

Supporting Information

Ruthenium-Based Catalysts for Water Oxidation: Key Role of Carboxy Group as Proton Acceptor

Yuting Liu, Xiao-Fang Su, Wei Guan, Li-Kai Yan*

Institute of Functional Material Chemistry & Local United Engineering Lab for Power Battery, Faculty
of Chemistry, Northeast Normal University, Changchun

130024, China

Table S1 Selected bond lengths (Å), bond angles (deg), dihedral angles (deg) and overpotentials (vs SHE) the experimental data and computed results calculated by M06,B3LYP and B3LYP-D3 hybrid functionals.

	Experimen t	M06	B3LYP	B3LYP- D3
Bond Distances (Å)				
Ru1-O1	2.146	2.168	2.166	2.167
Ru1-N1	2.070	2.103	2.119	2.098
Ru1-N2	1.969	2.003	2.012	2.002
Ru1-N3	2.059	2.103	2.118	2.098
Ru1-N4	1.979	2.003	2.011	2.003
Ru1-N5	2.060	2.111	2.145	2.116
O1-C16	1.289	1.295	1.303	1.303
O2-C16	1.241	1.228	1.234	1.234
Bond Angles (deg)				
O1-Ru1-N4	76.39	76.10	76.57	76.48
N1-Ru1-N2	79.30	78.62	78.55	78.90
N2-Ru1-N3	79.33	78.62	78.55	78.89
N4-Ru1-N5	79.90	79.33	78.85	79.47
Dihedral Angles (deg)				
O1-C16-C17-N4	2.5	0.0	0.0	0.0
N4-C21-C25-N5	1.1	0.0	0.0	0.0
N2-C10-C11-N3	1.0	-0.8	1.1	0.2
N1-C5-C6-N2	2.8	0.7	-1.1	-0.2
Overpotentials				
E _{red}	-1.39	-1.41	-1.46	-1.47
E _{ox}	1.10	1.00	0.95	0.96

${}^2\mathbf{1}(\text{LRu}^{\text{III}}\text{-OH}_2)$

Ru	0.31393000	-0.14772500	-0.40029600	N	0.45288600	1.91661600	-0.84185600
C	-4.61494600	-0.40611800	-0.63847000	C	-0.56768400	2.70605900	-1.19900500
C	-3.91782700	0.10937600	0.47027100	H	-1.22329900	4.64113000	-1.83973400
C	-2.51310900	0.05422000	0.42408800	H	1.10007600	5.58585600	-1.78548600
N	-1.81858200	-0.48281300	-0.62110600	H	2.98459000	4.12499700	-1.10091000
C	-2.50449800	-1.03261400	-1.62610700	H	-1.55542400	2.25345800	-1.21395300
C	-3.90796000	-0.97363500	-1.67033700	C	-4.55963700	0.66128100	1.62307600
H	-5.70137600	-0.36885100	-0.65538700	C	-3.83541900	1.10472900	2.68479900
H	-4.39689800	-1.40788500	-2.53581900	C	-2.40723600	1.03849400	2.67387500
O	-0.66905500	-2.32499300	-2.35515500	H	-5.64552900	0.70546200	1.63351400
C	3.05102800	-0.76311200	0.38642900	H	-4.32656800	1.51086600	3.56511900
N	2.27455900	0.24305000	-0.05436400	C	-1.59536300	1.44431900	3.74915600
C	2.75186800	1.46338200	-0.35703000	C	-0.22537200	1.33063200	3.65274000
C	4.11065900	1.72029700	-0.21524100	C	0.34324800	0.82932300	2.47811400
H	4.52184800	2.69758200	-0.44415200	N	-0.40567500	0.44476200	1.44763900
C	0.69844700	-4.14710000	1.26944100	C	-1.76003700	0.53152100	1.53166800
C	0.17668400	-2.96430100	0.76646800	H	-2.05805000	1.84088400	4.64940000
N	0.96460600	-1.92170100	0.47966200	H	0.42535300	1.62883200	4.46715400
C	2.30892100	-1.99222000	0.69058000	H	1.42108900	0.74596800	2.36885400
C	2.88286300	-3.15058000	1.19093100	H	0.52993400	-1.40602200	-2.58015600
C	2.06775000	-4.23923000	1.48051000	O	1.17161300	-0.66901300	-2.32043400
H	0.03339400	-4.97504700	1.48799400	C	-1.77469900	-1.81215600	-2.71756400
H	-0.88456700	-2.84045700	0.57197600	C	4.93875100	0.69634700	0.23250900
H	3.95340500	-3.20410200	1.35844100	H	6.00229400	0.87830800	0.34799100
H	2.50343600	-5.15210400	1.87450500	C	4.41746000	-0.55464200	0.54194500
C	-0.37296700	4.03386700	-1.55038200	H	5.06529600	-1.34669600	0.90166400
C	0.91509000	4.54992500	-1.51927900	O	-2.34506400	-1.89870400	-3.80507800
C	1.97383000	3.73281400	-1.13741100	H	1.09654300	0.02816800	-2.98659300
C	1.72132700	2.41276600	-0.79842600				

