Electronic Supplementary Material (ESI) for Chemical Science

SUPPORTING INFORMATION

Experimental and quantum chemical characterization of the water oxidation cycle catalysed by $[Ru^{II}(damp)(bpy)(H_2O)]^{2+}$

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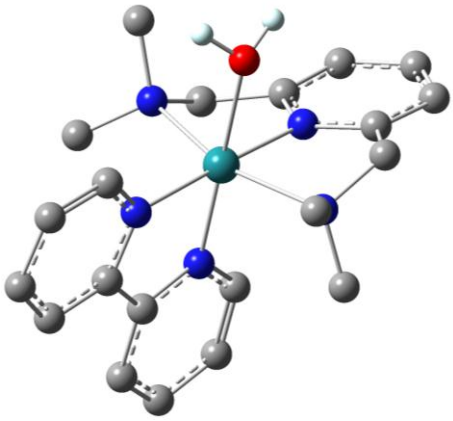
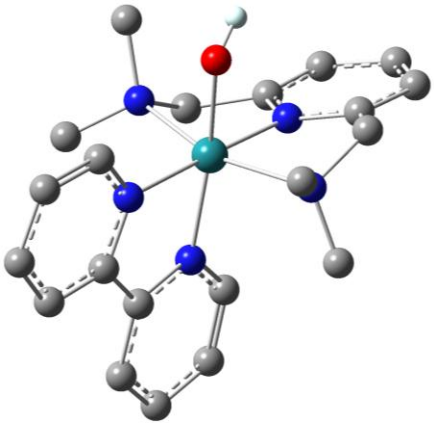
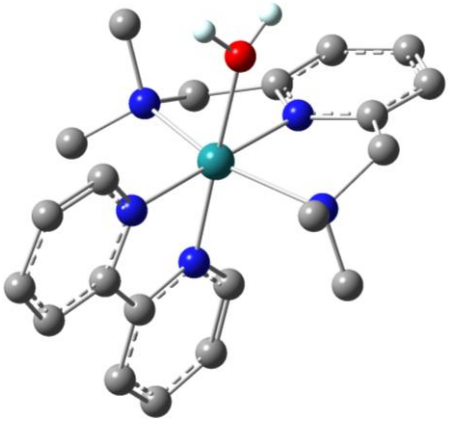
1. Images for the optimized structures at the DFT level of theory



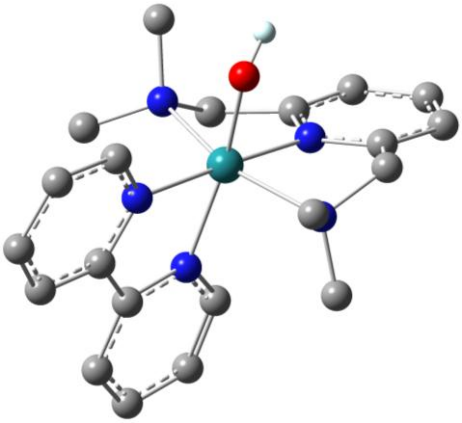
$[Ru^{II}\text{-}OH_2]^{2+}$



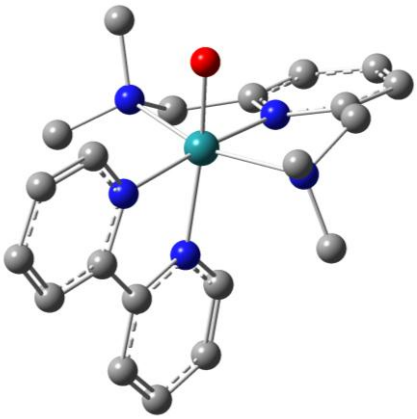
$[Ru^{II}\text{-}OH]^{+}$



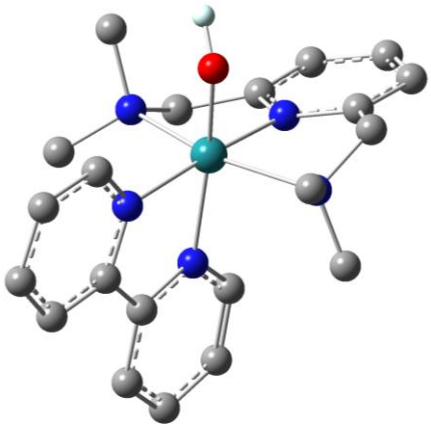
$[Ru^{III}\text{-}OH_2]^{3+}$



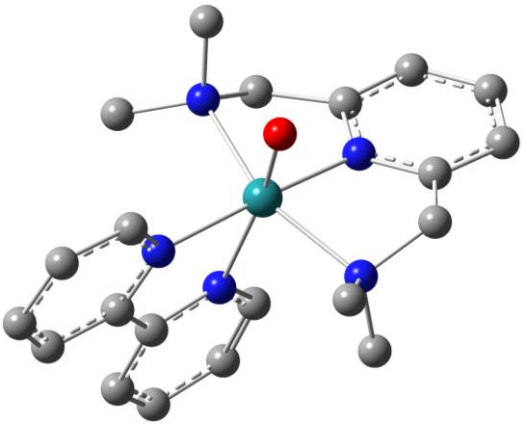
$[Ru^{III}\text{-}OH]^{2+}$



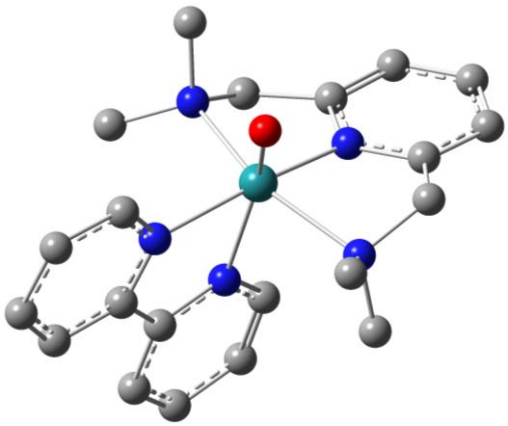
$[Ru^{III}\text{-}O]^{+}$



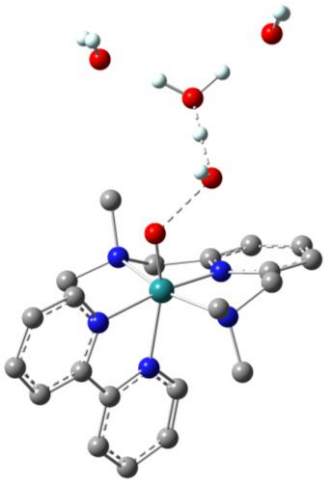
$[Ru^{IV}\text{-}OH]^{3+}$



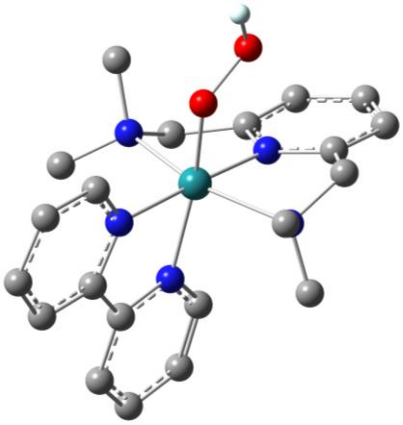
$[Ru^{IV}\text{-}O]^{2+}$



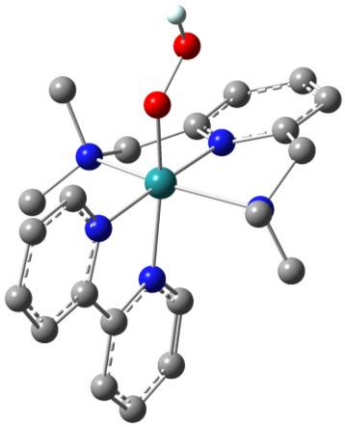
$[Ru^{V}\text{-}O]^{3+}$



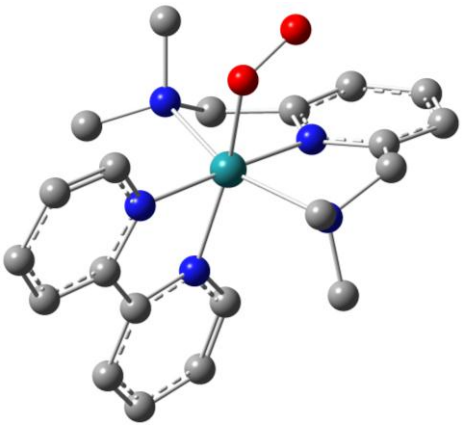
$[(Ru^{V}–O)(OH_2)_4]^{3+}$ O-O Bond Formation TS



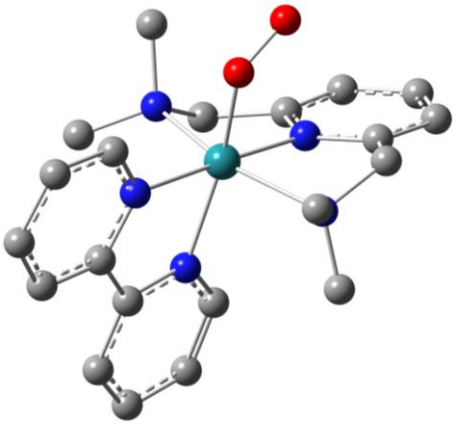
$[Ru^{III}\text{-}OOH]^{2+}$



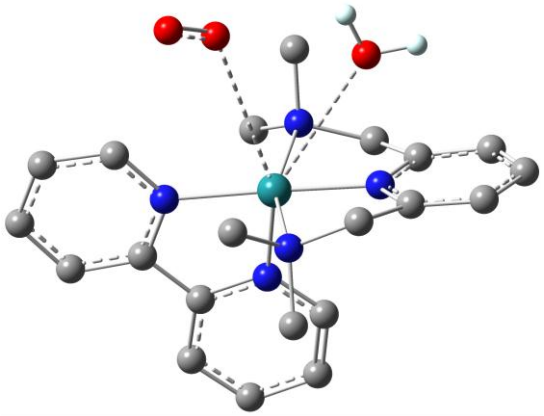
$[Ru^{IV}\text{-}OOH]^{3+}$



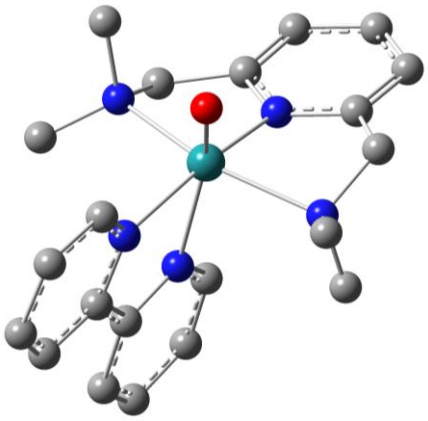
$[Ru^{III}\text{-}OO]^{+}$



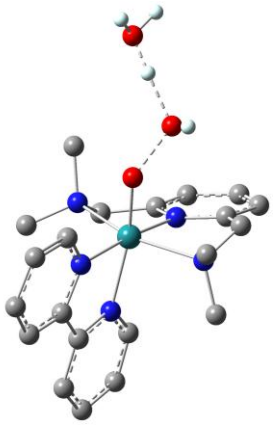
$[Ru^{IV}\text{-}OO]^{2+}$



$[(Ru^{IV}–OO)(H_2O)]^{2+}$ O_2 Release TS



$[Ru^{VI}\text{-}O]^{4+}$



$[(Ru^{VI}\text{–}O)(OH_2)_2]^{4+}$ O-O Bond Formation TS

2. Cartesian Coordinates and Energies

$[Ru^{II}–OH_2]^{2+}$ (Singlet)

Energy: -1261.11440197 a.u.

