

Supporting Information

Understanding the Excited State Decay Mechanism of Complex Systems: A General First-Order Kinetic Model

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Cartesian Coordinates and Structures

All the Cartesian coordinates for the optimized geometries of S_0 , S_1 , T_1 , T_2 , 3MC , TS, and conical intersections for the $\text{Ru}(\text{bpz})_3^{2+}$ complex are shown below.

S_0	N 0.206537000 1.783307000 -1.058066000
	N 0.305547000 4.279053000 -2.289470000
Ru	0.008301000 0.004407000 0.002074000

C 1.007645000 2.001564000 -2.110012000	C -1.481340000 -2.450230000 0.582484000
C -0.553445000 2.814010000 -0.601647000	C 0.228857000 -2.204437000 2.127455000
C -0.485700000 4.060691000 -1.240995000	C -0.157983000 -3.407228000 2.724139000
C 1.048806000 3.257649000 -2.720666000	C -1.839186000 -3.654152000 1.207139000
H 1.614666000 1.170125000 -2.471218000	H 1.067186000 -1.619813000 2.509207000
H -1.088607000 4.901111000 -0.885498000	H 0.387659000 -3.784492000 3.595240000
H 1.705666000 3.424860000 -3.580653000	H -2.681310000 -4.244173000 0.834893000
N -1.274975000 1.252366000 1.058955000	N 1.446667000 -1.058814000 -1.060472000
N -3.011309000 3.087180000 2.230383000	N 3.549184000 -2.421914000 -2.275529000
C -1.395871000 2.511219000 0.559766000	C 2.713356000 -0.956345000 -0.576651000
C -2.007276000 0.920541000 2.130986000	C 1.238439000 -1.828473000 -2.137381000
C -2.873100000 1.850327000 2.712642000	C 2.301155000 -2.506109000 -2.740716000
C -2.280931000 3.414621000 1.166287000	C 3.753502000 -1.656036000 -1.205537000
H -1.901411000 -0.090158000 2.528076000	H 0.221003000 -1.900363000 -2.524597000
H -3.466236000 1.569511000 3.589134000	H 2.120210000 -3.130664000 -3.621692000
H -2.397884000 4.427782000 0.771457000	H 4.777085000 -1.590070000 -0.826106000
N -1.642502000 -0.708596000 -1.047634000	N 1.732061000 0.482007000 1.060663000
N -3.884167000 -1.848128000 -2.245384000	N 4.179159000 0.992735000 2.286615000
C -2.233943000 -0.125564000 -2.099410000	C 1.813630000 1.290503000 2.126257000
C -2.168089000 -1.870222000 -0.575778000	C 2.875200000 -0.084649000 0.591451000
C -3.295399000 -2.424816000 -1.199693000	C 4.095034000 0.190200000 1.227381000
C -3.358479000 -0.705515000 -2.692005000	C 3.046542000 1.538824000 2.734522000
H -1.805757000 0.804399000 -2.476333000	H 0.890767000 1.736724000 2.500012000
H -3.727808000 -3.361297000 -0.835859000	H 5.025442000 -0.252835000 0.860862000
H -3.833635000 -0.220488000 -3.551057000	H 3.101712000 2.199630000 3.605895000
N -0.430755000 -1.732517000 1.060856000	
N -1.183920000 -4.127251000 2.265228000	

S₁

Ru 0.032373000 0.043084000 -0.000295000	H -3.862933000 -0.127010000 -3.500219000
N 0.230301000 1.867970000 -1.015155000	N -0.375360000 -1.694442000 1.051587000
N 0.265132000 4.355373000 -2.237378000	N -1.108252000 -4.133830000 2.201037000
C 1.067414000 2.115718000 -2.028251000	C -1.450026000 -2.413153000 0.548986000
C -0.597381000 2.855733000 -0.587574000	C 0.313763000 -2.205566000 2.093974000
C -0.559994000 4.105757000 -1.223266000	C -0.051356000 -3.407237000 2.667264000
C 1.072890000 3.374089000 -2.639693000	C -1.775284000 -3.647827000 1.179599000
H 1.727632000 1.311811000 -2.358291000	H 1.156908000 -1.625548000 2.474728000
H -1.215562000 4.917308000 -0.895777000	H 0.504630000 -3.805742000 3.520068000
H 1.754719000 3.573446000 -3.472579000	H -2.620968000 -4.233804000 0.804395000
N -1.327752000 1.246335000 1.018637000	N 1.441564000 -1.101758000 -1.021141000
N -3.148688000 2.986430000 2.169499000	N 3.456535000 -2.624230000 -2.158222000
C -1.466718000 2.508654000 0.539340000	C 2.706162000 -1.041516000 -0.531359000
C -2.080025000 0.853381000 2.052436000	C 1.181534000 -1.903435000 -2.060041000
C -2.991392000 1.744559000 2.628774000	C 2.209878000 -2.661526000 -2.629616000
C -2.399586000 3.368968000 1.138112000	C 3.707063000 -1.827328000 -1.122249000
H -1.951968000 -0.165487000 2.420991000	H 0.158675000 -1.936371000 -2.438125000
H -3.603087000 1.425868000 3.478789000	H 1.998917000 -3.313138000 -3.483530000
H -2.536275000 4.388359000 0.766734000	H 4.731464000 -1.805460000 -0.740709000
N -1.616394000 -0.648527000 -1.049610000	N 1.800450000 0.538721000 1.015694000
N -3.880880000 -1.798917000 -2.214659000	N 4.250080000 0.974244000 2.238028000
C -2.249625000 -0.046362000 -2.078747000	C 1.912799000 1.414201000 2.020745000
C -2.127257000 -1.842834000 -0.563108000	C 2.907103000 -0.126601000 0.594862000
C -3.278801000 -2.382365000 -1.204031000	C 4.134438000 0.110466000 1.232145000
C -3.365380000 -0.616168000 -2.658516000	C 3.154039000 1.623861000 2.630984000
H -1.836465000 0.895305000 -2.445982000	H 1.015313000 1.941838000 2.348655000
H -3.697290000 -3.329256000 -0.846306000	H 5.039540000 -0.412887000 0.911583000