${}^2\text{2}(\text{H}^{\text{L}}\text{Ru}^{\text{III}}\text{-OH})$

Ru	-0.35455700	0.16325800	-0.42286100	N	-0.44133500	-1.84844100	-1.03043700
C	4.64113100	0.31989800	-0.34918500	C	0.56866100	-2.61519000	-1.45182000
C	3.86011900	-0.19770100	0.69430500	H	1.22473400	-4.51577300	-2.19505000
C	2.45420900	-0.09715000	0.57634100	H	-1.09090200	-5.47971800	-2.13748200
N	1.83969300	0.50260500	-0.48151100	H	-2.96683000	-4.06250200	-1.34461200
C	2.62140600	1.03974900	-1.42427700	H	1.55302800	-2.15332400	-1.46687500
C	4.01997200	0.94158700	-1.40621300	C	4.43846300	-0.80755000	1.85120300
H	5.72408000	0.24190100	-0.30395100	C	3.65703300	-1.27815900	2.85545100
H	4.58853000	1.38136600	-2.21788500	C	2.23199900	-1.19087400	2.77338300
O	1.03322000	2.60808700	-2.28745200	H	5.52175700	-0.87327900	1.90812500
C	-3.06441400	0.75432200	0.35096400	H	4.09692700	-1.72962900	3.74098900
N	-2.28468100	-0.23293700	-0.13094700	C	1.37939000	-1.64928000	3.79487000
C	-2.74465700	-1.44473800	-0.48953800	C	0.01547100	-1.53844000	3.64463700
C	-4.10184900	-1.72115800	-0.34773300	C	-0.49537000	-0.98811300	2.46492000
H	-4.50844700	-2.68848200	-0.62309000	N	0.28956900	-0.54359800	1.48880600
C	-0.82598800	4.23020200	1.22279900	C	1.63661700	-0.62422100	1.62931200
C	-0.26766100	3.07998100	0.67973200	H	1.80909000	-2.08619000	4.69297200
N	-1.00305200	1.99826900	0.41182600	H	-0.66970400	-1.87984200	4.41282000
C	-2.34089800	2.00060500	0.67186100	H	-1.56879500	-0.91033700	2.30890300
C	-2.95430500	3.11940700	1.21432100	H	-0.45598400	1.48297500	-2.45109900
C	-2.18670100	4.24650900	1.49164000	O	-0.87919700	0.63980600	-2.22483700
H	-0.19684100	5.08906800	1.42907600	C	1.99493600	1.89324100	-2.48009300
H	0.78997900	3.01128600	0.44156000	C	-4.93308700	-0.72686200	0.15325400
H	-4.01918900	3.11671400	1.42303300	H	-5.99410200	-0.92411900	0.26899600
H	-2.65468400	5.12855000	1.91798700	C	-4.42484800	0.52103100	0.50761300
C	0.37708300	-3.92866600	-1.85893300	H	-5.08451300	1.29053600	0.89430500
C	-0.90604500	-4.45670300	-1.82488200	O	2.66051500	1.82989600	-3.62329600
C	-1.95837000	-3.66367600	-1.38339800	H	2.26097500	2.45922500	-4.24807900
C	-1.70500900	-2.35727900	-0.98790600				