Ru	0.10003800	-0.47651300	0.16025100
N	2.04978900	-0.05955000	0.03255600
C	2.77017500	-0.60460300	-0.97722800
C	4.12784900	-0.33218600	-1.08994900
C	4.73725900	0.47462900	-0.12816000
C	3.98404500	1.00038400	0.92279400
C	2.62378100	0.72621300	0.97575700
N	-0.63412300	1.30589200	-0.45377300
C	0.11336300	2.37144700	-0.82445400
C	-0.43274600	3.58411800	-1.20838100
C	-1.81930200	3.72480000	-1.22309400
C	-2.59901300	2.63721100	-0.85747300
C	-2.00043700	1.43494800	-0.47744600
N	-1.95523000	-0.82773900	0.24684200
C	-2.56558300	-1.97813400	0.59529800
C	-3.94219500	-2.12682400	0.64365700
C	-4.74565100	-1.03755000	0.31187400
C	-4.13399300	0.15136200	-0.06035400
C	-2.74125400	0.23915800	-0.08882100
H	4.70534200	-0.75409000	-1.90940600
H	5.80063300	0.69001300	-0.19504700
H	4.44857500	1.62360200	1.68357800
H	1.19076900	2.21770200	-0.81399700
H	0.22411500	4.40099800	-1.49429000
H	-2.28320000	4.66202900	-1.51856200
H	-3.68235900	2.71983300	-0.86735400
H	-1.90821300	-2.81372600	0.82968400
H	-4.37217500	-3.08164000	0.93316000
H	-5.82929400	-1.11528500	0.33768300
H	-4.74183800	1.01048700	-0.33102300
N	0.46639900	0.38639300	2.17997500
C	0.84411000	-0.64332800	3.17119600
H	1.05372400	-0.18661700	4.14861400
H	0.01953800	-1.35322600	3.29269000
H	1.74568300	-1.16770900	2.84000200
C	-0.65291600	1.17212600	2.74567200
H	-1.50265100	0.50649900	2.92290500
H	-0.36463400	1.63898100	3.69789200
H	-0.94899400	1.95589100	2.04326000
C	1.64123900	1.29683100	1.96041000

H	2.11911200	1.54396900	2.91976600
H	1.23761700	2.23853200	1.56205500
C	1.98643400	-1.55448700	-1.84327300
H	2.07512400	-2.57180500	-1.43891900
H	2.38647600	-1.59562100	-2.86666700
N	0.52045400	-1.22509400	-1.87469500
C	0.29625200	-0.19281700	-2.91158400
H	0.55927700	-0.58202100	-3.90469100
H	-0.75696100	0.10182300	-2.91324700
H	0.91317300	0.68572700	-2.70135900
C	-0.24002100	-2.43714100	-2.25286600
H	-1.29963200	-2.17907700	-2.33326500
H	0.10176800	-2.82961700	-3.22081300
H	-0.10921300	-3.20529400	-1.48690500
O	0.77443500	-2.55255900	0.75626200
H	0.27820400	-3.03539200	1.43612000
H	1.70348000	-2.63416600	1.02919500

$[Ru^{II}–OH]^{+}$ (Singlet)

Energy: -1260.80928193 a.u.

Ru	0.12745400	-0.47006200	0.11975100
N	2.04911900	-0.05071900	0.00531600
C	2.76594200	-0.54460600	-1.03516800
C	4.12383000	-0.27874800	-1.13489300
C	4.75063400	0.45582700	-0.12559000
C	4.00612600	0.90914200	0.96451500
C	2.64397700	0.64846600	1.00474400
N	-0.66930000	1.37683100	-0.33731300
C	0.01990400	2.51357600	-0.60936800
C	-0.57986700	3.72015400	-0.91590100
C	-1.97414300	3.79298100	-0.95963300
C	-2.69941600	2.64255600	-0.68971200
C	-2.04563500	1.44867800	-0.37910100
N	-1.90220900	-0.84583400	0.21524600
C	-2.43374000	-2.04268200	0.53893200
C	-3.80161100	-2.25427500	0.58799000
C	-4.66252400	-1.19504400	0.29535200
C	-4.12105500	0.03884600	-0.03323200
C	-2.73344800	0.20099900	-0.06708000
H	4.69200400	-0.65945200	-1.98097400
H	5.81613000	0.66199800	-0.18237900
H	4.47928500	1.46473700	1.77142400
H	1.10513600	2.41189700	-0.58915400
H	0.03918800	4.58880000	-1.12487100
H	-2.48014700	4.72354600	-1.20162400

H	-3.78611300	2.66654200	-0.71817300
H	-1.69433000	-2.81608700	0.74936900
H	-4.18516300	-3.23700800	0.84923400
H	-5.74090700	-1.33000100	0.32383600
H	-4.77452900	0.87716100	-0.26172400
N	0.53663700	0.14812800	2.20573700
C	0.98385100	-0.97778200	3.05054600
H	1.17608100	-0.62898600	4.07647600
H	0.21862600	-1.75673600	3.05372600
H	1.90817600	-1.39718900	2.64291900
C	-0.59299300	0.81709300	2.87473900
H	-1.40551000	0.09555900	3.00191000
H	-0.29877600	1.19941500	3.86422600
H	-0.94677200	1.64935400	2.25875500
C	1.66580300	1.11983200	2.04232700
H	2.15353200	1.31213000	3.01089800
H	1.21293300	2.06830500	1.71718600
C	1.96297900	-1.44553100	-1.93145100
H	1.99389000	-2.46165800	-1.51921600
H	2.36908700	-1.48321400	-2.95409800
N	0.51489100	-1.06321400	-1.96289200
C	0.32861200	0.04534600	-2.91448000
H	0.59580600	-0.26837000	-3.93492400
H	-0.71742100	0.36599200	-2.90165300
H	0.95975200	0.89208400	-2.62529500
C	-0.28133800	-2.22817600	-2.39435200
H	-1.32788100	-1.92229400	-2.48846000
H	0.06835200	-2.60444600	-3.36759900
H	-0.19092500	-3.00331000	-1.62838400
O	0.51244300	-2.42795700	0.51338200
H	1.39369000	-2.57864600	0.88467300

$[Ru^{III}–OH_2]^{3+}$ (Doublet)

Energy: -1260.65937478 a.u.

Ru	0.08735600	-0.50332600	0.15200400
N	2.09045200	-0.09617700	0.05134300
C	2.80409700	-0.60027500	-0.98478800
C	4.17044200	-0.36288500	-1.06950500
C	4.78885700	0.37980800	-0.06264300
C	4.03630100	0.88715900	0.99828400
C	2.66884000	0.64598400	1.02629600
N	-0.66841900	1.30616800	-0.39834600
C	0.08299500	2.38816800	-0.70010800
C	-0.47322100	3.60993900	-1.04377200
C	-1.86211200	3.72831800	-1.08704200

C	-2.64100900	2.61867900	-0.78268100
C	-2.03457800	1.41055000	-0.43575800
N	-1.96332000	-0.86983000	0.24355500
C	-2.54856700	-2.03936300	0.57914100
C	-3.92294500	-2.21148200	0.61079200
C	-4.73929400	-1.13042600	0.27789700
C	-4.14948700	0.07933300	-0.07371900
C	-2.76041400	0.19474700	-0.08616400
H	4.74561500	-0.75810500	-1.90394900
H	5.85956000	0.56717000	-0.10639100
H	4.50762200	1.47043900	1.78634600
H	1.16135400	2.24631600	-0.67367300
H	0.17618700	4.44935400	-1.27807100
H	-2.33165600	4.67178700	-1.35588700
H	-3.72467800	2.69377600	-0.81234600
H	-1.88179400	-2.86439800	0.81994900
H	-4.34153400	-3.17520800	0.88842800
H	-5.82242700	-1.22920600	0.28976900
H	-4.77517300	0.92738700	-0.33859700
N	0.45817100	0.38372800	2.14436100
C	0.72047000	-0.72548300	3.10400400
H	0.87774600	-0.31814400	4.11062300
H	-0.14294100	-1.39707200	3.13928500
H	1.61857600	-1.27331100	2.80910400
C	-0.64017400	1.21994700	2.69996500
H	-1.53505000	0.60507200	2.82862400
H	-0.34845400	1.61994600	3.67893200
H	-0.85445400	2.05659100	2.03131000
C	1.70095500	1.22258400	2.01762300
H	2.15369600	1.35709400	3.00932000
H	1.38699400	2.22255600	1.68663800
C	1.99718400	-1.44445600	-1.92744600
H	2.02220900	-2.49619200	-1.61424100
H	2.39894200	-1.41741100	-2.94892300
N	0.55267000	-1.01228500	-1.94168100
C	0.39653600	0.09313000	-2.92388500
H	0.64036200	-0.27192200	-3.92886700
H	-0.63656300	0.44891600	-2.92259900
H	1.07355700	0.91496200	-2.67626700
C	-0.30001300	-2.15287600	-2.38191000
H	-1.33623600	-1.81642700	-2.46977800
H	0.03503300	-2.51217900	-3.36339700
H	-0.22764700	-2.97373200	-1.66426000
O	0.79529900	-2.56476600	0.63211100
H	1.73208800	-2.71007800	0.85377900
H	0.30695000	-3.22132000	1.15794900

$[Ru^{III}–OH]^{2+}$ (Doublet)

Energy: -1260.50657165 a.u.

Ru	0.13992800	-0.48109700	0.18217800
N	2.09607700	-0.07702400	0.01365100
C	2.78147500	-0.68536300	-0.98019000
C	4.14303800	-0.44403200	-1.12461500
C	4.77638300	0.39575900	-0.20904400
C	4.05064600	0.98808500	0.82777000
C	2.68795500	0.74145300	0.91259700
N	-0.70555200	1.35867300	-0.45823500
C	-0.01859900	2.44914100	-0.85619400
C	-0.63095800	3.61702200	-1.27918400
C	-2.02415100	3.66904900	-1.29222500
C	-2.74358000	2.55064300	-0.89416800
C	-2.07207700	1.39721000	-0.48293500
N	-1.91883400	-0.85495900	0.29171900
C	-2.44685700	-2.02820200	0.68655100
C	-3.81738100	-2.23811400	0.75142600
C	-4.67569300	-1.20104300	0.39539400
C	-4.13388300	0.01144200	-0.01351400
C	-2.74824900	0.16834400	-0.05963900
H	4.70340100	-0.91688500	-1.92764000
H	5.84320700	0.58586600	-0.29819700
H	4.54062500	1.63402000	1.55249500
H	1.06724100	2.35569000	-0.83870000
H	-0.02752900	4.46466700	-1.59140300
H	-2.54331200	4.56888100	-1.61279600
H	-3.82960700	2.57420900	-0.90678800
H	-1.72139800	-2.79518400	0.95241700
H	-4.19862400	-3.20146500	1.07859600
H	-5.75401100	-1.33257400	0.43542200
H	-4.79040100	0.83027500	-0.29466700
N	0.55231000	0.44989200	2.15649600
C	0.95570500	-0.56950200	3.15884500
H	1.14914500	-0.08729300	4.12600100
H	0.16008600	-1.30904600	3.27374700
H	1.87434100	-1.06719000	2.83458200
C	-0.55392000	1.24513800	2.73744900
H	-1.39398700	0.57983100	2.95525300
H	-0.23551600	1.72770700	3.67124400
H	-0.87221000	2.01594000	2.03069100
C	1.72354200	1.35185800	1.89190600
H	2.21472300	1.61833100	2.83869200

H	1.32115800	2.28612700	1.47526500
C	1.95939100	-1.65706500	-1.77976700
H	1.98877200	-2.63616500	-1.28336000
H	2.35446500	-1.79280900	-2.79623800
N	0.50941400	-1.25676100	-1.84156700
C	0.33870900	-0.23191100	-2.89693900
H	0.60403600	-0.64808300	-3.87765500
H	-0.70391200	0.09682700	-2.92224000
H	0.98422700	0.62809900	-2.69202800
C	-0.30726100	-2.44536900	-2.18187600
H	-1.34995600	-2.13766200	-2.29884400
H	0.03764600	-2.89128900	-3.12432800
H	-0.22611900	-3.17635400	-1.37381800
O	0.51358000	-2.28027000	0.78840600
H	1.33873300	-2.41005100	1.28687600

$[Ru^{III}–O]^{+}$ (Doublet)

Energy: -1260.16909739 a.u.