H 3.243388000 2.336845000 3.456786000

T₁

Ru 0.010694000 -0.029439000 -0.008577000

N 0.234056000 1.713714000 -1.055184000

N 0.390350000 4.279692000 -2.190482000

C 1.068846000 1.970887000 -2.081126000

C -0.531257000 2.771224000 -0.550497000

C -0.412837000 4.051466000 -1.182687000

C 1.143932000 3.231583000 -2.646271000

H 1.668410000 1.143070000 -2.464098000

H -1.012576000 4.888272000 -0.810242000

H 1.813812000 3.419325000 -3.488911000

N -1.262626000 1.164363000 1.051746000

N -3.000684000 3.036396000 2.221480000

C -1.345845000 2.472701000 0.560783000

C -2.059142000 0.823342000 2.084096000

C -2.910602000 1.744428000 2.666845000

C -2.246418000 3.379564000 1.208724000

H -1.992932000 -0.200415000 2.456355000

H -3.537216000 1.457393000 3.514742000

H -2.319348000 4.410034000 0.846280000

N -1.674325000 -0.701620000 -1.038212000

N -3.983804000 -1.726339000 -2.181259000

C -2.253454000 -0.082824000 -2.074119000

C -2.233897000 -1.840539000 -0.554693000

C -3.402593000 -2.337330000 -1.151449000

C -3.416828000 -0.610787000 -2.642594000

H -1.788657000 0.829209000 -2.451819000

H -3.873082000 -3.252027000 -0.779697000

H -3.888768000 -0.103581000 -3.490424000

N -0.441471000 -1.802122000 1.028658000

N -1.261592000 -4.164224000 2.234218000

C -1.540578000 -2.459824000 0.579448000

C 0.239520000 -2.313729000 2.060108000

C -0.184346000 -3.504116000 2.660742000

C -1.933915000 -3.652002000 1.205548000

H 1.119209000 -1.773184000 2.415232000

H 0.373472000 -3.917431000 3.507367000

H -2.816429000 -4.197922000 0.860795000

N 1.487491000 -1.113559000 -1.037706000

N 3.616742000 -2.444546000 -2.218007000

C 2.754228000 -0.920043000 -0.589351000

C 1.283761000 -1.959130000 -2.053683000

C 2.365315000 -2.622925000 -2.642339000

C 3.813322000 -1.604795000 -1.203381000

H 0.260569000 -2.102230000 -2.406342000

H 2.195099000 -3.311607000 -3.476397000

H 4.842004000 -1.468457000 -0.858013000

N 1.734370000 0.527305000 1.020197000

N 4.163794000 1.230296000 2.155595000

C 1.782072000 1.376255000 2.053759000

C 2.893498000 0.010924000 0.535947000

C 4.109249000 0.386504000 1.127312000

C 3.013419000 1.719259000 2.620576000
H 0.840055000 1.776784000 2.431476000
H 5.057360000 -0.007642000 0.750566000
H 3.050574000 2.410397000 3.468963000

T₂

Ru 0.016543000 -0.002601000 -0.000851000
N 0.187961000 1.793337000 -1.101836000
N 0.223515000 4.261871000 -2.373667000
C 0.957866000 1.996443000 -2.176237000
C -0.575958000 2.817919000 -0.643360000
C -0.539748000 4.055298000 -1.301979000
C 0.966148000 3.244663000 -2.809932000
H 1.568943000 1.168516000 -2.539111000
H -1.142782000 4.894963000 -0.944749000
H 1.598720000 3.404680000 -3.689261000
N -1.245004000 1.273929000 1.055228000
N -3.033263000 3.052747000 2.193098000
C -1.400427000 2.516906000 0.530544000
C -1.962730000 0.918804000 2.128600000
C -2.863578000 1.828286000 2.692835000
C -2.313412000 3.398232000 1.127155000
H -1.816560000 -0.083441000 2.534467000
H -3.451544000 1.540263000 3.570362000
H -2.463301000 4.403431000 0.723173000
N -1.599964000 -0.688249000 -1.074698000
N -3.942212000 -1.760398000 -2.169261000

C -2.216711000 -0.096793000 -2.127942000
C -2.164434000 -1.841012000 -0.549292000
C -3.349275000 -2.336959000 -1.141862000
C -3.367303000 -0.630084000 -2.667325000
H -1.762393000 0.805585000 -2.539026000
H -3.816829000 -3.239028000 -0.734522000
H -3.848729000 -0.149737000 -3.522933000
N -0.412907000 -1.703890000 1.072920000
N -1.155725000 -4.147016000 2.215171000
C -1.484336000 -2.423352000 0.567829000
C 0.263873000 -2.217621000 2.128942000
C -0.107825000 -3.419752000 2.692679000
C -1.813496000 -3.653715000 1.183770000
H 1.102192000 -1.639894000 2.520427000
H 0.438913000 -3.818779000 3.550784000
H -2.649380000 -4.242649000 0.793151000
N 1.489663000 -1.024486000 -1.059983000
N 3.556635000 -2.445087000 -2.229601000
C 2.746139000 -0.947951000 -0.550600000
C 1.261522000 -1.792068000 -2.133468000
C 2.315754000 -2.505212000 -2.713677000
C 3.774776000 -1.678474000 -1.162759000
H 0.244990000 -1.833317000 -2.527773000
H 2.131748000 -3.133647000 -3.591133000
H 4.795011000 -1.641286000 -0.770683000
N 1.754827000 0.458303000 1.106240000
N 4.184528000 0.949691000 2.357247000

C 1.817407000 1.231321000 2.195733000

C 2.901150000 -0.089664000 0.627732000

MECP_{T₁-T₂}

Ru -1.815938080 -0.004634233 -1.443026484

N -1.584358104 1.756240728 -2.471000221

N -1.409018979 4.271385315 -3.638625617

C -0.764149377 1.978427665 -3.511033693

C -2.325596505 2.803152684 -1.991528474

C -2.206747722 4.057165106 -2.611112600

C -0.686371649 3.225540101 -4.089771345

H -0.182066015 1.147698777 -3.879429953

H -2.781947039 4.898082064 -2.245591695

H -0.030388363 3.393948583 -4.932679152

N -3.116612476 1.220678428 -0.409784987

N -4.790865850 3.088077338 0.786579812

C -3.170301947 2.507885070 -0.869934928

C -3.900872965 0.881255159 0.624576581

C -4.724535791 1.812870137 1.218278217

C -4.029312685 3.420166073 -0.237361987

H -3.854627967 -0.135755410 0.983131040

H -5.344865564 1.533238020 2.058696346

H -4.086986973 4.442708070 -0.587116097

N -3.499915538 -0.702057982 -2.458438157

N -5.765261539 -1.795785570 -3.605412237

C -4.109558129 -0.092435975 -3.476121588

C -4.013215346 -1.864881007 -1.994014434

C -5.156760700 -2.395950092 -2.589092086

C -5.244810224 -0.652756427 -4.046807447

H -3.691652288 0.834091060 -3.839492452

H -5.585787376 -3.323619669 -2.234237104

H -5.734247009 -0.157850576 -4.875845439

N -2.226804913 -1.774667732 -0.423142394

N -2.949576058 -4.167458827 0.757803141

C -3.297698704 -2.467553119 -0.874333857

C -1.526146686 -2.268020612 0.599330641

C -1.901074802 -3.468661830 1.187981442

C -3.639984565 -3.673322982 -0.263449816

H -0.676365549 -1.703684658 0.952421245

H -1.334514003 -3.863000355 2.021777480

H -4.490373138 -4.245734566 -0.608436251

N -0.380915650 -1.083710739 -2.464140992

N 1.743768527 -2.454866746 -3.617143391

C 0.892074230 -0.931692274 -1.985683420

C -0.576897401 -1.917462762 -3.496964111

C 0.481027354 -2.589763273 -4.069305572

C 1.936862147 -1.642825699 -2.596238866

H -1.583567828 -2.030427136 -3.870202371

H 0.314872196 -3.251209849 -4.908459785

H 2.949998073 -1.539989722 -2.229766734

N -0.126813920 0.515933755 -0.403003415

N 2.312412973 1.121950687 0.780128763

C -0.055023865 1.370277652 0.630909485

C 1.033822132 -0.043689449 -0.867904469

C 2.244555722 0.290400233 -0.240497420
C 1.155789043 1.661198466 1.217978541
H -0.975101867 1.805663677 0.989095624
H 3.173913815 -0.136590098 -0.594812098
H 1.204239772 2.342024525 2.056570975