${}^23(\text{LRu}^{\text{III}}\text{-OH})$

Ru	-0.33753700	0.15377100	-0.45011500	C	-1.72249800	-2.37162000	-0.90547400
C	4.63508200	0.36301100	-0.39061700	N	-0.45652300	-1.87371300	-0.99239300
C	3.86652900	-0.13086500	0.68104900	C	0.53820600	-2.66244500	-1.41010600
C	2.46458400	-0.07177200	0.55605900	H	1.16416800	-4.59132900	-2.10512900
N	1.83557000	0.46690000	-0.53341900	H	-1.15695900	-5.53499200	-1.96615100
C	2.58863900	0.98198100	-1.50842900	H	-3.00431900	-4.07750900	-1.17888100
C	3.99531800	0.90558900	-1.47343100	H	1.52451800	-2.20707700	-1.46111300
H	5.72040500	0.31373700	-0.34035400	C	4.45478600	-0.67583600	1.86442500
H	4.53841800	1.29795100	-2.32674600	C	3.68404800	-1.12502100	2.88872500
O	1.02900000	2.51892900	-2.39103200	C	2.25939300	-1.07169500	2.80057000
C	-3.02858500	0.78419200	0.37908500	H	5.53973900	-0.71327100	1.92618000
N	-2.27081100	-0.21343700	-0.11606700	H	4.13252500	-1.52946900	3.79272000
C	-2.74390900	-1.43816100	-0.40695000	C	1.40993000	-1.50179200	3.83741600
C	-4.09178900	-1.71325800	-0.18986500	C	0.04473000	-1.41967400	3.68061100
H	-4.50709700	-2.69131600	-0.40901300	C	-0.47158500	-0.92109200	2.47981800
C	-0.77149200	4.30595200	0.97588500	N	0.30756800	-0.50465400	1.48776900
C	-0.22933900	3.12867300	0.47382100	C	1.65724100	-0.56365200	1.63034200
N	-0.96636900	2.02798300	0.31301600	H	1.84394600	-1.89459900	4.75398200
C	-2.29344900	2.04199100	0.62205400	H	-0.63652400	-1.74067900	4.46119600
C	-2.89061600	3.18800300	1.12512400	H	-1.54625200	-0.86102800	2.32043900
C	-2.11794700	4.33079600	1.30823400	H	-0.30536500	1.42029200	-2.46144900
H	-0.14139900	5.18038500	1.09682100	O	-0.83316800	0.61601200	-2.25634600
H	0.80807600	3.05166900	0.16219600	C	1.96384000	1.72815700	-2.68760700
H	-3.94787400	3.19596900	1.36997700	C	-4.90025700	-0.70606000	0.32308700
H	-2.57227200	5.23418200	1.70388400	H	-5.95271300	-0.90277400	0.50172900
C	0.32839300	-3.98678100	-1.76987400	C	-4.37791800	0.55199600	0.61578100
C	-0.95763100	-4.50383800	-1.69114100	H	-5.01770100	1.32943700	1.01992500
C	-1.99385700	-3.68866400	-1.25257100	O	2.48206300	1.50058800	-3.79057100