Ru	0.13040700	-0.54648700	0.12338600
O	0.46687800	-2.30860300	0.47277300
N	2.06329700	-0.08336200	0.03720300
C	2.78686800	-0.54016100	-1.00887000
C	4.13318600	-0.21899600	-1.10556000
C	4.72159500	0.53599600	-0.08745100
C	3.96366300	0.94970000	1.00784700
C	2.61368500	0.62393400	1.04845700
N	-0.63468700	1.38631400	-0.31854000
C	0.08648900	2.51294100	-0.55917300
C	-0.47421200	3.73640100	-0.85749300
C	-1.86995600	3.84536400	-0.93077800
C	-2.62716200	2.71167200	-0.69345200
C	-2.00898400	1.49527300	-0.38458900
N	-1.94647800	-0.81628700	0.17304000
C	-2.52542700	-1.99454900	0.48289900
C	-3.89806100	-2.15972700	0.52514700
C	-4.71625700	-1.06176000	0.24281200
C	-4.12917100	0.15244300	-0.06770700
C	-2.73303700	0.26857500	-0.09866300
H	4.72078200	-0.56840200	-1.95131000
H	5.77761000	0.78840900	-0.14182100
H	4.41664700	1.51473600	1.81930800
H	1.16987300	2.38849400	-0.52119100
H	0.16985400	4.59262800	-1.04037700
H	-2.34650900	4.79155300	-1.17133000
H	-3.71202500	2.76360000	-0.74639800

H	-1.81999400	-2.79961000	0.68991800
H	-4.31766700	-3.13098800	0.77187100
H	-5.79924400	-1.15523300	0.26797100
H	-4.75020100	1.01801900	-0.28334500
N	0.51378700	0.01952400	2.22708500
C	0.99077000	-1.14337500	3.00799300
H	1.24752400	-0.82674500	4.02983500
H	0.20834200	-1.90367400	3.03106500
H	1.86201600	-1.58246900	2.51705300
C	-0.62646600	0.63778300	2.92536700
H	-1.42145100	-0.10634600	3.02875000
H	-0.33580000	0.98909100	3.92698200
H	-1.00132300	1.48328700	2.34006600
C	1.62165100	1.02194500	2.10504400
H	2.10757900	1.17541700	3.08116100
H	1.15366200	1.97840100	1.82752600
C	2.01253800	-1.46616200	-1.90312500
H	2.04613900	-2.46594600	-1.45023900
H	2.44323800	-1.52806100	-2.91403200
N	0.56226400	-1.09978800	-1.97580700
C	0.38299200	0.02418700	-2.90974200
H	0.68015200	-0.26496500	-3.92903000
H	-0.66786400	0.32846900	-2.91485700
H	0.99105500	0.87572500	-2.58750400
C	-0.20488000	-2.26928000	-2.44442800
H	-1.25425200	-1.97911700	-2.55390400
H	0.17177300	-2.62392100	-3.41528500
H	-0.11908000	-3.05614400	-1.69011100

[Ru^{IV}–OH]$^{3+}$ (Triplet)

Energy: -1260.02557739 a.u.

Ru	0.12355000	-0.56568900	0.14972400
N	2.08135300	-0.10395500	0.06502700
C	2.80531200	-0.62198500	-0.96054500
C	4.16883800	-0.36993700	-1.02475800
C	4.76027500	0.39392300	-0.01492600
C	3.99314500	0.89938000	1.04025100
C	2.63072000	0.64112300	1.05888900
N	-0.60617700	1.33778800	-0.40810500
C	0.16128500	2.40769400	-0.72382500
C	-0.37316500	3.63220100	-1.08379700
C	-1.76195500	3.76881700	-1.12920800
C	-2.55893400	2.67499600	-0.81348200
C	-1.97256100	1.46144100	-0.45209800
N	-1.97025800	-0.82826500	0.22003400

C	-2.57285900	-1.98493800	0.56160900
C	-3.95545400	-2.11138400	0.59583500
C	-4.74277900	-1.00968500	0.26908000
C	-4.12133600	0.18443500	-0.08388700
C	-2.72932000	0.26051900	-0.10408600
H	4.76630900	-0.77639500	-1.83779700
H	5.82984900	0.59237400	-0.04581200
H	4.45448900	1.48593600	1.83176800
H	1.23859100	2.25317600	-0.69329700
H	0.28748900	4.45993600	-1.32800600
H	-2.21753400	4.71588600	-1.41040900
H	-3.64081300	2.76791900	-0.84970000
H	-1.91188600	-2.81658000	0.79474200
H	-4.39845600	-3.06474600	0.87258400
H	-5.82819500	-1.07716800	0.28707600
H	-4.72477700	1.05051700	-0.34147100
N	0.43221100	0.27930300	2.18068600
C	0.76836000	-0.83288700	3.12083700
H	0.93864300	-0.42531500	4.12467000
H	-0.06471400	-1.53915400	3.17226000
H	1.68562100	-1.33368400	2.79652300
C	-0.69730100	1.05143200	2.76273200
H	-1.55405800	0.38751400	2.90408600
H	-0.40838200	1.46155300	3.73836100
H	-0.96864200	1.87804300	2.10143900
C	1.63750800	1.17737500	2.04942800
H	2.08799100	1.33041900	3.03926900
H	1.27652500	2.16190600	1.71994100
C	2.01958500	-1.52250400	-1.86592900
H	2.04216400	-2.54428900	-1.46201600
H	2.43976000	-1.56515000	-2.87912300
N	0.56983900	-1.10732100	-1.93705200
C	0.42776400	0.00025400	-2.91917500
H	0.69887400	-0.36267300	-3.91781100
H	-0.60933400	0.34374200	-2.94193300
H	1.09059000	0.82886700	-2.65537700
C	-0.25793600	-2.26076100	-2.39544900
H	-1.29296600	-1.93182900	-2.51758900
H	0.11359400	-2.61525100	-3.36497700
H	-0.20117300	-3.07183300	-1.66707500
O	0.40030200	-2.38046200	0.55793200
H	0.90789100	-2.73961400	1.30925500

$[Ru^{IV}–O]^{2+}$ (Singlet)

Energy: -1259.87281125 a.u.

Ru	0.15438200	-0.55876800	0.15136800
O	0.46795400	-2.22621600	0.61485200
N	2.09862300	-0.06705200	0.04349200
C	2.82443500	-0.58439500	-0.97158600
C	4.17867300	-0.28926000	-1.06115800
C	4.75714900	0.50732800	-0.07187500
C	3.98935100	0.99642500	0.98710700
C	2.63504000	0.69383700	1.02261000
N	-0.68889200	1.39447900	-0.41432200
C	0.00932800	2.50180700	-0.73321300
C	-0.58835800	3.70333800	-1.07845800
C	-1.98034500	3.76673400	-1.10197700
C	-2.71254300	2.63081300	-0.78285700
C	-2.05093500	1.44956200	-0.44001800
N	-1.94083300	-0.85250300	0.21354300
C	-2.49545400	-2.03046600	0.55742200
C	-3.86930100	-2.21490800	0.61370800
C	-4.70345800	-1.14433800	0.30411000
C	-4.13376600	0.07297400	-0.04824100
C	-2.74500100	0.20447500	-0.08793600
H	4.77738700	-0.69032600	-1.87523900
H	5.81866400	0.73862700	-0.11882800
H	4.44088400	1.59894900	1.77150700
H	1.09516800	2.40016200	-0.71457200
H	0.02415300	4.56562300	-1.32630600
H	-2.48997900	4.68927100	-1.36897500
H	-3.79797100	2.66665700	-0.80257000
H	-1.78864200	-2.82624100	0.78710400
H	-4.27023100	-3.18420000	0.89674000
H	-5.78459200	-1.25316600	0.33716900
H	-4.77245700	0.91767000	-0.29016800
N	0.49562900	0.20477100	2.19938900
C	0.93523300	-0.90959000	3.08356400
H	1.18108500	-0.51670400	4.07851400
H	0.12974000	-1.64190500	3.16634000
H	1.80770600	-1.40470200	2.65172700
C	-0.64251500	0.89753400	2.84352800
H	-1.45624300	0.18247300	2.99151400
H	-0.34733300	1.30144800	3.82111300
H	-0.98746200	1.71880000	2.20852000
C	1.63329400	1.17393700	2.03548000
H	2.10203000	1.36819800	3.01045800
H	1.19957900	2.12741700	1.70036900
C	2.05419200	-1.53748900	-1.83911000
H	2.10337600	-2.53329900	-1.37714100
H	2.47860400	-1.61847900	-2.84929500

N	0.59632100	-1.17380000	-1.92046900
C	0.42045800	-0.08653400	-2.90915100
H	0.72159400	-0.42874700	-3.90790000
H	-0.63063300	0.21351600	-2.93950900
H	1.03388200	0.77596000	-2.63066800
C	-0.17329000	-2.36147300	-2.36192300
H	-1.22427100	-2.08130500	-2.47392700
H	0.20160700	-2.72525200	-3.32759600
H	-0.08116500	-3.14805200	-1.60894600

$[Ru^{IV}–O]^{2+}$ (Triplet)

Energy: -1259.88551341 a.u.

Ru	0.15558900	-0.55698300	0.15168000
O	0.48157800	-2.22138700	0.62014600
N	2.10313300	-0.06343400	0.04460100
C	2.83121700	-0.58469000	-0.96594600
C	4.18588200	-0.29000200	-1.05353500
C	4.76168500	0.51097700	-0.06644500
C	3.99082300	1.00560500	0.98759200
C	2.63628200	0.70297800	1.02044900
N	-0.69855800	1.39706800	-0.42197500
C	-0.00857600	2.50736200	-0.74515300
C	-0.61504600	3.70395800	-1.09312600
C	-2.00736200	3.75665600	-1.11431700
C	-2.73114000	2.61664200	-0.79033600
C	-2.06056400	1.44100900	-0.44482400
N	-1.93800100	-0.86045700	0.21725300
C	-2.48762800	-2.03912300	0.56581100
C	-3.86070200	-2.22921000	0.62494400
C	-4.69955000	-1.16318600	0.31290000
C	-4.13510100	0.05515300	-0.04459900
C	-2.74697400	0.19243000	-0.08691100
H	4.78661800	-0.69443400	-1.86445600
H	5.82338900	0.74181000	-0.11139900
H	4.43995300	1.61242700	1.77005800
H	1.07802000	2.41311500	-0.72762900
H	-0.00937800	4.57001400	-1.34455700
H	-2.52428300	4.67461500	-1.38322700
H	-3.81676300	2.64544900	-0.80843700
H	-1.77783400	-2.83168600	0.79712100
H	-4.25722000	-3.19914500	0.91191900
H	-5.78019600	-1.27610600	0.34790800
H	-4.77787500	0.89615600	-0.28847100
N	0.49457600	0.21977700	2.19679700
C	0.93450900	-0.88950900	3.08674800

H	1.17914300	-0.49181500	4.08014400
H	0.12950600	-1.62208700	3.17279200
H	1.80796900	-1.38578300	2.65829300
C	-0.64416600	0.91513000	2.83708700
H	-1.45763400	0.20043500	2.98826100
H	-0.34952600	1.32386300	3.81285300
H	-0.98930700	1.73325500	2.19817700
C	1.63163500	1.18891400	2.02792200
H	2.09793300	1.39087800	3.00252000
H	1.19726700	2.13931700	1.68502800
C	2.06318700	-1.54028000	-1.83282500
H	2.11250200	-2.53526600	-1.36931200
H	2.48955100	-1.62272700	-2.84210300
N	0.60517100	-1.17785100	-1.91835400
C	0.43104700	-0.09152400	-2.90839000
H	0.73747000	-0.43336700	-3.90568300
H	-0.62062000	0.20591000	-2.94379600
H	1.04125300	0.77253600	-2.62765500
C	-0.16189600	-2.36648300	-2.36085900
H	-1.21309300	-2.08802800	-2.47501600
H	0.21528700	-2.73023800	-3.32570400
H	-0.07028800	-3.15330300	-1.60809200

$[Ru^{V}–O]^{3+}$ (Doublet)

Energy: -1259.39769690 a.u.