MECP_{S₀-S₁}

Ru 0.547494195 0.026457716 -0.085193183
N 0.820274161 1.826955679 -1.089504688
N 0.828556710 4.356384519 -2.195048594
C 1.566583416 2.092549705 -2.163101741
C 0.096886613 2.824414041 -0.527459003
C 0.102073354 4.090966736 -1.119767473
C 1.570674989 3.366978986 -2.705899789
H 2.138649882 1.282064367 -2.591948233
H -0.482078751 4.898393212 -0.696784952
H 2.178358919 3.586611439 -3.573723591
N -0.125704813 1.293179973 1.294887061
N -2.297237305 2.722753600 2.340865001
C -0.595343676 2.447368094 0.685685562
C -0.762802822 0.892417689 2.432949866
C -1.818849059 1.610583697 2.934242126
C -1.685050649 3.120224671 1.235744232
H -0.377637479 0.019188102 2.934914827
H -2.295238273 1.289002988 3.851388454
H -2.067376834 4.006604291 0.744069909
N -0.539134163 -0.915265366 -1.454712742

N -3.132321880 -1.389894207 -2.414572656
C -1.005079067 -0.310663753 -2.587995334
C -1.405263658 -1.791828164 -0.812347335
C -2.688244079 -1.987056728 -1.319763359
C -2.273377833 -0.560264634 -3.043911928
H -0.323041331 0.331697872 -3.122256001
H -3.369100354 -2.650786813 -0.800982540
H -2.615779907 -0.087527828 -3.955417361
N 0.186231775 -1.760818214 0.918883415
N -0.718677248 -4.116328613 2.033130456
C -0.874846557 -2.409184900 0.383798299
C 0.817316149 -2.297394163 1.964670360
C 0.359944240 -3.485142925 2.511882258
C -1.328409539 -3.588702298 0.982241041
H 1.667354189 -1.765207060 2.367818048
H 0.869597510 -3.926883833 3.357874018
H -2.188160951 -4.112603982 0.584108179
N 2.342098054 -1.189807059 -1.036120182
N 4.414023705 -2.703916096 -2.083544327
C 3.602283982 -1.007409687 -0.619514090
C 2.113691887 -2.117822607 -1.959778259
C 3.156815987 -2.873159442 -2.483200184
C 4.634812595 -1.778894512 -1.157071644
H 1.098396140 -2.265089912 -2.289525301
H 2.957837680 -3.624103018 -3.237102751
H 5.655886086 -1.649258742 -0.825393463
N 2.674746068 0.583596299 0.875033651

N 5.158803294 1.327865010 1.850979199
 C 2.788944599 1.512941475 1.817048102
 C 3.792222324 0.011303067 0.410637747
 C 5.037651107 0.399566397 0.909434156
 C 4.037858090 1.880800837 2.305908726
 H 1.888415745 1.972372141 2.190709663
 H 5.950277563 -0.045221384 0.535982969
 H 4.119435560 2.636993342 3.076209343

³MC

Ru 0.224907000 0.367292000 0.737449000
 N 0.674789000 2.127657000 -0.277598000
 N 1.049139000 4.577189000 -1.524362000
 C 1.397259000 2.227458000 -1.398749000
 C 0.124701000 3.257670000 0.232828000
 C 0.330275000 4.476464000 -0.412781000
 C 1.577709000 3.455829000 -2.014859000
 H 1.829109000 1.324935000 -1.803792000
 H -0.101791000 5.387819000 -0.021999000
 H 2.163480000 3.526226000 -2.922374000
 N -0.798448000 1.792326000 1.860756000
 N -1.962969000 3.876950000 3.273298000
 C -0.662786000 3.075701000 1.442954000
 C -1.507912000 1.561404000 2.970558000
 C -2.085926000 2.609778000 3.669474000
 C -1.258155000 4.105131000 2.171632000
 H -1.610608000 0.538510000 3.299723000

H -2.658778000 2.412611000 4.566484000
 H -1.155426000 5.135062000 1.856605000
 N -1.965859000 -0.260881000 -0.162535000
 N -4.601702000 -0.957669000 -0.576206000
 C -2.704962000 0.392082000 -1.050470000
 C -2.516809000 -1.260046000 0.537385000
 C -3.855681000 -1.597756000 0.318893000
 C -4.031510000 0.033274000 -1.261565000
 H -2.235132000 1.201882000 -1.593981000
 H -4.336882000 -2.387504000 0.879717000
 H -4.636639000 0.555852000 -1.991838000
 N -0.444789000 -1.374087000 1.780934000
 N -1.244552000 -3.681139000 3.097444000
 C -1.652012000 -1.926976000 1.524812000
 C 0.343958000 -1.965329000 2.684986000
 C -0.064524000 -3.114259000 3.343526000
 C -2.023877000 -3.093183000 2.197818000
 H 1.303765000 -1.510549000 2.882915000
 H 0.580387000 -3.579537000 4.077863000
 H -2.975813000 -3.564944000 1.994791000
 N 1.483828000 -0.956098000 -0.369808000
 N 3.071098000 -2.784864000 -1.726160000
 C 2.811752000 -1.027909000 -0.125208000
 C 0.964531000 -1.781982000 -1.285270000
 C 1.764120000 -2.686599000 -1.965114000
 C 3.582906000 -1.965830000 -0.815319000
 H -0.096382000 -1.712539000 -1.475941000

H 1.331322000 -3.341893000 -2.710102000
H 4.640752000 -2.060688000 -0.610797000
N 2.512898000 0.535823000 1.662496000
N 5.223774000 1.001769000 1.896532000
C 2.976036000 1.398863000 2.558688000
C 3.380840000 -0.103831000 0.868425000
C 4.749836000 0.149035000 0.993241000
C 4.342819000 1.622448000 2.681336000
H 2.253032000 1.911160000 3.180530000
H 5.472120000 -0.330840000 0.346311000
H 4.725733000 2.314259000 3.421163000

TS

Ru 0.015070000 0.042423000 0.021430000
N 0.341292000 1.877334000 -0.918695000
N 0.550521000 4.401612000 -2.073874000
C 1.267883000 2.133209000 -1.855294000
C -0.498834000 2.882419000 -0.551581000
C -0.369493000 4.147013000 -1.147353000
C 1.362393000 3.401827000 -2.428984000
H 1.936927000 1.324537000 -2.151275000
H -1.036413000 4.964367000 -0.860734000
H 2.120738000 3.598150000 -3.192523000
N -1.453542000 1.238664000 0.889062000
N -3.338021000 3.020363000 1.900906000
C -1.492863000 2.528921000 0.458849000
C -2.341397000 0.850539000 1.818067000

