177000	C -3.599312000 0.944537000 -7.775640000
C -1.408917000 -1.457619000 -1.194199000	C -8.481601000 -1.009299000 -2.428935000
N -3.312381000 2.757464000 0.395410000	F -4.215466000 1.944108000 -8.441233000
C -3.778074000 3.868844000 1.004377000	F -4.323611000 -0.169677000 -7.969243000
C -3.721586000 4.051217000 2.356403000	F -2.402212000 0.758050000 -8.355956000
C -3.130439000 3.030789000 3.146342000	F -9.411006000 -0.828602000 -1.478133000
C -2.639776000 1.902884000 2.552709000	F -9.058401000 -0.751031000 -3.615975000
C -2.722131000 1.754241000 1.153566000	F -8.148345000 -2.316920000 -2.423648000
C -0.557275000 -2.738332000 0.788288000	C -2.979980000 5.272865000 -2.214365000
C -3.051179000 3.224643000 4.629695000	C -1.660271000 4.856378000 -1.888147000
F -1.259842000 -3.862495000 0.512671000	C -0.602792000 5.782692000 -1.895091000
F -0.419488000 -2.677388000 2.124242000	C -0.882427000 7.143347000 -2.239510000
F 0.679411000 -2.928491000 0.269919000	C -2.142853000 7.541455000 -2.554551000
F -4.279456000 3.379539000 5.178884000	C -3.233224000 6.614403000 -2.551153000
F -2.462531000 2.196561000 5.264648000	C -5.203203000 4.677533000 -2.486859000
F -2.351590000 4.339772000 4.947764000	N -3.959917000 4.328126000 -2.180784000
C -2.316751000 2.369025000 -4.529224000	

C -4.561315000 6.960220000 -2.863748000
 C -5.538518000 5.991733000 -2.831171000
 N -1.477903000 3.544243000 -1.571144000
 C -0.262610000 3.115688000 -1.246821000
 C 0.840626000 3.973966000 -1.235880000
 C 0.676514000 5.302767000 -1.557128000
 H -2.146538000 -0.238760000 -2.776866000
 H -1.483414000 -0.538231000 2.074290000
 H -1.103304000 -2.261124000 -1.846002000
 H -4.219491000 4.617504000 0.364982000
 H -4.118348000 4.951152000 2.799912000
 H -2.185687000 1.126786000 3.147641000
 H -1.492305000 2.949002000 -4.142892000
 H -5.282736000 0.302596000 -5.744553000
 H -1.606643000 2.368082000 -6.543249000
 H -5.539909000 1.488400000 0.191284000
 H -7.604252000 0.147189000 -0.087019000
 H -6.634626000 -0.248116000 -4.249387000
 H -0.062473000 7.849746000 -2.242444000
 H -2.347702000 8.571973000 -2.814239000
 H -5.956451000 3.903332000 -2.450069000
 H -4.800283000 7.983041000 -3.125900000
 H -6.567466000 6.224356000 -3.065887000
 H -0.161384000 2.069565000 -0.998503000
 H 1.809987000 3.576247000 -0.971189000
 H 1.518580000 5.983166000 -1.552277000

T₂

Ru -3.239412000 2.390140000 -1.610065000
 C -1.904023000 -0.357607000 -1.709646000
 N -2.325755000 0.675452000 -0.950273000
 C -2.140651000 0.638583000 0.421812000
 C -1.474662000 -0.455171000 0.998304000
 C -1.035427000 -1.483144000 0.205589000
 C -1.260880000 -1.446445000 -1.191651000
 N -3.341394000 2.698689000 0.411806000
 C -3.887263000 3.767229000 1.032585000
 C -3.802388000 3.964661000 2.381158000
 C -3.106383000 3.001417000 3.152672000
 C -2.547794000 1.907985000 2.543738000
 C -2.663701000 1.744645000 1.154282000
 C -0.319760000 -2.662209000 0.790054000
 C -2.990269000 3.210016000 4.631083000
 F -0.987328000 -3.817138000 0.555505000
 F -0.149933000 -2.569126000 2.120628000
 F 0.909435000 -2.819314000 0.243405000
 F -4.205041000 3.355291000 5.211404000
 F -2.371537000 2.195636000 5.259792000
 F -2.296211000 4.337092000 4.922071000
 C -2.179390000 2.106016000 -4.464099000
 N -3.192773000 1.849979000 -3.630165000
 C -4.295664000 1.212283000 -4.089405000
 C -4.397359000 0.825537000 -5.418687000
 C -3.345892000 1.100408000 -6.278084000