$^{24}(\text{HLRu}^{\text{III}}-\text{O})$

Ru	-0.37781700	-0.17373900	-0.37843700	C	-2.59923000	-1.72892700	0.69897600
C	4.48363500	-0.77979700	-0.62445000	N	-1.26114800	-1.87849100	0.47406800
C	3.87019200	-0.15970200	0.47948800	C	-0.66052100	-3.03245800	0.79739800
C	2.46132000	-0.13025400	0.50281400	H	-0.82301600	-5.00181500	1.62382000
N	1.70029900	-0.69669200	-0.46999400	H	-3.28237700	-4.75251300	2.06553800
C	2.30330300	-1.33507800	-1.46778600	H	-4.40611400	-2.62803100	1.44942000
C	3.70162900	-1.36759900	-1.59368100	H	0.39672700	-3.10107900	0.55707300
H	5.56833600	-0.80220700	-0.69518800	C	4.59990400	0.43635600	1.55673100
H	4.14535700	-1.87476500	-2.44509800	C	3.95352300	1.01813300	2.60130400
O	0.89245400	-3.17681900	-1.99457900	C	2.52361100	1.06569400	2.64898000
C	-2.55399400	1.70600900	-0.52585000	H	5.68610700	0.40681400	1.52136700
N	-2.22950400	0.43445300	-0.17082800	H	4.51134100	1.46305900	3.42191100
C	-3.15354300	-0.42684500	0.33198600	C	1.80336500	1.65310700	3.70666200
C	-4.47019700	-0.01063000	0.49425200	C	0.42634900	1.66065800	3.67079800
H	-5.21559800	-0.68871400	0.89867600	C	-0.23045600	1.09247400	2.57081600
C	0.84117200	3.80152500	-1.88716200	N	0.42231700	0.53327100	1.56036900
C	0.87175900	2.48102600	-1.46838400	C	1.77976400	0.50602100	1.59139100
N	-0.22150200	1.83922000	-1.03893700	H	2.34338900	2.09624400	4.54020900
C	-1.41880200	2.49004900	-1.01647400	H	-0.15656700	2.10443400	4.47110800
C	-1.51175200	3.81867100	-1.42541800	H	-1.31781300	1.09433500	2.50314100
C	-0.37398000	4.47935900	-1.86207600	O	-0.57378300	-0.76001200	-2.12817800
H	1.75236100	4.28143600	-2.22823400	C	1.48120500	-2.19397400	-2.38625800
H	1.79452400	1.90465200	-1.48067800	C	-4.82331700	1.28591200	0.13417600
H	-2.46902800	4.33040200	-1.40296300	H	-5.84820400	1.62225400	0.25344700
H	-0.43546600	5.51478000	-2.18348100	C	-3.86103500	2.15337300	-0.37490300
C	-1.34987000	-4.08663800	1.37441700	H	-4.13072700	3.16831300	-0.65068400
C	-2.71368600	-3.94443300	1.61512200	O	1.70268500	-1.90201700	-3.66948600
C	-3.34284400	-2.75790000	1.27222700	H	1.24160800	-2.56943000	-4.20354000

$^{25}(\text{LRu}^{\text{III}}\text{-O})$

Ru	-0.37540600	-0.26437000	-0.49918300	C	-2.65573900	-1.70250400	0.61056300
C	4.57215100	-0.66838600	-0.18030600	N	-1.32901400	-1.91955100	0.36857300
C	3.80200400	0.00787700	0.78808800	C	-0.77548900	-3.10032000	0.68683500
C	2.40079700	-0.05585900	0.65886900	H	-1.02460500	-5.05174500	1.53431400
N	1.77903200	-0.76620000	-0.32827100	H	-3.45526500	-4.67094100	2.03377500
C	2.52447100	-1.46788200	-1.18130500	H	-4.49112000	-2.50723900	1.40228100
C	3.93518000	-1.39225900	-1.15336500	H	0.26251100	-3.22141000	0.38015000
H	5.65793100	-0.61482000	-0.13329000	C	4.38748400	0.74034800	1.86668500
H	4.48719100	-1.93444300	-1.91560700	C	3.61370600	1.36820600	2.79076500
O	2.23876700	-2.32031800	-3.35184700	C	2.18929300	1.31979100	2.69529400
C	-2.45456500	1.70628500	-0.68834900	H	5.47268500	0.77495700	1.93373600
N	-2.18986000	0.41164300	-0.33441700	H	4.06067300	1.91534900	3.61744100
C	-3.14877100	-0.38575200	0.22799400	C	1.33755700	1.93895400	3.63041300
C	-4.42400000	0.11955200	0.44587200	C	-0.02712900	1.85237300	3.47324300
H	-5.18712200	-0.50375200	0.90308600	C	-0.53903000	1.15812200	2.36912500
C	1.01500600	3.60167400	-2.14788900	N	0.23876100	0.56490800	1.47360100
C	0.99194000	2.29860400	-1.67984200	C	1.58628700	0.62643500	1.62281200
N	-0.12548700	1.72120900	-1.22061100	H	1.77175600	2.47889500	4.46909300
C	-1.29561700	2.42176700	-1.21513800	H	-0.70946600	2.31453500	4.17905400
C	-1.33324200	3.73920100	-1.67411700	H	-1.61466700	1.08824100	2.20720600
C	-0.17194400	4.33191300	-2.14101700	O	-0.51869500	-0.89784600	-2.21428900
H	1.94318800	4.02978400	-2.51164800	C	1.90705700	-2.46483000	-2.15875400
H	1.88785900	1.68009800	-1.67012200	C	-4.71496700	1.43278900	0.08478100
H	-2.26781600	4.29173700	-1.66769300	H	-5.70834800	1.83645500	0.25167700
H	-0.19103500	5.35648200	-2.50080800	C	-3.72237100	2.23221400	-0.47957600
C	-1.50658800	-4.11025500	1.29103500	H	-3.93885100	3.26248300	-0.74661400
C	-2.85740300	-3.89651200	1.56182300	O	1.24937900	-3.37613200	-1.61110600
C	-3.43728200	-2.68855900	1.21276700				