Ru	0.15547900	-0.63115700	0.14760200
O	0.15791500	-2.30558800	0.33673500
N	2.07934500	-0.09587200	0.10225100
C	2.83118500	-0.55452200	-0.93980200
C	4.19080000	-0.28296300	-0.95716600
C	4.75314400	0.43483200	0.10323500
C	3.96209000	0.86898800	1.17272200
C	2.60429400	0.59478700	1.15255000
N	-0.60388500	1.34195800	-0.37935500
C	0.18807600	2.40591300	-0.65693900
C	-0.31909100	3.65407500	-0.97457700
C	-1.70362700	3.82042600	-1.02893800
C	-2.52404100	2.73325400	-0.75397200
C	-1.95894400	1.49882100	-0.42974100
N	-1.99668800	-0.80147100	0.18458000
C	-2.62216200	-1.95124600	0.51110200
C	-4.00673200	-2.05437200	0.54187600
C	-4.77471900	-0.93635500	0.22838600
C	-4.12902200	0.24989000	-0.10512400
C	-2.73496200	0.30065100	-0.11848200

H	4.81114600	-0.64518100	-1.77413100
H	5.82042200	0.64881100	0.10202700
H	4.40206500	1.41195300	2.00634300
H	1.26255500	2.23615800	-0.61984000
H	0.36122000	4.47712900	-1.17785700
H	-2.13772400	4.78456700	-1.28525700
H	-3.60367100	2.84707300	-0.79425200
H	-1.98314500	-2.80092000	0.74109000
H	-4.46406800	-3.00571200	0.80243900
H	-5.86125700	-0.98463900	0.24136600
H	-4.71298700	1.13265800	-0.35042600
N	0.40282300	0.11448200	2.19609800
C	0.75178200	-1.08518800	3.03062400
H	0.94831200	-0.76122100	4.05937600
H	-0.08709800	-1.78449300	3.02975000
H	1.64068200	-1.57904500	2.62980000
C	-0.75471700	0.81062100	2.81616800
H	-1.59281000	0.11487400	2.90072200
H	-0.48390400	1.15492000	3.82196100
H	-1.04068200	1.67544600	2.21201400
C	1.58751900	1.04578700	2.15678700
H	2.01645300	1.13114300	3.16405700
H	1.21423000	2.04556600	1.89151700
C	2.09178500	-1.44154100	-1.89489600
H	2.14145400	-2.47589400	-1.52340300
H	2.54287800	-1.44106700	-2.89594900
N	0.63707400	-1.06708200	-1.99057900
C	0.48899300	0.09069700	-2.91030400
H	0.78718900	-0.20934500	-3.92219000
H	-0.55511100	0.41195100	-2.93599900
H	1.12688900	0.91828400	-2.58975600
C	-0.13795400	-2.21284800	-2.54904200
H	-1.18743100	-1.92184700	-2.64153400
H	0.24558700	-2.46664600	-3.54456200
H	-0.04843600	-3.08126300	-1.89343500

[Ru^{V}–O]$^{3+}$ (Quartet)

Energy: -1259.39053920 a.u.

Ru	0.10103400	-0.55507700	0.10295600
O	0.44517500	-2.25765900	0.43242900
N	2.10292300	-0.04539400	0.02157600
C	2.84851700	-0.52022700	-1.00519400
C	4.20412100	-0.22927700	-1.06910300
C	4.77985400	0.52523400	-0.04549800
C	4.00098300	0.96818800	1.02639200

C	2.64747400	0.66634000	1.03920300
N	-0.72543700	1.44337000	-0.29267400
C	-0.03633900	2.57776700	-0.53149800
C	-0.65116100	3.79482200	-0.79150000
C	-2.04324900	3.84404600	-0.81232000
C	-2.76604300	2.67713500	-0.57470300
C	-2.09071100	1.48444200	-0.31569400
N	-1.94820900	-0.87394200	0.16208400
C	-2.48668500	-2.09331600	0.42012900
C	-3.85431000	-2.29463500	0.46823100
C	-4.70075500	-1.20653900	0.24374400
C	-4.14948500	0.04788900	-0.01818900
C	-2.76790700	0.20812200	-0.05629400
H	4.80592100	-0.60070000	-1.89552000
H	5.84317800	0.75432800	-0.07337800
H	4.44561100	1.53081600	1.84427900
H	1.05032600	2.49061100	-0.52193200
H	-0.04859100	4.68008100	-0.97712200
H	-2.56368100	4.77773000	-1.01462400
H	-3.85195800	2.70594400	-0.59577000
H	-1.77430800	-2.89949300	0.58584900
H	-4.24615700	-3.28652400	0.67843400
H	-5.78151200	-1.33034100	0.27359800
H	-4.80630400	0.89612100	-0.18957700
N	0.58949700	-0.00590200	2.18493000
C	1.11953900	-1.18962500	2.92723300
H	1.37195200	-0.88263700	3.94930500
H	0.35815400	-1.97089100	2.96291500
H	2.01052400	-1.57767800	2.42864600
C	-0.60024300	0.53098200	2.90012500
H	-1.34902100	-0.25794700	3.00583900
H	-0.30198000	0.86139400	3.90368600
H	-1.01469700	1.38489000	2.35778700
C	1.65478200	1.05040900	2.09082000
H	2.12128000	1.18139500	3.07608800
H	1.16232700	2.00107800	1.84262800
C	2.08745700	-1.41547400	-1.92842000
H	2.11294400	-2.44328600	-1.53926500
H	2.50110600	-1.43566300	-2.94486100
N	0.64439300	-0.99490800	-1.98751800
C	0.49840300	0.18972500	-2.87497100
H	0.79002900	-0.08673200	-3.89571400
H	-0.54364700	0.51835900	-2.88681200
H	1.14487200	1.00105900	-2.53000000
C	-0.18382100	-2.11832000	-2.51009300
H	-1.22207400	-1.79142500	-2.60845700

H	0.18643400	-2.40855100	-3.50184200
H	-0.11234800	-2.97596400	-1.83685200

$[(Ru^{V}–O)(OH_2)_4]^{3+}$ O-O Bond Formation Transition State Structure (Doublet)

Energy: -1565.11678419 a.u.

Ru	-0.27342500	0.10081700	0.17659400
O	0.93033900	1.28914100	0.57025600
N	0.86241600	-1.53672000	-0.02795400
C	1.30637700	-2.14763400	1.09654300
C	2.07953900	-3.29594500	0.98368400
C	2.39344400	-3.77240600	-0.28987300
C	1.93353300	-3.11193900	-1.43303700
C	1.14640200	-1.98100800	-1.27709000
N	-2.15498100	-0.87428800	-0.35076900
C	-2.28980400	-2.18183600	-0.66079800
C	-3.50497400	-2.75915500	-0.99065500
C	-4.64295500	-1.95372800	-0.99834100
C	-4.51858400	-0.60939500	-0.67140700
C	-3.26608900	-0.08378600	-0.34848600
N	-1.75240300	1.64546200	0.30935500
C	-1.45911000	2.91576100	0.64762800
C	-2.42335600	3.91117900	0.71589300
C	-3.74486200	3.58680100	0.42292500
C	-4.05169200	2.27809200	0.06935500
C	-3.04127200	1.31736600	0.01587900
H	2.43809600	-3.80665500	1.87416800
H	3.00046200	-4.66912000	-0.39474700
H	2.17769000	-3.48133400	-2.42629000
H	-1.37996000	-2.78057600	-0.62615200
H	-3.55606700	-3.81765200	-1.23051800
H	-5.61602000	-2.36875800	-1.25064300
H	-5.39897000	0.02671200	-0.66608100
H	-0.41183200	3.11438100	0.86518200
H	-2.13506400	4.92113200	0.99434600
H	-4.52731400	4.34050800	0.46718000
H	-5.07796100	2.00946500	-0.16416600
N	0.19646000	0.21176800	-1.98910600
C	1.44646500	0.99906300	-2.18666000
H	1.71532500	0.99321500	-3.25043600
H	1.28489400	2.02793400	-1.85778300
H	2.25710600	0.55920800	-1.60032700
C	-0.86004000	0.76909100	-2.86779600
H	-1.02669000	1.81713100	-2.60541200
H	-0.55229800	0.71421400	-3.91991300
H	-1.78831000	0.20526600	-2.74131400

C	0.46662900	-1.21555000	-2.37719600
H	1.04531100	-1.24365400	-3.31066400
H	-0.50299200	-1.68342300	-2.60056100
C	0.97496900	-1.42094300	2.36283200
H	1.77788200	-0.68998800	2.53245100
H	0.92856700	-2.09260000	3.22990000
N	-0.31642800	-0.64842400	2.24833700
C	-1.45311900	-1.56086000	2.53427400
H	-1.39071600	-1.91845700	3.56947700
H	-2.39747000	-1.02619600	2.40231900
H	-1.42287200	-2.42256100	1.86155000
C	-0.32232300	0.44198900	3.25753900
H	-1.28009200	0.96694300	3.21332900
H	-0.19328900	0.02613700	4.26464300
H	0.48986400	1.13956200	3.04302000
O	2.79521900	0.82176200	1.24577400
H	2.76178400	1.61495000	1.80828300
H	3.75760700	1.04987000	0.34153000
O	4.57443600	1.15815000	-0.42241100
H	5.47727100	0.89269800	-0.04440500
H	4.62830600	2.09943800	-0.78005500
O	6.87324000	0.37841700	0.57695400
H	7.40430600	0.87214800	1.21805300
H	7.51630200	-0.08352900	0.01998200
O	4.51012000	3.58602300	-1.47145200
H	4.88743500	3.67771000	-2.35940800
H	4.81303500	4.37644700	-0.99995700

$[Ru^{III}–OOH]^{2+}$ (Doublet)

Energy: -1335.64651976 a.u.