C -2.217117000 1.747961000 -5.799923000	C 0.824801000 3.974650000 -1.392941000
N -5.057523000 1.428093000 -1.840952000	C 0.624629000 5.312905000 -1.646873000
C -5.932214000 1.239994000 -0.846049000	H -2.087304000 -0.281624000 -2.770028000
C -7.129604000 0.573756000 -1.039849000	H -1.313643000 -0.484945000 2.064154000
C -7.423053000 0.101152000 -2.309445000	H -0.935988000 -2.244690000 -1.840483000
C -6.519477000 0.292510000 -3.343385000	H -4.411253000 4.470745000 0.404541000
C -5.331522000 0.959030000 -3.083294000	H -4.258794000 4.831175000 2.833468000
C -3.457311000 0.734291000 -7.739415000	H -2.018048000 1.173259000 3.128640000
C -8.703940000 -0.653604000 -2.582999000	H -1.318236000 2.608004000 -4.051283000
F -4.074474000 1.716151000 -8.430620000	H -5.278483000 0.317729000 -5.779752000
F -4.172189000 -0.389390000 -7.920603000	H -1.376641000 1.976997000 -6.438407000
F -2.253490000 0.545775000 -8.302859000	H -5.661483000 1.632918000 0.121817000
F -9.619988000 -0.460119000 -1.622655000	H -7.807430000 0.440887000 -0.209776000
F -9.254210000 -0.280423000 -3.752702000	H -6.739616000 -0.071739000 -4.335357000
F -8.471150000 -1.980486000 -2.657696000	H -0.180355000 7.870875000 -2.203071000
C -3.057319000 5.247883000 -2.149217000	H -2.499264000 8.576464000 -2.649896000
C -1.718196000 4.841994000 -1.891935000	H -6.021423000 3.846378000 -2.311356000
C -0.676534000 5.784414000 -1.909890000	H -4.952212000 7.963723000 -2.875613000
C -0.989199000 7.151953000 -2.190674000	H -6.690544000 6.174971000 -2.809289000
C -2.268061000 7.540772000 -2.437031000	H -0.133927000 2.041381000 -1.217755000
C -3.342992000 6.596751000 -2.421750000	H 1.810858000 3.583014000 -1.187738000
C -5.279271000 4.630231000 -2.349389000	H 1.455089000 6.007524000 -1.649691000
N -4.019917000 4.286265000 -2.112419000	
C -4.688845000 6.935270000 -2.663681000	[Ru(4,4'-BTFMB) ₂ (TAP)] ²⁺
C -5.648995000 5.951585000 -2.627152000	S ₀
N -1.500115000 3.520845000 -1.645218000	Ru -4.959824000 2.725345000 -2.459031000
C -0.262861000 3.097246000 -1.404090000	C -2.264072000 3.742130000 0.679824000