¹6(LRu^{IV}-OH₂)

Ru	0.31161700	-0.33016000	-0.58320600	N	-0.42313300	1.61434900	-1.14627400
C	-4.41109800	-1.31359700	-0.19843100	C	-1.62027600	1.90384900	-1.66886400
C	-3.76286500	-0.57802700	0.81592100	H	-2.96336000	3.38900900	-2.42071300
C	-2.37776300	-0.38934200	0.67288600	H	-1.32535900	5.25284800	-2.03092100
N	-1.69715500	-0.87522400	-0.37407700	H	0.91168200	4.70945700	-1.10165300
C	-2.29701900	-1.64278700	-1.27294100	H	-2.30660100	1.07922900	-1.83151700
C	-3.67322900	-1.87090600	-1.22861300	C	-4.37212700	-0.04750500	1.99730900
H	-5.48360000	-1.47700100	-0.13973000	C	-3.61723500	0.54658100	2.96435500
H	-4.12294600	-2.50354200	-1.98776000	C	-2.19138600	0.66473400	2.84690300
O	-0.05977400	-1.98414600	-1.74496500	H	-5.44665600	-0.14898700	2.11855300
C	3.02855200	0.27047200	0.25387600	H	-4.08519600	0.92505600	3.86900300
N	1.89447900	0.86749200	-0.17641000	C	-1.33289000	1.16053800	3.84524100
C	1.79478400	2.18542400	-0.44047900	C	0.02689700	1.14558400	3.62170500
C	2.90107800	2.99811000	-0.23338000	C	0.54332900	0.67139800	2.40959000
H	2.85227300	4.06404900	-0.42485100	N	-0.24623700	0.22510100	1.43208100
C	2.41014600	-3.82301200	1.00975300	C	-1.58855200	0.21569900	1.66587100
C	1.43472200	-2.98920600	0.47691600	H	-1.74037700	1.53015600	4.78244900
N	1.68536600	-1.70241400	0.22903700	H	0.72560900	1.49857100	4.37180700
C	2.90596000	-1.16830200	0.50344000	H	1.61624300	0.66851300	2.25604100
C	3.91864600	-1.95659700	1.02603500	H	1.26097900	-1.05114000	-2.90375200
C	3.66640900	-3.30163800	1.27765300	O	1.45770900	-0.20157000	-2.46658400
H	2.17357800	-4.86385200	1.20046300	C	-1.29376000	-2.28126300	-2.15781200
H	0.44031200	-3.34885000	0.23344100	C	4.08222700	2.41736700	0.21737300
H	4.89171900	-1.52793500	1.24105600	H	4.95578600	3.03962000	0.38177600
H	4.44962300	-3.93183700	1.68639700	C	4.15934100	1.04979300	0.45794600
C	-1.98051700	3.20252500	-2.00276400	H	5.08489600	0.60403900	0.80509500
C	-1.07167000	4.22598900	-1.78810900	O	-1.51492300	-3.03394000	-3.07105000
C	0.18082300	3.92453700	-1.26309600	H	1.14467400	0.49094000	-3.07134100
C	0.48717900	2.60971800	-0.95203200				