C -3.281511000 1.752450000 2.318034000
C -2.454746000 3.405959000 0.984035000
H -2.303588000 -0.182102000 2.166060000
H -4.001377000 1.424676000 3.073623000
H -2.500125000 4.443870000 0.644533000
N -1.852195000 -0.888244000 -1.219976000
N -4.385859000 -1.795591000 -1.878096000
C -2.549600000 -0.304083000 -2.194051000
C -2.397715000 -1.922164000 -0.555369000
C -3.688069000 -2.365135000 -0.896415000
C -3.824125000 -0.773208000 -2.529419000
H -2.088267000 0.541682000 -2.711449000
H -4.165857000 -3.184874000 -0.353567000
H -4.391080000 -0.305688000 -3.340322000
N -0.515139000 -1.798277000 0.962340000
N -1.146713000 -4.249045000 2.119039000
C -1.586985000 -2.507971000 0.529252000
C 0.226906000 -2.305361000 1.958808000
C -0.102744000 -3.530797000 2.539141000
C -1.876159000 -3.747127000 1.125928000
H 1.085512000 -1.723412000 2.297523000
H 0.503013000 -3.926712000 3.359512000
H -2.719032000 -4.346101000 0.771738000
N 1.578318000 -1.058514000 -0.923062000
N 3.604030000 -2.566711000 -2.088733000
C 2.858056000 -0.944788000 -0.487479000
C 1.316512000 -1.909727000 -1.926459000

C 2.340684000 -2.656421000 -2.510447000	C 3.118779000 0.009674000 0.607049000
C 3.859168000 -1.725041000 -1.090151000	C 4.403531000 0.419055000 1.006183000
H 0.282766000 -1.988537000 -2.266545000	C 3.497083000 1.775792000 2.605612000
H 2.116356000 -3.340043000 -3.334437000	H 1.314025000 1.798388000 2.696533000
H 4.892298000 -1.665133000 -0.739038000	H 5.298826000 0.040314000 0.506163000
N 2.038628000 0.515464000 1.228458000	H 3.640339000 2.487343000 3.424595000
N 4.582985000 1.289391000 1.998527000	
C 2.208811000 1.395372000 2.214325000	

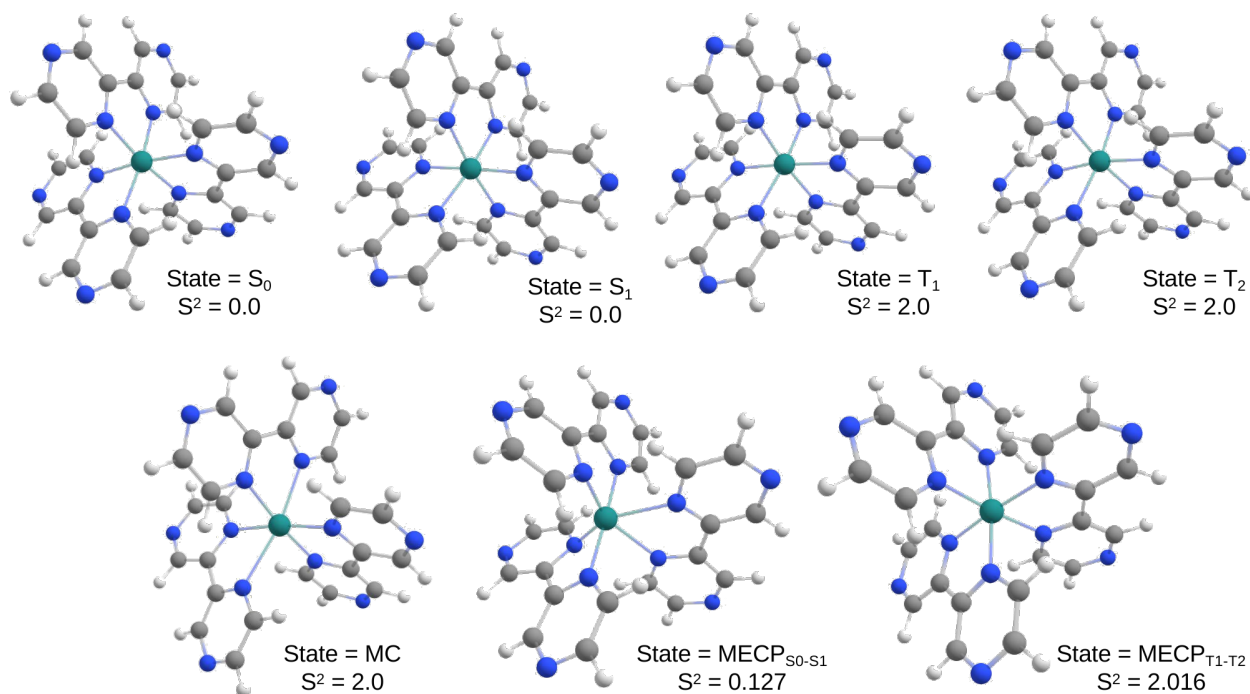


Figure S1: Structure and spin contamination of the states involved in the excited state decay model.

Kinetic Equations

The eighteen kinetic equations solved in this work are detailed below. For reference, $[M@N](t)$ is the population concentration of state M at the state N geometry at a given time t , and $k_{M \rightarrow S}^N$ is the rate constant for the transition $M \rightarrow S$ (subscript) at the geometry of state N

(superscript).

$$\begin{aligned} \frac{d[S_1 @ S_0](t)}{dt} = & -(k_{S_1 \rightarrow T_1}^{S_0} + k_{S_1 \rightarrow T_2}^{S_0} + k_{S_1 \rightarrow S_0}^{S_0} + k_F^{S_0} + k_{S_1, GR})[S_1 @ S_0](t) \\ & + k_{T_1 \rightarrow S_1}^{S_0}[T_1 @ S_0](t) + k_{T_2 \rightarrow S_1}^{S_0}[T_2 @ S_0](t) \end{aligned} \quad (S1)$$

$$\begin{aligned} \frac{d[T_1 @ S_0](t)}{dt} = & -(k_{T_1 \rightarrow S_1}^{S_0} + k_{T_1 \rightarrow T_2}^{S_0} + k_{T_1 \rightarrow S_0}^{S_0} + k_P^{S_0} + k_{T_1, GR})[T_1 @ S_0](t) \\ & + k_{S_1 \rightarrow T_1}^{S_0}[S_1 @ S_0](t) + k_{T_2 \rightarrow T_1}^{S_0}[T_2 @ S_0](t) \end{aligned} \quad (S2)$$

$$\begin{aligned} \frac{d[T_2 @ S_0](t)}{dt} = & -(k_{T_2 \rightarrow S_1}^{S_0} + k_{T_2 \rightarrow T_1}^{S_0} + k_{T_2, GR})[T_2 @ S_0](t) + k_{S_1 \rightarrow T_2}^{S_0}[S_1 @ S_0](t) \\ & + k_{T_1 \rightarrow T_2}^{S_0}[T_1 @ S_0](t) \end{aligned} \quad (S3)$$