C -1.212848000 4.412540000 0.082532000	C -5.750819000 5.567327000 -1.718241000
C -1.222518000 4.618659000 -1.291342000	C -6.600300000 6.647632000 -1.586022000
C -2.292194000 4.139495000 -2.021741000	C -7.910855000 6.519268000 -2.029595000
N -3.317365000 3.490067000 -1.451909000	C -8.326841000 5.326609000 -2.591589000
C -3.312760000 3.288134000 -0.112063000	C -8.858656000 7.683435000 -1.877495000
C -5.799551000 1.615628000 2.165694000	F -10.070562000 7.433978000 -2.396373000
C -4.660931000 2.291856000 1.767561000	F -9.034182000 7.997526000 -0.576633000
C -4.479986000 2.575804000 0.418388000	F -8.377867000 8.785885000 -2.486704000
N -5.396475000 2.199665000 -0.506007000	C -10.567297000 1.035026000 -4.891476000
C -6.498768000 1.547637000 -0.109224000	F -10.635278000 1.371383000 -6.197998000
C -6.737758000 1.234923000 1.214645000	F -11.568729000 1.678659000 -4.265152000
C -0.057768000 4.933769000 0.901013000	F -10.818112000 -0.282745000 -4.808998000
C -6.033718000 1.277883000 3.617661000	C -4.562847000 4.213652000 -5.159762000
F 0.006993000 6.280494000 0.845825000	C -4.020049000 4.292528000 -6.455875000
F 1.118395000 4.463818000 0.438876000	N -3.245702000 3.359973000 -6.974957000
F -0.148347000 4.590611000 2.195149000	C -2.983665000 2.282967000 -6.201414000
F -6.041731000 -0.057545000 3.812088000	C -3.526611000 2.189749000 -4.909601000
F -5.090660000 1.793829000 4.421154000	N -4.313416000 3.167640000 -4.385537000
F -7.225691000 1.743287000 4.042758000	C -2.150373000 1.217975000 -6.671877000
C -6.958268000 0.849891000 -3.801216000	C -1.887673000 0.135891000 -5.890722000
N -6.744893000 2.065566000 -3.281345000	C -2.439637000 0.024460000 -4.574298000
C -7.754555000 2.971687000 -3.276160000	C -3.260791000 1.060778000 -4.100910000
C -9.007328000 2.653041000 -3.783565000	N -3.831093000 1.024063000 -2.866492000
C -9.220363000 1.389599000 -4.309439000	N -2.182654000 -1.050929000 -3.796744000
C -8.180460000 0.471415000 -4.326561000	C -2.736542000 -1.066629000 -2.600153000
C -7.421282000 4.276629000 -2.695676000	C -3.566390000 -0.036905000 -2.118144000
N -6.145537000 4.405501000 -2.258476000	H -2.267492000 3.573830000 1.744584000

H -0.419766000 5.137978000 -1.795275000	C -4.578608000 2.274068000 1.843864000
H -2.337568000 4.281564000 -3.090107000	C -4.437688000 2.587197000 0.497568000
H -3.926625000 2.595165000 2.496586000	N -5.412847000 2.280465000 -0.391837000
H -7.203592000 1.267508000 -0.876137000	C -6.534870000 1.679956000 0.024261000
H -7.641390000 0.707384000 1.485356000	C -6.731912000 1.338060000 1.347715000
H -6.128988000 0.159905000 -3.784087000	C 0.112961000 4.732874000 0.797810000
H -9.808079000 3.375804000 -3.763535000	C -5.926211000 1.259142000 3.715307000
H -8.304107000 -0.522981000 -4.729305000	F 0.234846000 6.074323000 0.752997000
H -4.726328000 5.627815000 -1.387017000	F 1.235982000 4.213765000 0.266638000
H -6.235903000 7.563494000 -1.142705000	F 0.071375000 4.373181000 2.088626000
H -9.340136000 5.213398000 -2.941909000	F -5.901804000 -0.080319000 3.862925000
H -5.185873000 5.003626000 -4.767488000	F -4.974843000 1.770469000 4.509729000
H -4.240840000 5.160897000 -7.064721000	F -7.115614000 1.689318000 4.174903000
H -1.736147000 1.303732000 -7.667438000	C -6.885093000 0.871807000 -3.795561000
H -1.256826000 -0.669405000 -6.242235000	N -6.742288000 2.087942000 -3.259171000
H -2.538634000 -1.920340000 -1.963324000	C -7.759729000 2.980981000 -3.318182000
H -4.006879000 -0.091351000 -1.133780000	C -8.967482000 2.643517000 -3.912100000
	C -9.114881000 1.377104000 -4.454822000
S₁	C -8.062578000 0.475969000 -4.404100000
	C -7.478677000 4.285890000 -2.714661000
Ru -5.007700000 2.770826000 -2.361002000	N -6.255436000 4.409030000 -2.145730000
C -2.160618000 3.653710000 0.677339000	C -5.911740000 5.551807000 -1.537768000
C -1.109063000 4.279144000 0.032403000	C -6.762788000 6.638547000 -1.491753000
C -1.170810000 4.503260000 -1.336556000	C -8.009383000 6.528434000 -2.093927000
C -2.294664000 4.085597000 -2.022873000	C -8.377943000 5.344341000 -2.705980000
N -3.318151000 3.485964000 -1.402363000	C -8.947643000 7.713417000 -2.066586000
C -3.266326000 3.262563000 -0.068018000	F -10.093048000 7.474013000 -2.720774000
C -5.734529000 1.641657000 2.265067000	