$^{37}(\text{HLRu}^{\text{IV}}\text{-OH})$

Ru	-0.34493400	0.20786800	-0.47842900	C	-1.59891100	-2.34873200	-1.10037900
C	4.62127200	0.25613000	-0.16009900	N	-0.34669500	-1.80139800	-1.12203700
C	3.78491700	-0.30649400	0.81562800	C	0.69423800	-2.51566600	-1.56303300
C	2.38979000	-0.15226600	0.64697700	H	1.41004000	-4.36930800	-2.36100000
N	1.84387300	0.53538700	-0.39170600	H	-0.86940200	-5.41289800	-2.32532300
C	2.67283900	1.12326000	-1.26444600	H	-2.79838000	-4.08350500	-1.50901700
C	4.06444900	0.97660400	-1.19109000	H	1.66210500	-2.02294100	-1.56962900
H	5.69867300	0.14175400	-0.07980400	C	4.28864000	-1.00504000	1.95484000
H	4.68324700	1.46122500	-1.93733400	C	3.44539600	-1.49661800	2.89917400
O	1.07654500	2.70017700	-2.08452200	C	2.03029200	-1.34200100	2.76658100
C	-3.07145800	0.71477800	0.26786200	H	5.36458000	-1.11831300	2.05223200
N	-2.26292500	-0.25012300	-0.22166600	H	3.82886700	-2.01238600	3.77509100
C	-2.67226300	-1.47847600	-0.60076100	C	1.11516500	-1.79805300	3.73461900
C	-4.01875900	-1.79154500	-0.47856400	C	-0.23570600	-1.60218000	3.54607900
H	-4.39556000	-2.76653900	-0.76685000	C	-0.67723900	-0.97585200	2.38016900
C	-0.88006000	4.15299800	1.35021600	N	0.17019700	-0.54606400	1.44370500
C	-0.29346900	3.03040600	0.78291900	C	1.50945600	-0.70024200	1.62883600
N	-1.02419600	1.96678500	0.43044200	H	1.48581500	-2.29566700	4.62697600
C	-2.37750100	1.95490500	0.63859300	H	-0.96486200	-1.93443400	4.27609600
C	-3.01075800	3.05167400	1.19702800	H	-1.73921200	-0.82950000	2.20386500
C	-2.25238900	4.16364400	1.55275100	H	-0.37257600	1.71158200	-2.41110100
H	-0.25984700	4.99949100	1.62234600	O	-0.66486100	0.78907200	-2.22476800
H	0.77422600	2.97520300	0.59723900	C	2.10571900	2.07706400	-2.26795800
H	-4.08305200	3.04348800	1.36044800	C	-4.88519100	-0.82241700	0.02244500
H	-2.73735300	5.02879900	1.99350900	H	-5.94035100	-1.05494300	0.12323600
C	0.54365100	-3.82174500	-2.00782600	C	-4.42571700	0.43660800	0.39980300
C	-0.72042400	-4.39244500	-1.98722000	H	-5.11505400	1.17560000	0.79260600
C	-1.80493200	-3.64817100	-1.53018200	O	2.87996900	2.20587200	-3.32422400
H	2.50392500	2.88325900	-3.91351900				

¹8(LRu^{IV}-OH)