$$\begin{aligned} \frac{d[S_0 @ S_0](t)}{dt} = & (k_{S_1 \rightarrow S_0}^{S_0} + k_F^{S_0})[S_1 @ S_0](t) + (k_{T_1 \rightarrow S_0}^{S_0} + k_P^{S_0})[T_1 @ S_0](t) \\ & + \{[S_0 @ S_1](t) + [S_0 @ T_1](t) + [S_0 @ T_2](t) + [S_0 @^3 MC]\}k_{S_0, GR} \end{aligned} \quad (S4)$$

$$\begin{aligned} \frac{d[S_1 @ S_1](t)}{dt} = & -(k_{S_1 \rightarrow T_1}^{S_1} + k_{S_1 \rightarrow T_2}^{S_1} + k_{S_1 \rightarrow S_0}^{S_1} + k_F^{S_1})[S_1 @ S_1](t) \\ & + k_{T_1 \rightarrow S_1}^{S_1}[T_1 @ S_1](t) + k_{T_2 \rightarrow S_1}^{S_1}[T_2 @ S_1](t) \\ & + \{[S_1 @ S_0](t) + [S_1 @ T_1](t) + [S_1 @ T_2](t)\}k_{S_1, GR} \end{aligned} \quad (S5)$$

$$\begin{aligned} \frac{d[T_1 @ S_1](t)}{dt} = & -(k_{T_1 \rightarrow S_1}^{S_1} + k_{T_1 \rightarrow T_2}^{S_1} + k_{T_1 \rightarrow S_0}^{S_1} + k_P^{S_1} + k_{T_1, GR})[T_1 @ S_1](t) \\ & + k_{S_1 \rightarrow T_1}^{S_1}[S_1 @ S_1](t) + k_{T_2 \rightarrow T_1}^{S_1}[T_2 @ S_1](t) \end{aligned} \quad (S6)$$

$$\begin{aligned} \frac{d[T_2 @ S_1](t)}{dt} = & -(k_{T_2 \rightarrow S_1}^{S_1} + k_{T_2 \rightarrow T_1}^{S_1} + k_{T_2, GR})[T_2 @ S_1](t) + k_{S_1 \rightarrow T_2}^{S_1}[S_1 @ S_1](t) \\ & + k_{T_1 \rightarrow T_2}^{S_1}[T_1 @ S_1](t) \end{aligned} \quad (S7)$$

$$\begin{aligned} \frac{d[S_0 @ S_1](t)}{dt} = & -k_{S_0, GR}[S_0 @ S_1](t) + (k_{S_1 \rightarrow S_0}^{S_1} + k_F^{S_1})[S_1 @ S_1](t) \\ & + (k_{T_1 \rightarrow S_0}^{S_1} + k_p^{S_1})[T_1 @ S_1](t) \end{aligned} \quad (S8)$$

$$\begin{aligned} \frac{d[S_1 @ T_1](t)}{dt} = & -(k_{S_1 \rightarrow T_1}^{T_1} + k_{S_1 \rightarrow T_2}^{T_1} + k_{S_1 \rightarrow S_0}^{T_1} + k_F^{T_1} + k_{S_1, GR})[S_1 @ T_1](t) \\ & + k_{T_1 \rightarrow S_1}^{T_1}[T_1 @ T_1](t) + k_{T_2 \rightarrow S_1}^{T_1}[T_2 @ T_1](t) \end{aligned} \quad (S9)$$

$$\begin{aligned} \frac{d[T_1 @ T_1](t)}{dt} = & -(k_{T_1 \rightarrow S_1}^{T_1} + k_{T_1 \rightarrow T_2}^{T_1} + k_{T_1 \rightarrow S_0}^{T_1} + k_{T_1 \rightarrow ^3MC}^{T_1} + k_P^{T_1})[T_1 @ T_1](t) \\ & + k_{^3MC \rightarrow T_1}^{^3MC}[^3MC](t) + k_{S_1 \rightarrow T_1}^{T_1}[S_1 @ T_1](t) + k_{T_2 \rightarrow T_1}^{T_1}[T_2 @ T_1](t) \\ & + \{[T_1 @ S_0](t) + [T_1 @ S_1](t) + [T_1 @ T_2](t)\}k_{T_1, GR} \end{aligned} \quad (S10)$$

$$\begin{aligned} \frac{d[T_2 @ T_1](t)}{dt} = & -(k_{T_2 \rightarrow S_1}^{T_1} + k_{T_2 \rightarrow T_1}^{T_1} + k_{T_2, GR})[T_2 @ T_1](t) + k_{S_1 \rightarrow T_2}^{T_1}[S_1 @ T_1](t) \\ & + k_{T_1 \rightarrow T_2}^{T_1}[T_1 @ T_1](t) \end{aligned} \quad (S11)$$

$$\begin{aligned} \frac{d[S_0 @ T_1](t)}{dt} = & -k_{S_0, GR}[S_0 @ T_1](t) + (k_{S_1 \rightarrow S_0}^{T_1} + k_F^{T_1})[S_1 @ T_1](t) \\ & + (k_{T_1 \rightarrow S_0}^{T_1} + k_p^{T_1})[T_1 @ T_1](t) \end{aligned} \quad (S12)$$

$$\begin{aligned} \frac{d[S_1 @ T_2](t)}{dt} = & -(k_{S_1 \rightarrow T_1}^{T_2} + k_{S_1 \rightarrow T_2}^{T_2} + k_{S_1 \rightarrow S_0}^{T_2} + k_F^{T_2} + k_{S_1, GR})[S_1 @ T_2](t) \\ & + k_{T_1 \rightarrow S_1}^{T_2}[T_1 @ T_2](t) + k_{T_2 \rightarrow S_1}^{T_2}[T_2 @ T_2](t) \end{aligned} \quad (S13)$$

$$\begin{aligned} \frac{d[T_1 @ T_2](t)}{dt} = & -(k_{T_1 \rightarrow S_1}^{T_2} + k_{T_1 \rightarrow T_2}^{T_2} + k_{T_1 \rightarrow S_0}^{T_2} + k_P^{T_2} + k_{T_1, GR})[T_1 @ T_2](t) \\ & + k_{S_1 \rightarrow T_1}^{T_2}[S_1 @ T_2](t) + k_{T_2 \rightarrow T_1}^{T_2}[T_2 @ T_2](t) \end{aligned} \quad (S14)$$

$$\begin{aligned} \frac{d[T_2 @ T_2](t)}{dt} = & -(k_{T_2 \rightarrow S_1}^{T_2} + k_{T_2 \rightarrow T_1}^{T_2})[T_2 @ T_2](t) + k_{S_1 \rightarrow T_2}^{T_2}[S_1 @ T_2](t) \\ & + k_{T_1 \rightarrow T_2}^{T_2}[T_1 @ T_2](t) + \{[T_2 @ S_0](t) + [T_2 @ S_1](t) + [T_2 @ T_1](t)\}k_{T_2, GR} \end{aligned} \quad (S15)$$

$$\begin{aligned} \frac{d[S_0 @ T_2](t)}{dt} = & -k_{S_0, GR}[S_0 @ T_2](t) + (k_{S_1 \rightarrow S_0}^{T_2} + k_F^{T_2})[S_1 @ T_2](t) \\ & + (k_{T_1 \rightarrow S_0}^{T_2} + k_p^{T_2})[T_1 @ T_2](t) \end{aligned} \quad (S16)$$

$$\frac{d[{}^3MC](t)}{dt} = -(k_{{}^3MC \rightarrow T_1}^{3MC} + k_P^{3MC})[{}^3MC](t) + k_{T_1 \rightarrow {}^3MC}^{T_1}[T_1 @ T_1] \quad (S17)$$

$$\frac{d[S_0 @ {}^3MC](t)}{dt} = -k_{S_0, GR}[S_0 @ {}^3MC](t) + k_p^{3MC}[{}^3MC](t) \quad (S18)$$