Ru	0.10641500	-0.42569600	0.07262000
O	0.56494400	-2.25719500	0.38375400
N	2.02885200	0.15629500	-0.01989600
C	2.75706700	-0.19963800	-1.09844200
C	4.10108000	0.14448600	-1.16925800
C	4.67795500	0.82203400	-0.09578500
C	3.90902100	1.15810600	1.01949800
C	2.56263500	0.82029900	1.02734100
N	-0.84168300	1.42831700	-0.27544900
C	-0.21634300	2.60666900	-0.47595400
C	-0.89391300	3.79712400	-0.67914200
C	-2.28795900	3.77547700	-0.68314900
C	-2.94368200	2.56793700	-0.48586200
C	-2.20830400	1.39836300	-0.28120000
N	-1.92850400	-0.93486100	0.14505100

C	-2.40068200	-2.17446400	0.37342700
C	-3.75734900	-2.46164700	0.41353100
C	-4.66911600	-1.42914200	0.20838400
C	-4.18963900	-0.14681100	-0.02574100
C	-2.81348900	0.08451900	-0.05251900
H	4.69334500	-0.12967400	-2.03895800
H	5.73231900	1.08560900	-0.12520500
H	4.35096100	1.67898500	1.86554500
H	0.87265900	2.56758800	-0.47960700
H	-0.33946300	4.71826500	-0.83466900
H	-2.85712600	4.68833900	-0.84046200
H	-4.02952800	2.53662400	-0.48907300
H	-1.64344300	-2.94181100	0.52500500
H	-4.08689400	-3.47948500	0.60264600
H	-5.73925700	-1.61849600	0.23116900
H	-4.88771700	0.67006500	-0.18637700
N	0.42894800	0.20398300	2.16538100
C	0.86376000	-0.96123700	2.98038000
H	1.08881000	-0.63296500	4.00347300
H	0.05827500	-1.69958700	3.00671700
H	1.74885400	-1.41772000	2.53265500
C	-0.71922400	0.84225600	2.84838500
H	-1.53723200	0.12028700	2.92194700
H	-0.43690300	1.15748500	3.86177500
H	-1.05350900	1.71861200	2.28636000
C	1.56134100	1.18903200	2.08539400
H	2.02979100	1.29766000	3.07372200
H	1.11828200	2.16567300	1.84178600
C	2.01027400	-1.05622300	-2.07907100
H	2.13401800	-2.10345400	-1.77622600
H	2.40204700	-0.95776800	-3.10100700
N	0.53330900	-0.76603100	-2.06871300
C	0.27346800	0.41431800	-2.92365900
H	0.56055100	0.19925700	-3.96141800
H	-0.79080000	0.66366600	-2.89550900
H	0.85625100	1.26886600	-2.56699500
C	-0.19525200	-1.92813500	-2.62933200
H	-1.26166300	-1.69046000	-2.67768600
H	0.16312000	-2.15561600	-3.64225800
H	-0.04434300	-2.79576300	-1.98268700
O	1.96651600	-2.59618900	0.56664200
H	1.88829800	-3.55033200	0.75890900

$[Ru^{IV}–OOH]^{3+}$ (Singlet)

Energy: -1335.16793214 a.u.

Ru	0.09209700	-0.47334700	0.08107400
O	0.48787700	-2.28208300	0.34148500
N	2.05976300	0.07282200	-0.00220700
C	2.77180600	-0.28247600	-1.09508900
C	4.12938400	0.00071300	-1.16479700
C	4.73775800	0.63480800	-0.08061100
C	3.98204100	0.99997100	1.03525100
C	2.62211300	0.71712500	1.04442500
N	-0.79835800	1.39174700	-0.23109900
C	-0.13738000	2.56325100	-0.37926100
C	-0.78584100	3.77285800	-0.55551700
C	-2.18241700	3.78304600	-0.59011800
C	-2.87203500	2.58585100	-0.44144200
C	-2.17101600	1.39273800	-0.25568000
N	-1.95368500	-0.95406800	0.14438400
C	-2.45767300	-2.18737100	0.34717400
C	-3.82250900	-2.44086300	0.35919800
C	-4.70496700	-1.38223600	0.14993500
C	-4.19150900	-0.10631300	-0.05899100
C	-2.81104700	0.09392700	-0.05767900
H	4.70607600	-0.27752500	-2.04399600
H	5.80340200	0.85166200	-0.10724100
H	4.44521800	1.50377900	1.88074500
H	0.94943700	2.50140600	-0.37022500
H	-0.20888700	4.68675700	-0.67002600
H	-2.72659500	4.71445700	-0.73118800
H	-3.95818000	2.58433300	-0.46455300
H	-1.73198900	-2.98283000	0.50261900
H	-4.18045900	-3.45270900	0.53050300
H	-5.78011700	-1.54671700	0.15058700
H	-4.87004800	0.72637700	-0.22208600
N	0.42988000	0.25940300	2.12814500
C	0.74955200	-0.95592900	2.94459100
H	0.96152600	-0.64529100	3.97466300
H	-0.10944600	-1.63175900	2.95035600
H	1.62798000	-1.46216300	2.53796100
C	-0.69625400	0.97581800	2.78282300
H	-1.56818300	0.31845900	2.82945000
H	-0.40988200	1.24830300	3.80616800
H	-0.93806800	1.88929000	2.23561700
C	1.64438200	1.14888700	2.09531100
H	2.09356200	1.17598800	3.09694800
H	1.29691800	2.17042200	1.88723800
C	1.96319300	-1.02316300	-2.11607100
H	1.97361000	-2.09768300	-1.89501900
H	2.35752500	-0.90021200	-3.13300100

N	0.52200900	-0.56680500	-2.08332300
C	0.39928000	0.69265700	-2.86093100
H	0.66266200	0.49347500	-3.90678200
H	-0.62930800	1.05785500	-2.82477300
H	1.08444400	1.44710300	-2.46624200
C	-0.35046400	-1.59991200	-2.71520200
H	-1.38232300	-1.24029800	-2.73331300
H	-0.02172500	-1.77301900	-3.74804600
H	-0.28972800	-2.53806900	-2.15892500
O	1.81014100	-2.72106100	0.51713500
H	1.69053900	-3.69098100	0.64113100

$[Ru^{IV}–OOH]^{3+}$ (Triplet)

Energy: -1335.16728039 a.u.

Ru	0.05747800	-0.43837500	0.04869200
O	0.48984900	-2.31791300	0.29161900
N	2.03279800	0.15055800	-0.00107000
C	2.78420400	-0.15457200	-1.08331700
C	4.12495200	0.20511000	-1.12518700
C	4.68489300	0.85126000	-0.02333200
C	3.89795600	1.13843400	1.09344900
C	2.55699300	0.78269900	1.07634500
N	-0.81535900	1.46573700	-0.20189300
C	-0.15992300	2.63644700	-0.35098200
C	-0.81466800	3.84768600	-0.51532900
C	-2.20839100	3.85386500	-0.53423200
C	-2.89364200	2.65032500	-0.38744800
C	-2.18463700	1.46186300	-0.21976300
N	-1.95920100	-0.90955000	0.09758400
C	-2.45364400	-2.15723500	0.27340800
C	-3.81455000	-2.41358100	0.30851700
C	-4.69985200	-1.34630900	0.15495600
C	-4.19508000	-0.05804500	-0.02476800
C	-2.81965600	0.14970600	-0.04965000
H	4.72708600	-0.02840300	-2.00042000
H	5.73689800	1.12787100	-0.03225100
H	4.32287800	1.63420000	1.96334800
H	0.92773300	2.57872500	-0.34847100
H	-0.24072500	4.76330100	-0.63089800
H	-2.75817200	4.78351000	-0.66444300
H	-3.98003000	2.64552800	-0.40512100
H	-1.71548400	-2.94901800	0.38496600
H	-4.17021600	-3.43029200	0.45318200
H	-5.77514500	-1.51136800	0.17575100
H	-4.88245400	0.77519900	-0.14212000

N	0.48075500	0.02027000	2.16228300
C	0.98677200	-1.17834500	2.89227400
H	1.18155800	-0.90419400	3.93587000
H	0.23129200	-1.96698300	2.86611900
H	1.90995600	-1.53494700	2.43177300
C	-0.72005700	0.53630600	2.87751500
H	-1.48238900	-0.24570800	2.92227400
H	-0.44316300	0.80851800	3.90388400
H	-1.11177300	1.42307300	2.37378100
C	1.55216100	1.07497800	2.14730700
H	2.00910600	1.14084900	3.14343500
H	1.06188400	2.04097900	1.96149700
C	2.06129100	-0.95287100	-2.12139000
H	2.20537900	-2.02133400	-1.92301900
H	2.43196700	-0.75859700	-3.13615600
N	0.58108900	-0.67131400	-2.07880300
C	0.30114800	0.55530900	-2.87529300
H	0.56329400	0.37143500	-3.92429200
H	-0.76166100	0.80328700	-2.82009400
H	0.90200600	1.38877000	-2.50279800
C	-0.16253600	-1.81436400	-2.68008100
H	-1.22729700	-1.57163400	-2.72783400
H	0.20091200	-1.99120000	-3.70027800
H	-0.00779300	-2.71584800	-2.08321300
O	1.84231600	-2.69544500	0.33791100
H	1.77501100	-3.66224900	0.50215400

$[Ru^{III}–OO]^{+}$ (Doublet)

Energy: -1335.32667510 a.u.

Ru	0.10249400	-0.41251200	0.06253600
O	0.57235300	-2.32840100	0.35536500
N	2.00881200	0.16258300	-0.00186900
C	2.76378000	-0.17712100	-1.07074000
C	4.09777000	0.20011700	-1.13189900
C	4.65859200	0.88534700	-0.05404900
C	3.87428900	1.18758500	1.05920000
C	2.53561500	0.82270800	1.05444700
N	-0.83153300	1.45440600	-0.26255100
C	-0.21795600	2.64245800	-0.46131500
C	-0.89741400	3.83046300	-0.66338200
C	-2.29295600	3.81192600	-0.67000800
C	-2.94079200	2.60141500	-0.47511300
C	-2.20276900	1.43238700	-0.27260100
N	-1.90980600	-0.90143800	0.12210100
C	-2.38137600	-2.14674400	0.34611100

C	-3.73441500	-2.43473500	0.40065300
C	-4.65464300	-1.40224400	0.21607400
C	-4.17990900	-0.11948200	-0.01208500
C	-2.80372700	0.11855800	-0.05412000
H	4.69885200	-0.06247700	-1.99953500
H	5.70661200	1.17278800	-0.07668500
H	4.29707900	1.70454700	1.91778400
H	0.87190800	2.60744400	-0.46155800
H	-0.34180700	4.75181000	-0.81662900
H	-2.86335400	4.72361400	-0.82729900
H	-4.02707500	2.56186100	-0.47993800
H	-1.61210800	-2.90748200	0.47920800
H	-4.05898500	-3.45538400	0.58474400
H	-5.72392100	-1.59454000	0.25114300
H	-4.87904800	0.70048800	-0.15517900
N	0.46507600	0.07799700	2.19105500
C	1.00451300	-1.09378100	2.91579100
H	1.28149900	-0.80835500	3.94134100
H	0.24266100	-1.87702000	2.94446300
H	1.87337500	-1.49089400	2.38315700
C	-0.69786100	0.60525500	2.92503900
H	-1.46367700	-0.17378000	2.98414200
H	-0.41896700	0.90563300	3.94646200
H	-1.10771700	1.47206900	2.39666400
C	1.52117700	1.13529000	2.11595700
H	1.99008200	1.27902700	3.10185100
H	1.00606000	2.07508300	1.86634000
C	2.05352500	-1.06737300	-2.04565600
H	2.19539400	-2.09962100	-1.69813300
H	2.46404100	-0.98802100	-3.06355000
N	0.57584400	-0.81445000	-2.06565900
C	0.29729700	0.34892200	-2.92573700
H	0.60227100	0.14744800	-3.96378700
H	-0.77381700	0.57222400	-2.90471400
H	0.84809200	1.22022500	-2.55696900
C	-0.11052000	-1.99973700	-2.61429300
H	-1.18270200	-1.78953100	-2.67678600
H	0.26426500	-2.24088600	-3.62028900
H	0.05221200	-2.84903000	-1.94584000
O	1.83226800	-2.71506000	0.43498700

$[Ru^{III}–OO]^{+}$ (Quartet)

Energy: -1335.27453677 a.u.