F -9.264137000 8.048008000 -0.800983000	H -9.781387000 3.351068000 -3.946438000
F -8.373426000 8.791950000 -2.632647000	H -8.141148000 -0.517536000 -4.819628000
C -10.411403000 0.999775000 -5.134727000	H -4.930263000 5.594766000 -1.091388000
F -10.398031000 1.373620000 -6.430628000	H -6.445265000 7.546434000 -0.999074000
F -11.466774000 1.597818000 -4.557509000	H -9.344733000 5.247678000 -3.173191000
F -10.625019000 -0.325190000 -5.101512000	H -5.303579000 5.061258000 -4.696548000
C -4.687648000 4.269257000 -5.097803000	H -4.432489000 5.191305000 -7.005982000
C -4.193652000 4.335819000 -6.388869000	H -1.921791000 1.328700000 -7.656899000
N -3.409401000 3.377727000 -6.931147000	H -1.381315000 -0.622341000 -6.233024000
C -3.123041000 2.329240000 -6.162699000	H -2.491142000 -1.835086000 -1.879969000
C -3.615928000 2.229589000 -4.834928000	H -3.939394000 -0.027533000 -1.013885000
N -4.397765000 3.232725000 -4.298849000	
C -2.299795000 1.252890000 -6.645734000	T₁
C -2.004592000 0.182328000 -5.865537000	Ru -4.984719000 2.762919000 -2.372854000
C -2.506381000 0.072500000 -4.521826000	C -2.162426000 3.666098000 0.680972000
C -3.328394000 1.126747000 -4.043258000	C -1.105415000 4.285670000 0.038798000
N -3.861320000 1.079356000 -2.771066000	C -1.156519000 4.500622000 -1.332427000
N -2.212105000 -0.977390000 -3.758236000	C -2.275434000 4.078363000 -2.023471000
C -2.726889000 -0.987235000 -2.508668000	N -3.304056000 3.483171000 -1.405518000
C -3.535449000 0.021949000 -2.014860000	C -3.263620000 3.270342000 -0.068540000
H -2.119535000 3.470912000 1.739123000	C -5.744866000 1.674105000 2.268002000
H -0.366717000 4.988082000 -1.871596000	C -4.591367000 2.311185000 1.846729000
H -2.387137000 4.235863000 -3.086951000	C -4.438635000 2.598556000 0.495823000
H -3.802244000 2.520488000 2.550517000	N -5.398819000 2.264087000 -0.398490000
H -7.283205000 1.462626000 -0.722320000	C -6.515508000 1.654359000 0.016116000
H -7.648784000 0.848758000 1.643786000	C -6.725609000 1.337100000 1.344695000
H -6.041296000 0.203632000 -3.724323000	C 0.110875000 4.743789000 0.810802000