Kinetic decay of population over time

The set of figures shown below is a collection of important states populated throughout the simulation but not explicitly shown in the figures of the main manuscript. The graphs are

sorted by simulation time. The states not mentioned in the main manuscript or this section had negligible contributions.

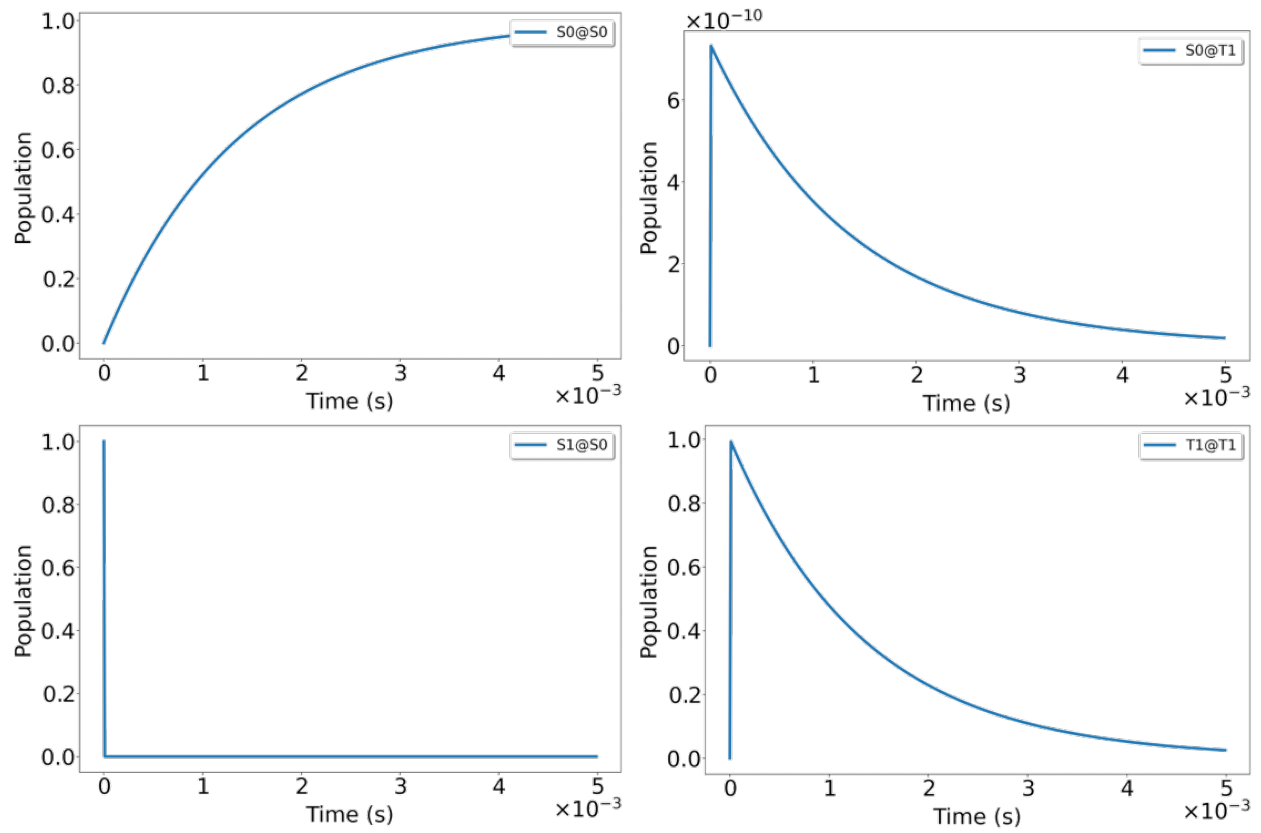


Figure S2: Evolution of states population over time for a time range from 0 to 5 ms using a propagation step of 10^{-5} .

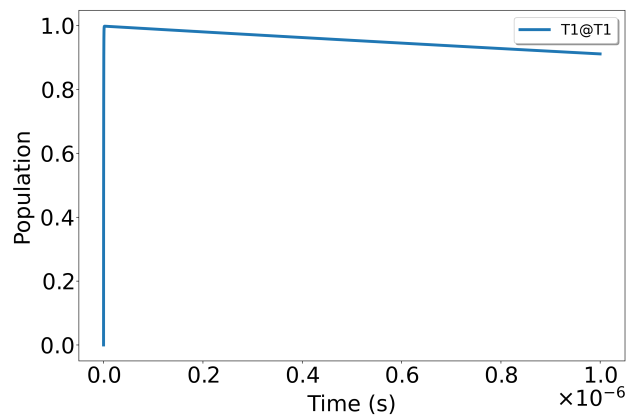


Figure S3: Evolution of states population over time for a time range from 0 to 1 μs using a propagation step of 10^{-10} .