Ru	0.08680900	-0.43279500	0.08958300
O	0.79165300	-2.21787300	0.54865000

N	1.99735900	0.15200300	0.00494000
C	2.76172600	-0.29705100	-1.01509300
C	4.10720500	0.04323000	-1.06759200
C	4.64781900	0.81422600	-0.03841700
C	3.84185900	1.23875000	1.02193200
C	2.49861200	0.89606700	1.01704000
N	-0.75152300	1.37564800	-0.41316900
C	-0.09580400	2.52997200	-0.68630000
C	-0.72420400	3.72725400	-0.92562300
C	-2.14306500	3.75728900	-0.89359600
C	-2.83189200	2.59967100	-0.63086200
C	-2.15629600	1.38195000	-0.38502500
N	-1.92807700	-0.92236600	0.15830600
C	-2.43925100	-2.13671800	0.44691300
C	-3.79350300	-2.38862000	0.51442100
C	-4.68392400	-1.32002900	0.27156600
C	-4.18275500	-0.07542700	-0.02551300
C	-2.78590500	0.14111500	-0.09001700
H	4.72841600	-0.30114000	-1.89116000
H	5.70187400	1.07922400	-0.05665700
H	4.25625700	1.82804700	1.83656900
H	0.99221200	2.45093800	-0.71644400
H	-0.13860900	4.61505900	-1.14281300
H	-2.67906500	4.68462400	-1.07820300
H	-3.91923700	2.60928300	-0.60442300
H	-1.70118000	-2.91805700	0.63106900
H	-4.14954100	-3.38617600	0.75229700
H	-5.75862000	-1.47832000	0.31809500
H	-4.86033700	0.75357500	-0.21581000
N	0.35005400	0.32348900	2.14529100
C	0.79140200	-0.76804100	3.04366700
H	0.97223600	-0.37465300	4.05418300
H	0.01206400	-1.53367700	3.08771600
H	1.70775100	-1.22430200	2.65998700
C	-0.83359700	0.97889600	2.73936600
H	-1.63603300	0.24153800	2.83102400
H	-0.59593600	1.37762600	3.73627600
H	-1.16960300	1.79364700	2.09245200
C	1.45846800	1.32809600	2.01317000
H	1.89897900	1.53500800	2.99983600
H	0.99609700	2.26360000	1.66588400
C	2.04445800	-1.21937700	-1.96328500
H	2.19035400	-2.24889000	-1.61141900
H	2.46041500	-1.16257700	-2.98008600
N	0.56307800	-0.97012300	-2.00282700
C	0.27960300	0.12434600	-2.95386300

H	0.57310200	-0.17283500	-3.97101400
H	-0.78858100	0.35590500	-2.93601800
H	0.83689100	1.02069300	-2.66712400
C	-0.12808200	-2.19269200	-2.46093900
H	-1.20215000	-1.99284700	-2.50836900
H	0.22716600	-2.49318000	-3.45751500
H	0.05426300	-3.00282700	-1.74983600
O	1.92806400	-2.77766200	0.71889700

$[Ru^{IV}–OO]^{2+}$ (Singlet)

Energy: -1335.01295145 a.u.

Ru	0.11588800	-0.44062400	0.09036200
O	0.56362400	-2.25500500	0.43700200
N	2.05549500	0.11604900	-0.01049000
C	2.78708000	-0.29076400	-1.06868300
C	4.13638900	0.03058300	-1.14452800
C	4.71617500	0.74446900	-0.09675500
C	3.94300000	1.14165300	0.99504400
C	2.59225600	0.82224800	1.00746500
N	-0.84650900	1.43410100	-0.30905600
C	-0.23046700	2.61077400	-0.53886300
C	-0.91656500	3.79211500	-0.76707900
C	-2.31037200	3.75860900	-0.76472900
C	-2.95712100	2.55126700	-0.53740300
C	-2.21136600	1.39206900	-0.30921100
N	-1.92733600	-0.93683700	0.17012400
C	-2.39913600	-2.17198600	0.42362900
C	-3.75599500	-2.45854800	0.46838000
C	-4.66677400	-1.43051700	0.24017800
C	-4.18681600	-0.15317100	-0.02055500
C	-2.81088100	0.07916100	-0.05052200
H	4.72961500	-0.28798500	-1.99823700
H	5.77471200	0.99026900	-0.12867400
H	4.38518100	1.69448400	1.82041600
H	0.85902800	2.57954400	-0.54534500
H	-0.37048100	4.71402900	-0.94603700
H	-2.88736300	4.66330600	-0.94046500
H	-4.04269600	2.51403900	-0.53590000
H	-1.64436900	-2.93858700	0.59149400
H	-4.08491700	-3.47240200	0.67881900
H	-5.73708900	-1.61891400	0.26535700
H	-4.88574000	0.65887800	-0.20003700
N	0.46070300	0.26477600	2.16021500
C	0.92076500	-0.88579900	2.98315500
H	1.17762200	-0.53938400	3.99224500

H	0.12110600	-1.62835200	3.05039400
H	1.79956000	-1.34848200	2.52524700
C	-0.68171800	0.90977500	2.84553700
H	-1.49450600	0.18522900	2.94575400
H	-0.38685200	1.24828300	3.84756400
H	-1.02748600	1.77156600	2.26811900
C	1.58970600	1.24773900	2.04152300
H	2.05318000	1.39881800	3.02656800
H	1.14734800	2.21203400	1.75251400
C	2.02840900	-1.15376700	-2.03381700
H	2.11699700	-2.20021900	-1.71423500
H	2.43319500	-1.09374500	-3.05336400
N	0.56171400	-0.80997700	-2.04939900
C	0.35542100	0.37116900	-2.91829800
H	0.65337500	0.13587700	-3.94839000
H	-0.70041200	0.65457300	-2.91149300
H	0.96088200	1.20865400	-2.55914500
C	-0.20212700	-1.95184800	-2.60931300
H	-1.26094400	-1.68313500	-2.65900500
H	0.15110200	-2.18903700	-3.62160100
H	-0.07801100	-2.82909200	-1.96903600
O	1.75778200	-2.69761600	0.61173100

$[Ru^{IV}–OO]^{2+}$ (Triplet)

Energy: -1335.01273898 a.u.

Ru	0.09353300	-0.41734900	0.06852900
O	0.80208300	-2.22698600	0.39211200
N	2.00943400	0.17637100	-0.01269800
C	2.75303100	-0.19565100	-1.07690300
C	4.10155000	0.13814900	-1.12517200
C	4.66436000	0.81670700	-0.04532300
C	3.88251800	1.15665200	1.06073300
C	2.53492200	0.82620400	1.05089600
N	-0.81308600	1.41383500	-0.28938800
C	-0.16955600	2.58034800	-0.50560900
C	-0.83136600	3.77694900	-0.72450800
C	-2.22505200	3.77785700	-0.72870400
C	-2.89766800	2.58233900	-0.51511800
C	-2.18301400	1.40384500	-0.29485100
N	-1.93052400	-0.92411500	0.14680000
C	-2.41156200	-2.15844000	0.39024400
C	-3.77062600	-2.43140400	0.44333000
C	-4.67387400	-1.39161700	0.23604600
C	-4.18440200	-0.11550500	-0.01325900
C	-2.80681100	0.10188900	-0.05275500

H	4.70742700	-0.14512500	-1.98252000
H	5.72094100	1.07296800	-0.05924400
H	4.31766200	1.67021700	1.91468600
H	0.91820600	2.52644000	-0.50864900
H	-0.26160500	4.68652700	-0.89226900
H	-2.78034200	4.69676100	-0.89893100
H	-3.98392800	2.56476600	-0.51885400
H	-1.66457700	-2.93560300	0.54343400
H	-4.10802100	-3.44446700	0.64399100
H	-5.74541100	-1.57082600	0.26914900
H	-4.87582100	0.70693800	-0.17484700
N	0.41668600	0.16197800	2.18249700
C	0.88614800	-0.99603300	2.98717300
H	1.07204300	-0.68114600	4.02227500
H	0.12042500	-1.77621200	2.98252100
H	1.80855600	-1.40128700	2.56442400
C	-0.74552600	0.76494300	2.87275000
H	-1.54015000	0.01787200	2.95268100
H	-0.46923900	1.09281000	3.88392200
H	-1.11065700	1.62819300	2.30895200
C	1.52330100	1.17622300	2.10626000
H	1.99046600	1.29755300	3.09382700
H	1.05704600	2.14143200	1.86072600
C	2.02466100	-1.04715100	-2.07935700
H	2.19569200	-2.10104800	-1.82415300
H	2.41250200	-0.90214400	-3.09728000
N	0.53679600	-0.81532000	-2.06368000
C	0.22561700	0.33306200	-2.94466000
H	0.50756600	0.10537100	-3.98119700
H	-0.84683800	0.54445100	-2.90873800
H	0.77963800	1.21707500	-2.61515700
C	-0.14510700	-2.01813000	-2.59755800
H	-1.22118600	-1.82794800	-2.63915200
H	0.21225700	-2.25010000	-3.60984200
H	0.04821000	-2.87246700	-1.94374400
O	1.92032500	-2.80729900	0.50689800

[(Ru^{IV}–OO)(H$_2$O)]$^{2+}$ O$_2$ Release Transition State Structure (Triplet)

Energy: -1411.40297977 a.u.

Ru	-0.05083900	0.14575300	0.04671500
O	-0.57533100	3.84936300	0.36852000
N	-1.93258100	-0.52923600	-0.01451600
C	-2.66555200	-0.33493000	-1.13305300
C	-3.98309600	-0.77288300	-1.18382600
C	-4.54259800	-1.36075000	-0.04874400

C	-3.78479900	-1.49782400	1.11577700
C	-2.46073300	-1.08067100	1.10221700
N	0.91630200	-1.58281600	-0.16714200
C	0.30148600	-2.78350300	-0.28934300
C	0.99802600	-3.97170600	-0.42277700
C	2.39163600	-3.94232100	-0.43857400
C	3.03026000	-2.71721200	-0.31725600
C	2.28886200	-1.54297000	-0.18015500
N	1.93860600	0.78048200	0.10630100
C	2.38178700	2.04216600	0.27336600
C	3.72725000	2.37491900	0.30243600
C	4.67439900	1.36416500	0.15058700
C	4.23368100	0.05846000	-0.01651200
C	2.86525800	-0.21367100	-0.03234400
H	-4.57074500	-0.63953500	-2.08935800
H	-5.57463700	-1.70249000	-0.06732200
H	-4.21574300	-1.93389900	2.01404300
H	-0.78554400	-2.76075400	-0.29065600
H	0.44797500	-4.90380500	-0.51764200
H	2.96850800	-4.85705700	-0.54482300
H	4.11568700	-2.66597600	-0.32640700
H	1.61006300	2.79900700	0.38754200
H	4.02201800	3.41142300	0.44092000
H	5.73753200	1.58910300	0.16453500
H	4.95387100	-0.74716600	-0.13254900
N	-0.39501300	-0.18402500	2.16333900
C	-0.91408500	1.10112700	2.68884000
H	-1.25008800	0.99133800	3.72987100
H	-0.11147500	1.84536400	2.66131400
H	-1.75120400	1.44757700	2.06965900
C	0.75265300	-0.62353600	2.98443700
H	1.52436600	0.15079200	2.96341600
H	0.44889300	-0.79254100	4.02664300
H	1.16245700	-1.55332900	2.57798600
C	-1.46931700	-1.23152800	2.22077500
H	-1.95754300	-1.22400500	3.20614900
H	-0.96269900	-2.20368400	2.12955400
C	-1.98395500	0.50627500	-2.17307900
H	-2.25655900	1.54910800	-1.95891400
H	-2.33098400	0.27780300	-3.19076600
N	-0.48508700	0.41552000	-2.10527000
C	-0.03975400	-0.73129500	-2.92751500
H	-0.30473400	-0.57582700	-3.98231700
H	1.04575200	-0.84106700	-2.84735900
H	-0.51994200	-1.64905700	-2.57483500
C	0.09585100	1.65377500	-2.66847500

H	1.18604200	1.56896900	-2.67113300
H	-0.24999000	1.82304700	-3.69806800
H	-0.19790000	2.50898100	-2.05189500
O	-0.04267900	4.79227200	-0.18977400
O	-2.97367300	2.27773800	0.29090200
H	-2.99510600	3.23435500	0.43651000
H	-3.89703500	2.00920300	0.40361500

[Ru^{VI}–O]$^{4+}$ (Singlet)

Energy: -1258.75648632 a.u.