C -5.944366000 1.319890000 3.723840000	C -4.682943000 4.255494000 -5.098536000
F 0.227500000 6.085764000 0.766605000	C -4.206788000 4.311938000 -6.398098000
F 1.238605000 4.228881000 0.285617000	N -3.440540000 3.347817000 -6.949532000
F 0.063739000 4.383952000 2.101454000	C -3.149723000 2.299174000 -6.183428000
F -5.863713000 -0.013381000 3.907114000	C -3.625316000 2.210980000 -4.849111000
F -5.028013000 1.891635000 4.519309000	N -4.390298000 3.220201000 -4.301448000
F -7.158105000 1.708757000 4.155604000	C -2.342566000 1.214423000 -6.669990000
C -6.867977000 0.876642000 -3.822597000	C -2.045970000 0.148364000 -5.883669000
N -6.727335000 2.087218000 -3.272265000	C -2.531051000 0.052297000 -4.532382000
C -7.744934000 2.980359000 -3.324480000	C -3.340794000 1.112623000 -4.054835000
C -8.947890000 2.650644000 -3.932514000	N -3.866384000 1.088306000 -2.775238000
C -9.092870000 1.390556000 -4.491089000	N -2.230762000 -0.990595000 -3.761470000
C -8.042025000 0.487695000 -4.442252000	C -2.731899000 -0.977894000 -2.501272000
C -7.469993000 4.279290000 -2.701994000	C -3.527182000 0.034299000 -2.007507000
N -6.241523000 4.407481000 -2.148254000	H -2.128210000 3.491304000 1.744503000
C -5.898956000 5.548200000 -1.536821000	H -0.347926000 4.981087000 -1.864976000
C -6.758703000 6.627574000 -1.468602000	H -2.359825000 4.219380000 -3.089709000
C -8.014647000 6.510048000 -2.049076000	H -3.826392000 2.580474000 2.557744000
C -8.381215000 5.327398000 -2.665878000	H -7.251877000 1.410484000 -0.734737000
C -8.966027000 7.683140000 -1.991415000	H -7.639656000 0.840865000 1.638762000
F -10.112157000 7.444801000 -2.645367000	H -6.025232000 0.206772000 -3.754086000
F -9.280584000 7.986105000 -0.716938000	H -9.760596000 3.359700000 -3.967150000
F -8.408176000 8.781558000 -2.535619000	H -8.118472000 -0.501681000 -4.868460000
C -10.384315000 1.022683000 -5.185394000	H -4.911370000 5.597549000 -1.103896000
F -10.359636000 1.408682000 -6.477720000	H -6.441087000 7.534531000 -0.973793000
F -11.443479000 1.617470000 -4.611394000	H -9.356314000 5.224759000 -3.114578000
F -10.601163000 -0.302220000 -5.166782000	H -5.285537000 5.054249000 -4.691731000

H -4.446770000 5.167049000 -7.014326000
H -1.976462000 1.279122000 -7.685890000
H -1.432695000 -0.663314000 -6.251677000
H -2.489607000 -1.819054000 -1.867238000
H -3.918055000 -0.003315000 -1.001861000

T₂

Ru -4.967740000 2.745334000 -2.387565000
C -2.244023000 3.727724000 0.734463000
C -1.214027000 4.417118000 0.118924000
C -1.265491000 4.668094000 -1.246003000
C -2.359474000 4.215586000 -1.957388000
N -3.355814000 3.541640000 -1.365541000
C -3.314454000 3.292141000 -0.035405000
C -5.706668000 1.481209000 2.233954000
C -4.603873000 2.218727000 1.841837000
C -4.454963000 2.540129000 0.498282000
N -5.370426000 2.151728000 -0.419550000
C -6.433279000 1.436697000 -0.032824000
C -6.636894000 1.078024000 1.286504000
C -0.026553000 4.910868000 0.914433000
C -5.911364000 1.094936000 3.680235000
F 0.052628000 6.255170000 0.872572000
F 1.124848000 4.427966000 0.410388000
F -0.087794000 4.548380000 2.203678000
F -5.842016000 -0.242331000 3.834663000
F -4.995171000 1.642408000 4.492394000

F -7.125088000 1.482911000 4.116123000
C -6.940695000 0.835964000 -3.653820000
N -6.755751000 2.073817000 -3.179316000
C -7.747062000 2.994781000 -3.265376000
C -8.968797000 2.664942000 -3.831356000
C -9.155686000 1.381668000 -4.324021000
C -8.131326000 0.451602000 -4.243514000
C -7.422141000 4.318763000 -2.722205000
N -6.171574000 4.449734000 -2.221988000
C -5.780929000 5.624300000 -1.714692000
C -6.613659000 6.727979000 -1.690802000
C -7.893591000 6.602903000 -2.211542000
C -8.307600000 5.388480000 -2.729531000
C -8.820256000 7.796213000 -2.195814000
F -9.963590000 7.563531000 -2.857298000
F -9.145247000 8.137590000 -0.933039000
F -8.235107000 8.869388000 -2.759886000
C -10.468723000 1.019968000 -4.981579000
F -10.470445000 1.395089000 -6.277022000
F -11.505500000 1.632644000 -4.386434000
F -10.699467000 -0.301382000 -4.944799000
C -4.609299000 4.295401000 -5.077300000
C -4.135676000 4.360161000 -6.374940000
N -3.394412000 3.387182000 -6.943928000
C -3.130810000 2.314924000 -6.188887000
C -3.609149000 2.213977000 -4.863495000
N -4.351019000 3.232093000 -4.295479000