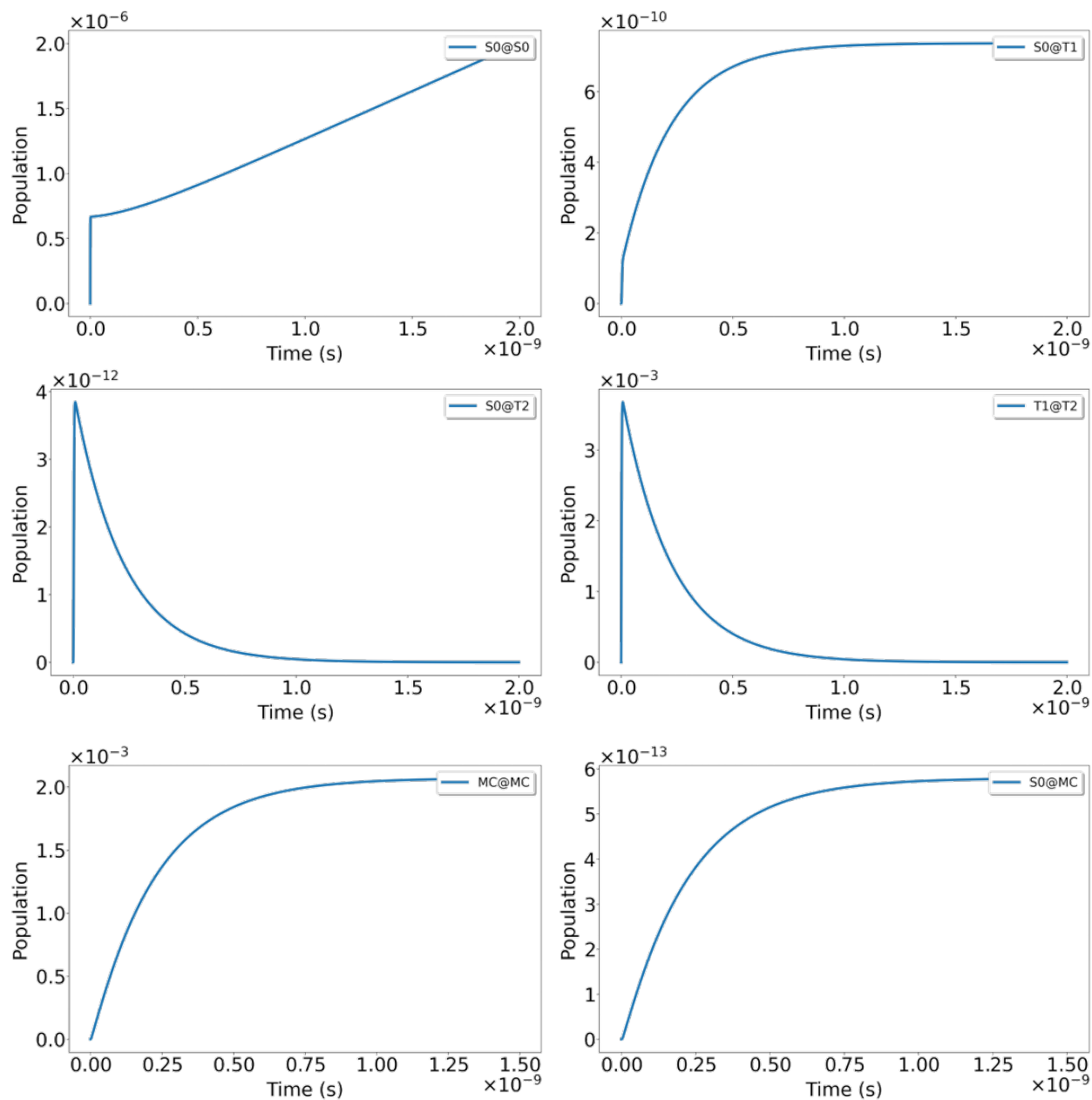


Figure S4: Evolution of states population over time for a time range from 0 to 2 ns using a propagation step of 10^{-13} .

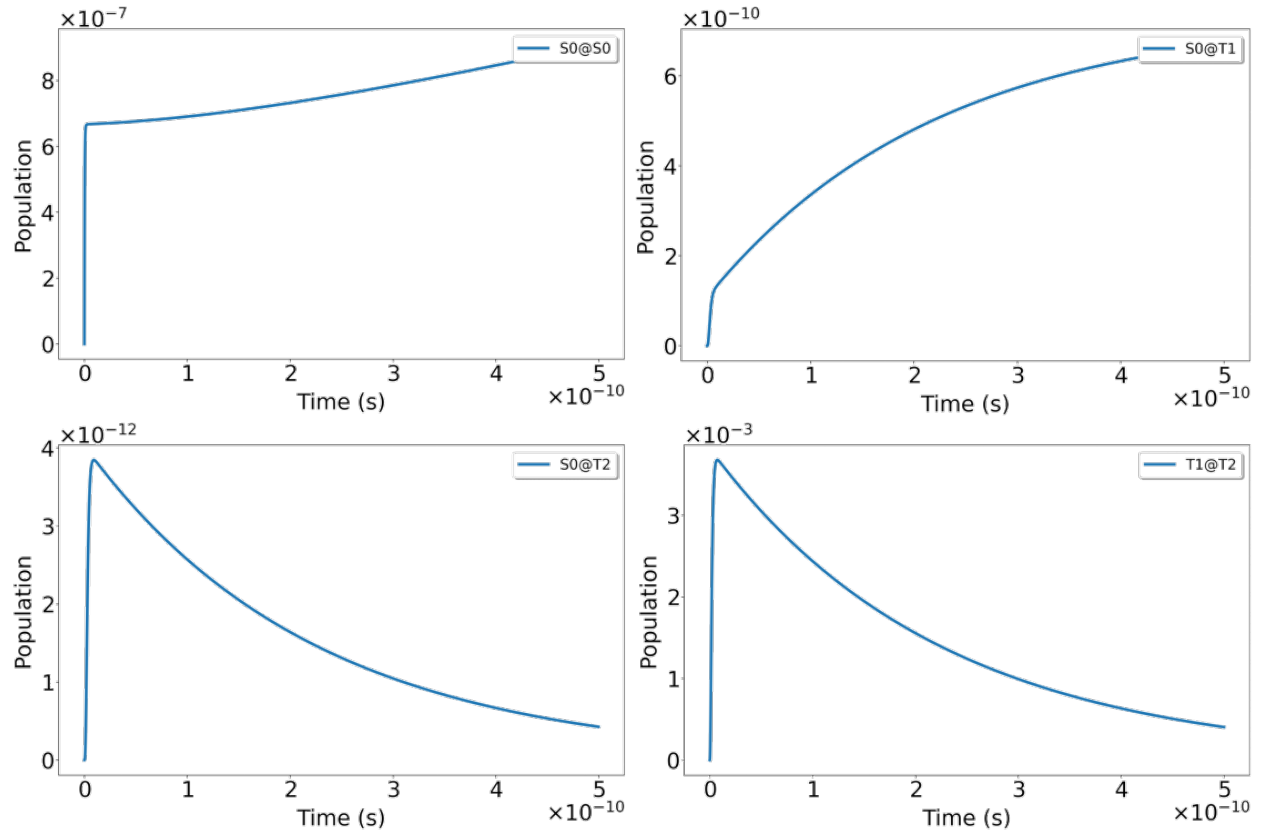


Figure S5: Evolution of states population over time for a time range from 0 to 5×10^{-10} s using a propagation step of 10^{-13} .