Ru	0.19624100	-0.59316200	0.25579200
O	0.14387200	-2.15770400	0.80808700
N	2.09710400	-0.07431400	0.05325200
C	2.82505500	-0.71779500	-0.92252400
C	4.18802700	-0.49118300	-1.00761300
C	4.79580300	0.37864300	-0.09096700
C	4.03698300	1.00521700	0.91175400
C	2.67462700	0.77511100	0.96654900
N	-0.65245300	1.25998300	-0.54834200
C	0.09354000	2.29867700	-0.97271600
C	-0.46031300	3.49518200	-1.44072000
C	-1.85024700	3.63342200	-1.48357300
C	-2.63383400	2.56871300	-1.05683500
C	-2.02851900	1.38869200	-0.58627200
N	-1.99997400	-0.80298900	0.32460400
C	-2.60901100	-1.91761200	0.75368300
C	-4.01329600	-2.04463100	0.79545100
C	-4.80940500	-0.98288100	0.36656600
C	-4.17985400	0.17068100	-0.08605500
C	-2.76788200	0.24585600	-0.10749600
H	4.78193400	-1.00421100	-1.76293200
H	5.86877900	0.56302800	-0.15045200
H	4.51370700	1.66199700	1.63806200
H	1.17439800	2.16992400	-0.95779200
H	0.20056700	4.29346800	-1.77612700
H	-2.31074400	4.55113600	-1.84783800
H	-3.71716900	2.65522500	-1.08641900
H	-1.97146100	-2.73695900	1.08311100
H	-4.44780600	-2.97001400	1.17338900
H	-5.89626300	-1.05210300	0.38562900
H	-4.78013700	1.00859700	-0.43264300
N	0.50955500	0.53081200	2.13952500
C	0.86591800	-0.51808100	3.16911500
H	1.09949600	-0.01148500	4.11333100
H	0.01422300	-1.18293200	3.32674300

H	1.73688200	-1.09261500	2.84368300
C	-0.62920900	1.33848500	2.65148700
H	-1.47181900	0.68180800	2.88042700
H	-0.32824300	1.84342700	3.57915000
H	-0.91526400	2.10263800	1.92410100
C	1.70547300	1.41663600	1.90732000
H	2.17111100	1.65245000	2.87425600
H	1.34736700	2.37372300	1.50096500
C	2.05470100	-1.73213100	-1.70483000
H	2.10865100	-2.70240200	-1.18688500
H	2.47086600	-1.88631600	-2.70950700
N	0.59837400	-1.35201100	-1.81567500
C	0.42662900	-0.34816300	-2.90140400
H	0.68476200	-0.81249400	-3.86169300
H	-0.61660100	-0.02660100	-2.94973700
H	1.08830600	0.50757000	-2.74305300
C	-0.21950400	-2.56119000	-2.14710600
H	-1.26842400	-2.27273500	-2.25179100
H	0.12003500	-2.96960600	-3.10774600
H	-0.10508100	-3.32402400	-1.37420700

$[Ru^{VI}–O]^{4+}$ (Triplet)

Energy: -1258.75099730 a.u.

Ru	0.22387800	-0.58652500	0.20422400
O	0.25943200	-2.13447000	0.84495400
N	2.09512700	-0.01370500	-0.01615600
C	2.82437900	-0.59666700	-1.02508900
C	4.17788600	-0.31585200	-1.12759200
C	4.77088600	0.53558100	-0.18569100
C	4.01252400	1.08602500	0.86209100
C	2.66084800	0.80244100	0.93586400
N	-0.72618400	1.34805300	-0.46770100
C	-0.03964800	2.42781100	-0.85819600
C	-0.64958300	3.63935600	-1.26824400
C	-2.03669600	3.73182600	-1.27088500
C	-2.76703600	2.61236600	-0.87598200
C	-2.09917200	1.42389700	-0.48022500
N	-1.97800100	-0.83384900	0.25562500
C	-2.55829900	-1.97628800	0.63057400
C	-3.96882100	-2.14309700	0.69243700
C	-4.80269200	-1.07747100	0.35081500
C	-4.20705100	0.11381800	-0.03926000
C	-2.78860200	0.22673500	-0.08341700
H	4.77409300	-0.77200800	-1.91659300
H	5.83539700	0.75998400	-0.25593200

H	4.48370000	1.71857300	1.61293300
H	1.04755000	2.34702000	-0.86321600
H	-0.02049000	4.47490100	-1.57441600
H	-2.54217600	4.64722700	-1.57653100
H	-3.85381800	2.65905800	-0.87877300
H	-1.89882500	-2.80129000	0.89976300
H	-4.37074800	-3.10586500	1.01029700
H	-5.88701400	-1.17507800	0.38911000
H	-4.83406300	0.95982600	-0.31136500
N	0.59507500	0.32553000	2.21100800
C	1.11707500	-0.73293400	3.14192900
H	1.39066600	-0.26827800	4.09650500
H	0.34105300	-1.47932800	3.32158900
H	1.99703800	-1.21829600	2.71162000
C	-0.55540100	1.00456300	2.86284800
H	-1.32219000	0.26448400	3.10564400
H	-0.23318100	1.47906300	3.79869800
H	-0.96216900	1.77825900	2.20508000
C	1.69309400	1.32242800	1.95325100
H	2.19542400	1.57241200	2.89788800
H	1.22977400	2.25716200	1.60145000
C	2.07679500	-1.61211000	-1.82916900
H	2.21652600	-2.59934000	-1.36115600
H	2.46158700	-1.69568500	-2.85449400
N	0.59624700	-1.32401800	-1.85753900
C	0.31509300	-0.31607100	-2.91886600
H	0.57426500	-0.73071700	-3.90081500
H	-0.75057600	-0.07217000	-2.92232400
H	0.91330700	0.58589500	-2.75541300
C	-0.14399700	-2.58121800	-2.18102100
H	-1.20922700	-2.35772000	-2.27902100
H	0.21100100	-2.98203400	-3.13890900
H	0.02166600	-3.32809100	-1.40078000

$[(Ru^{VI}–O)(OH_2)_2]^{4+}$ O-O Bond Formation Transition State Structure (Triplet)

Energy: -1411.62755471 a.u.

Ru	0.03852700	0.27544500	0.09036900
O	0.78511200	1.93204300	0.28901000
N	1.75193900	-0.86678700	0.06537800
C	2.41717200	-1.07765200	1.22944200
C	3.54800900	-1.88254100	1.24830200
C	3.99740400	-2.44688000	0.05189200
C	3.30733100	-2.20599900	-1.13918900
C	2.16905000	-1.41285100	-1.10698400
N	-1.32273200	-1.35108000	-0.17419500

C	-0.98271000	-2.65788200	-0.28692000
C	-1.91954700	-3.66729100	-0.45290800
C	-3.27075100	-3.32387200	-0.50138200
C	-3.63233000	-1.98197800	-0.37604100
C	-2.64811000	-1.00708700	-0.21217600
N	-1.82186100	1.22665400	0.10185900
C	-1.99295600	2.56457900	0.24810000
C	-3.24268700	3.15822900	0.24375400
C	-4.37306500	2.34854400	0.08205300
C	-4.20614100	0.97144100	-0.07152900
C	-2.92900800	0.41976200	-0.06052600
H	4.07447300	-2.06692900	2.18284900
H	4.88452900	-3.07800700	0.04796900
H	3.64828200	-2.63875900	-2.07788900
H	0.07987200	-2.88848100	-0.22595000
H	-1.59275200	-4.70109000	-0.53773600
H	-4.03581400	-4.08784800	-0.62945300
H	-4.68349300	-1.70692000	-0.40386200
H	-1.08237200	3.14676900	0.37043800
H	-3.33146300	4.23530400	0.36498000
H	-5.37145900	2.78324900	0.07544000
H	-5.08038400	0.33832600	-0.19828400
N	0.55010100	0.17934300	-2.06419600
C	1.46770900	1.29656700	-2.43050300
H	1.71522600	1.21909100	-3.49618500
H	0.97014100	2.25143400	-2.24801500
H	2.38253800	1.22319600	-1.83732800
C	-0.66187500	0.24173100	-2.93211800
H	-1.14699900	1.21421000	-2.81669400
H	-0.36026900	0.12663400	-3.98171000
H	-1.35190000	-0.56649000	-2.67895400
C	1.26448100	-1.12979200	-2.26550800
H	1.80457100	-1.10171800	-3.22128700
H	0.50164300	-1.91482900	-2.36349100
C	1.85327500	-0.33029300	2.39435900
H	2.30775600	0.66610800	2.44257100
H	2.05659400	-0.82519200	3.35290100
N	0.36442800	-0.15181500	2.24102800
C	-0.32369300	-1.39953200	2.68969500
H	-0.14449600	-1.53499200	3.76355900
H	-1.40041900	-1.31315000	2.52709400
H	0.07599500	-2.26430800	2.15494800
C	-0.10714100	0.98172300	3.08844300
H	-1.19828400	1.03218300	3.06085200
H	0.20651500	0.81293200	4.12680200
H	0.31892100	1.92210300	2.73276300

O	2.47673200	2.24782100	0.54510100
O	3.66825800	3.92804900	-1.01602800
H	2.32841900	2.73446300	1.38108300
H	3.13268600	3.28553300	-0.35292900
H	4.64495700	3.82426100	-0.95225300
H	3.45135900	4.88225700	-0.91378000

3. CASSCF/CASPT2 studied species

$[Ru^{II}\text{-}OH_2]^{2+}$ $[Ru^{III}\text{-}O]^{+}$ $[Ru^{IV}\text{-}O]^{2+}$ $[Ru^{V}\text{-}O]^{3+}$

$[Ru^{II}\text{-}OH_2]^{2+}$: oxidation state 2, singlet, (Active Space 6 electrons in 5 orbitals)

$[Ru^{III}\text{-}OH_2]^{3+}$: oxidation state 3, doublet, (Active Space 5 electrons in 5 orbitals)

$[Ru^{IV}\text{-}O]^{2+}$: oxidation state 4, triplet, (Active Space 10 electrons in 8 orbitals)

$[Ru^{V}\text{-}O]^{3+}$:oxidation state 5, doublet, (Active Space 9 electrons in 8 orbitals)

$[Ru^{VI}\text{-}O]^{4+}$:oxidation state 6, singlet, (Active Space 8 electrons in 8 orbitals)