C -2.346895000 1.224647000 -6.698379000	H -6.118687000 0.144944000 -3.550857000
C -2.069429000 0.136566000 -5.933934000	H -9.764175000 3.392337000 -3.888807000
C -2.556234000 0.028103000 -4.587659000	H -8.242811000 -0.555711000 -4.616421000
C -3.339018000 1.092836000 -4.086322000	H -4.777158000 5.684634000 -1.324638000
N -3.864901000 1.048126000 -2.810057000	H -6.254824000 7.658768000 -1.274651000
N -2.279473000 -1.043610000 -3.836846000	H -9.299016000 5.277550000 -3.138815000
C -2.779589000 -1.052441000 -2.586062000	H -5.187466000 5.103944000 -4.656208000
C -3.561135000 -0.031115000 -2.072000000	H -4.355281000 5.231398000 -6.976136000
H -2.209663000 3.526514000 1.793224000	H -1.980920000 1.302661000 -7.713360000
H -0.479082000 5.204579000 -1.757984000	H -1.474219000 -0.680541000 -6.318871000
H -2.449708000 4.390765000 -3.018030000	H -2.557716000 -1.911654000 -1.968586000
H -3.874305000 2.538129000 2.569176000	H -3.956407000 -0.085902000 -1.068863000
H -7.138615000 1.146237000 -0.795339000	
H -7.510509000 0.500637000 1.554430000	

References

- (1) Wei, X.; Cui, W.-b.; Qin, G.-y.; Zhang, X.-e.; Sun, F.-y.; Li, H.; Guo, J.-f.; Ren, A.-m. Theoretical investigation of Ru (II) complexes with long lifetime and a large two-photon absorption cross-section in photodynamic therapy. *Journal of medicinal chemistry* **2023**, *66*, 4167–4178.
- (2) Xu, H.; Zheng, K.-C.; Chen, Y.; Li, Y.-Z.; Lin, L.-J.; Li, H.; Zhang, P.-X.; Ji, L.-N. Effects of ligand planarity on the interaction of polypyridyl Ru (II) complexes with DNA. *Dalton Transactions* **2003**, 2260–2268.
- (3) Barretta, P.; Scoditti, S.; Belletto, D.; Ponte, F.; Vigna, V.; Mazzone, G.; Sicilia, E. Ruthenium complexes bearing nile red chromophore and one of its derivative: Theoret-

- ical evaluation of PDT-related properties. *Journal of Computational Chemistry* **2024**, *45*, 2034–2041.
- (4) Ponte, F.; Belletto, D.; Leonetti, R.; Sanna, N.; Scoditti, S.; Mazzone, G.; Sicilia, E. DFT Computational Analysis of the Mechanism of Action of Ru (II) Polypyridyl Complexes as Photoactivated Chemotherapy Agents: From Photoinduced Ligand Solvolysis to DNA Binding. *Inorganic Chemistry* **2024**, *63*, 20643–20653.
- (5) Salassa, L.; Garino, C.; Salassa, G.; Gobetto, R.; Nervi, C. Mechanism of ligand photodissociation in photoactivable [Ru (bpy) 2L2] 2+ complexes: a density functional theory study. *Journal of the American Chemical Society* **2008**, *130*, 9590–9597.
- (6) Furue, M.; Maruyama, K.; Oguni, T.; Naiki, M.; Kamachi, M. Trifluoromethyl-substituted 2, 2'-bipyridine ligands. Synthetic control of excited-state properties of ruthenium (II) tris-chelate complexes. *Inorganic chemistry* **1992**, *31*, 3792–3795.