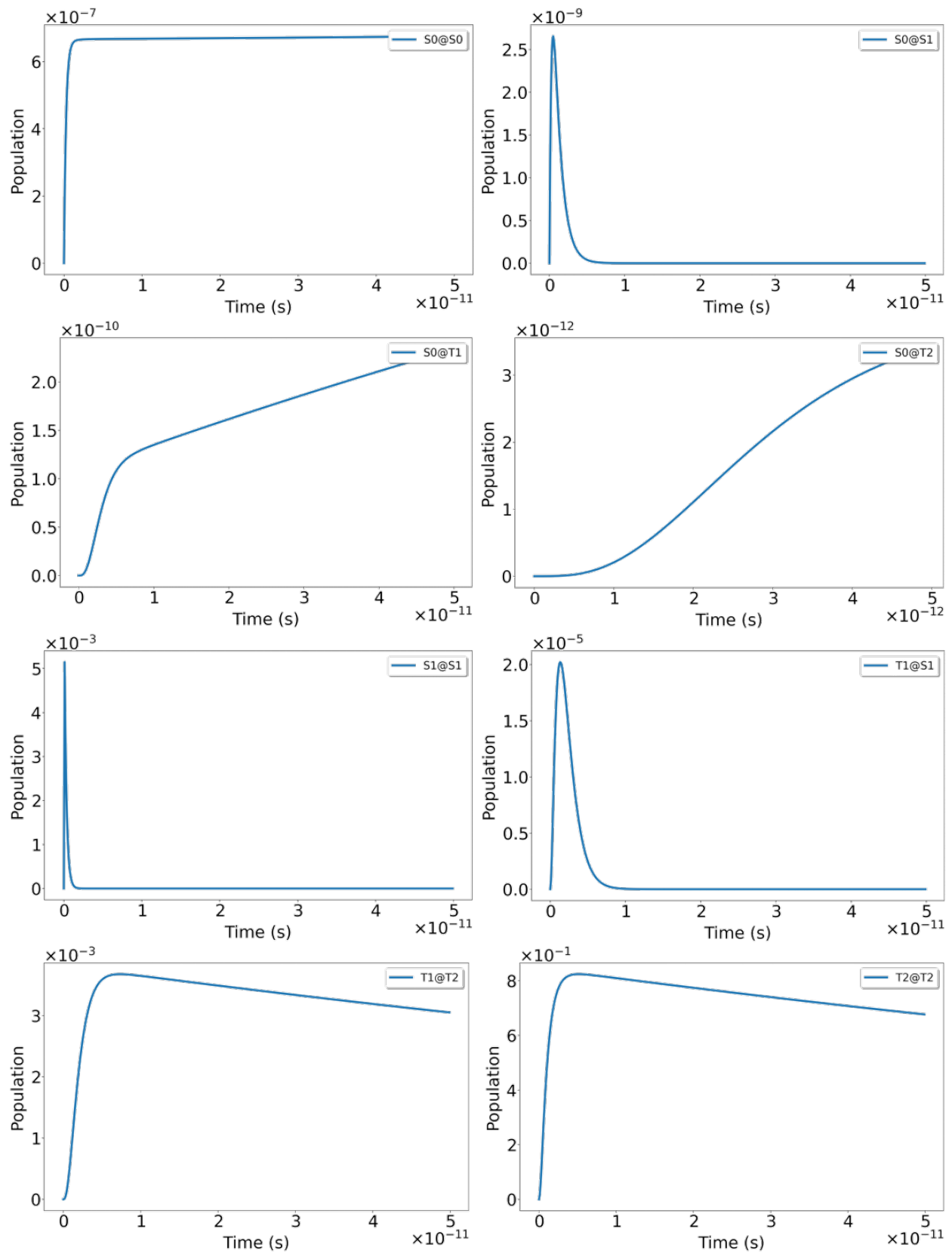


Figure S6: Evolution of states population over time for a time range from 0 to 5×10^{-11} s using a propagation step of 10^{-13} .

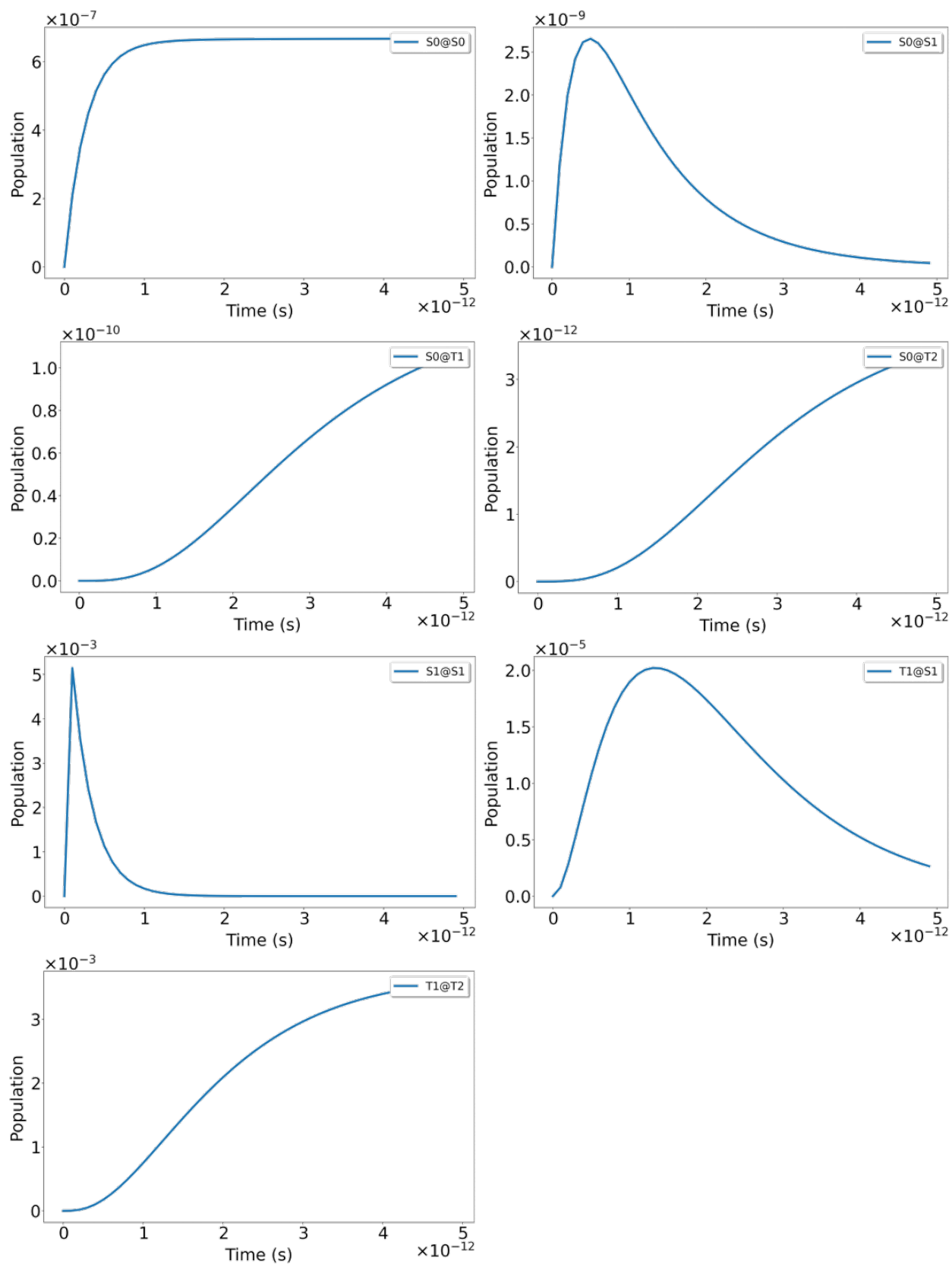


Figure S7: Evolution of states population over time for a time range from 0 to 5 ps using a propagation step of 10^{-13} .