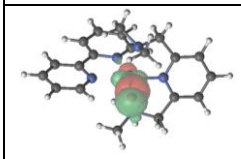
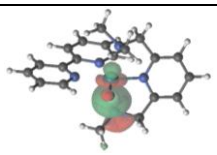
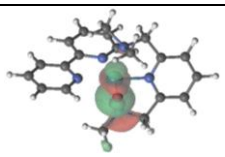
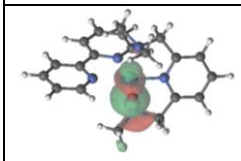
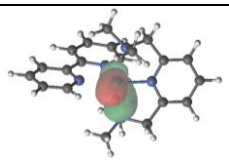
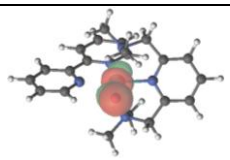
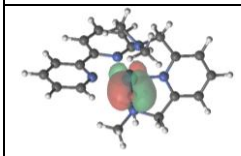
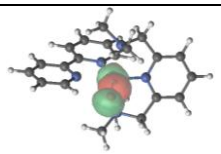
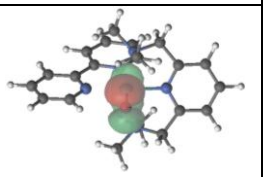
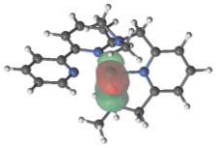
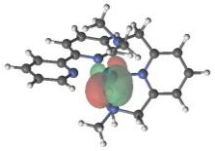
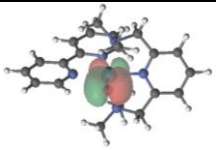
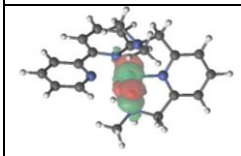
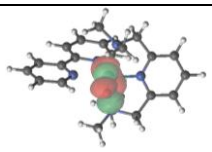
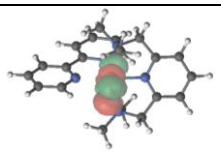
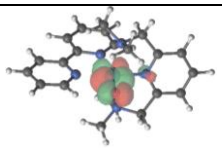
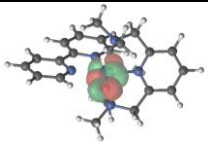
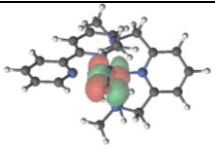
4. CASSCF/PT2 Energies and Population Analysis results:

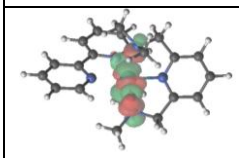
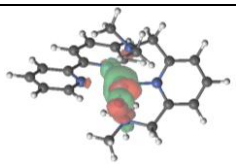
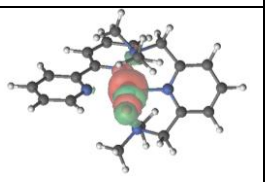
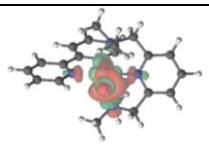
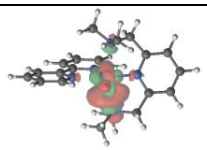
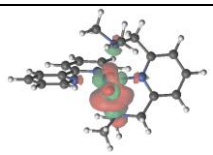
species	spin	Active Space	CASSCF Energy (hartrees)	CASSCF/CASPT2 Energy (hartrees)	reference weight	CI weights
$[Ru^{VI}\text{-}O]^{4+}$	S	8in8	-5.684,208	-5.688,497	0,402	79.4, 3.70, 3.92, 2.85, 1.17
$[Ru^{V}\text{-}O]^{3+}$	D	9in8	-5.684,905	-5.689,196	0,406	87.28, 3.2, 1.3, 1.1
$[Ru^{IV}\text{-}O]^{2+}$	T	10in8	-5.685,382	-5.689,694	0,405	89.86,2.83,1.02
$[Ru^{III}\text{-}OH_2]^{3+}$	D	5in5	-5.686,096	-5.690,431	0,406	97.0
$[Ru^{II}\text{-}OH_2]^{2+}$	S	6in5	-5.686,538	-5.690,899	0,405	98.58

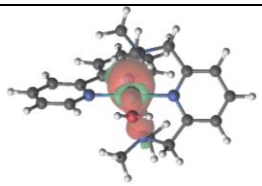
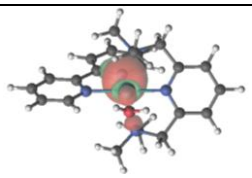
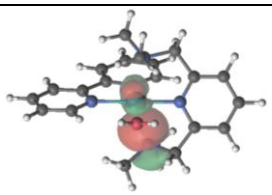
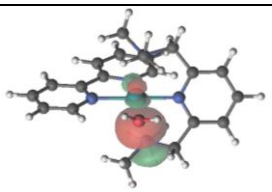
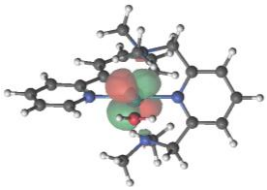
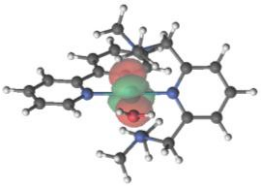
species	Mulliken charge Ru	Mulliken charge O	Mulliken spin/population Ru	Mulliken spin/population O
$[Ru^{VI}\text{-}O]^{4+}$	42,51	7,91	---	---
$[Ru^{V}\text{-}O]^{3+}$	42,49	8,17	0,574	0,394
$[Ru^{IV}\text{-}O]^{2+}$	42,64	8,38	1,011	0,961
$[Ru^{III}\text{-}OH_2]^{3+}$	42,67	7,52	0,969	0,001
$[Ru^{II}\text{-}OH_2]^{2+}$	42,94	7,49	---	---

species	LoProp charges Ru	Loprop charges O	EBO
$[Ru^{VI}\text{-}O]^{4+}$	1,714	0,010	2.625
$[Ru^{V}\text{-}O]^{3+}$	1,552	-0,219	2.26
$[Ru^{IV}\text{-}O]^{2+}$	1,257	-0,452	1.81
$[Ru^{III}\text{-}OH_2]^{3+}$	1,320	-0,668	1
$[Ru^{II}\text{-}OH_2]^{2+}$	0,834	-0,647	1

5. CASSCF Active Space Orbitals (orbital occupation):

DAMP6	DAMP5	DAMP4
		
(1.96)	(1.97)	(1.98)
		
(1.93)	(1.95)	(1.93)
		
(1.84)	(1.94)	(1.94)
		
(1.83)	(1.87)	(1.94)
		
(0.18)	(1.05)	(1.06)
		

(0.16)	(0.13)	(1.06)
		
(0.08)	(0.06)	(0.07)
		
(0.04)	(0.03)	(0.02)

DAMP3	DAMP2
	
(1.98)	(1.99)
	
(1.98)	(1.98)
	
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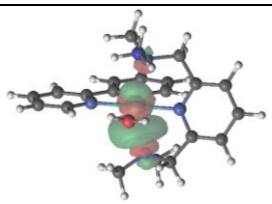
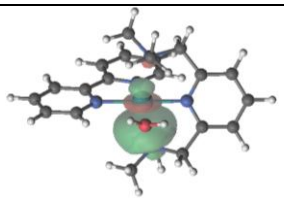
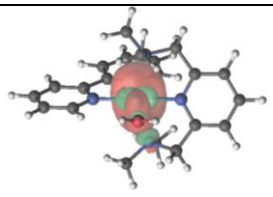
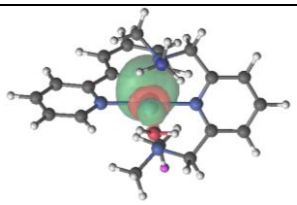
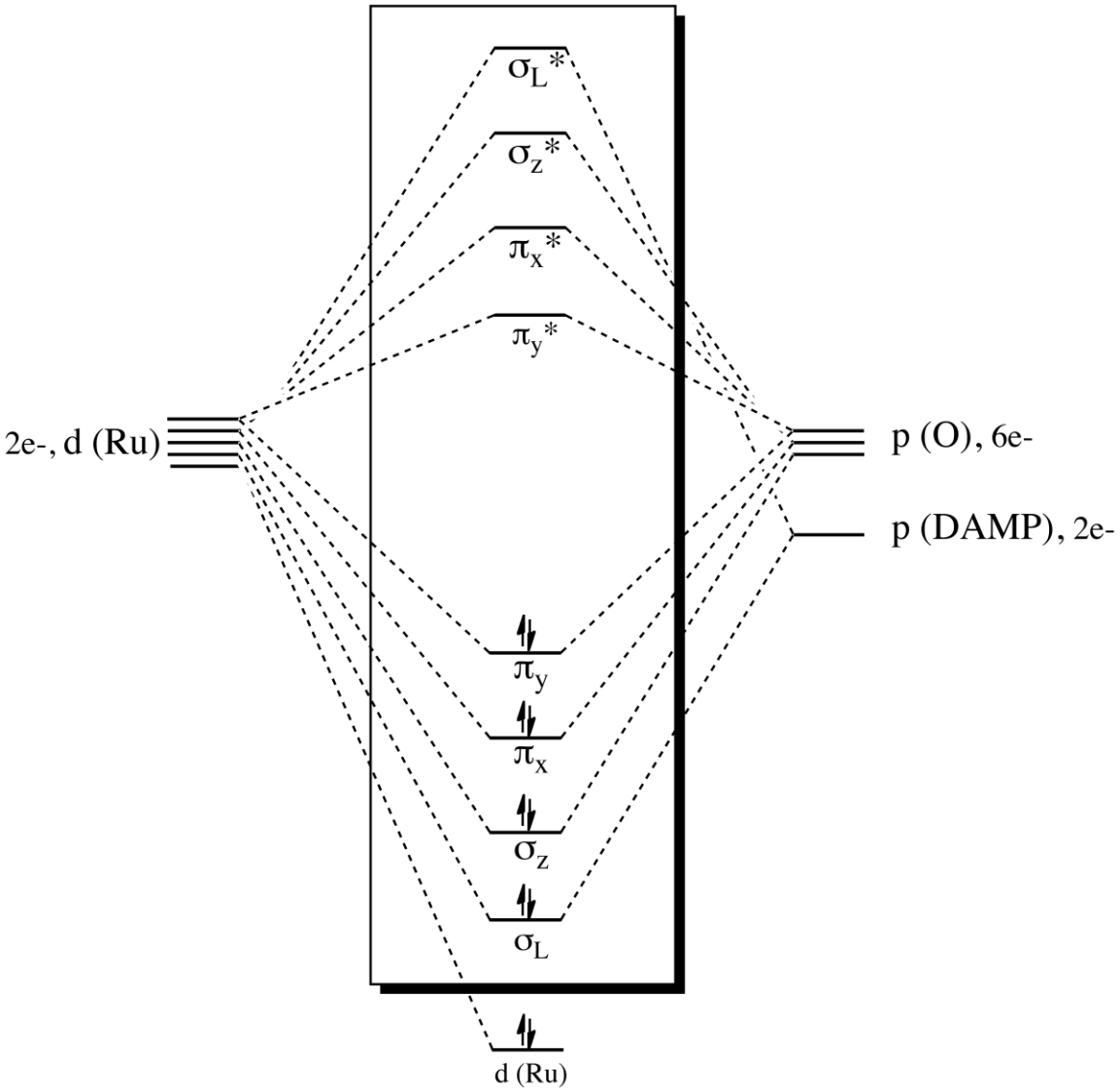
	
(0.02)	(0.02)
	
(0.02)	(0.01)

6. Schematic representation of the electronic structure of the species in oxiadtion state 6. In the square the orbitals observed in the active space, 8 electrons in 8 orbitals.



7. Schematic representation of the electronic structure of the species in oxiadtion state 2. In the square the orbitals observed in the active space, 6 electrons in 5 orbitals.