Ru	0.31467200	-0.13736800	-0.49468000	C	2.07889700	2.27538100	-0.58726700
C	-4.35494600	-0.77386100	-1.51276000	N	0.76374100	1.99927200	-0.40260300
C	-3.98594500	0.05279200	-0.42741200	C	-0.14480300	2.96778800	-0.53481300
C	-2.61198100	0.16295600	-0.17661600	H	-0.55594500	5.03080900	-0.93050600
N	-1.68790000	-0.43339100	-0.94287500	H	1.86965400	5.57915600	-1.27643700
C	-2.04088900	-1.32895300	-1.85185000	H	3.55682100	3.76774900	-1.04085200
C	-3.38976400	-1.50263700	-2.18713100	H	-1.18793200	2.69363800	-0.40022200
H	-5.40582000	-0.88961400	-1.76520900	C	-4.86785600	0.72070000	0.48462600
H	-3.64819100	-2.23110500	-2.94927000	C	-4.38452800	1.34559400	1.59700600
O	0.19420700	-1.98503800	-1.54814000	C	-2.98538900	1.34057400	1.92224400
C	2.95635600	-1.06243300	0.44885900	H	-5.93643900	0.69709500	0.28938000
N	2.33345600	0.00577400	-0.07333900	H	-5.06675400	1.82982400	2.29060600
C	2.98029600	1.14805000	-0.34784500	C	-2.41336300	1.83990000	3.10722700
C	4.36727000	1.19588200	-0.25978800	C	-1.05666400	1.69118700	3.32210500
H	4.90993600	2.10801600	-0.48460900	C	-0.25473800	1.05423500	2.36644700
C	0.07042200	-3.66504700	2.05098400	N	-0.77190100	0.58959900	1.23249000
C	-0.23663600	-2.47184000	1.41781500	C	-2.10477000	0.74628100	1.00765900
N	0.71792300	-1.68719200	0.90675300	H	-3.04160200	2.32415700	3.85033900
C	2.02155200	-2.05639200	0.97613800	H	-0.59194400	2.05540600	4.23177300
C	2.38752300	-3.24888000	1.58543800	H	0.81400800	0.92327600	2.51801900
C	1.40040000	-4.06169800	2.12558300	H	0.21319800	-0.06927600	-2.94410500
H	-0.72834400	-4.26966200	2.46572800	O	0.74867000	0.40216000	-2.28984400
H	-1.26297300	-2.13236800	1.31291800	C	-0.89136900	-2.21724200	-2.24563500
H	3.43221300	-3.53772700	1.63464900	C	5.04547400	0.05605800	0.15807900
H	1.66936400	-4.99865500	2.60307200	H	6.12841300	0.06851200	0.22640600
C	0.21404000	4.27286600	-0.83841600	C	4.34188200	-1.07571700	0.55619900
C	1.55713800	4.56966100	-1.02833400	H	4.86230300	-1.93480500	0.96565800
C	2.50132300	3.55987200	-0.89866100	O	-1.01242000	-3.10451200	-3.06873100

${}^3\text{9}(\text{H}^{\text{L}}\text{Ru}^{\text{IV}}-\text{O})$

Ru	-0.35010500	-0.22475200	-0.48011700	C	-3.29889800	-2.82538100	1.16806400
C	4.55533900	-0.59091300	-0.28554400	C	-2.56007800	-1.79318500	0.61037300
C	3.80715100	-0.00677800	0.75120700	N	-1.22175600	-1.93927400	0.38921500
C	2.40080800	-0.05550900	0.64966500	C	-0.60749500	-3.07985500	0.71099800
N	1.76738400	-0.67681500	-0.38302500	H	-0.76395200	-5.05582700	1.52817900
C	2.50394400	-1.27944900	-1.31525400	H	-3.22542400	-4.82866800	1.94424800
C	3.90463100	-1.22681400	-1.31761000	H	-4.36348500	-2.70824100	1.34201200
H	5.64081000	-0.54589800	-0.25567800	H	0.45428200	-3.13086900	0.48916300
H	4.44916500	-1.70839000	-2.12349200	C	4.41185400	0.63159900	1.87889000
O	1.11830300	-3.09459700	-1.98378700	C	3.64997600	1.18195700	2.85893000
C	-2.54085900	1.66168800	-0.58841200	C	2.22212500	1.15402300	2.78030100
N	-2.24671600	0.38938800	-0.26158700	H	5.49688700	0.65850500	1.93384000
C	-3.13331400	-0.48323500	0.25361000	H	4.11005800	1.65854200	3.72073900
C	-4.44854400	-0.07200500	0.43892000	C	1.38768200	1.70848500	3.77012100
H	-5.19302600	-0.74464400	0.85097700	C	0.02086000	1.65204000	3.61985300
C	0.85022300	3.75468700	-1.98928900	C	-0.51337600	1.05680000	2.47048800
C	0.88942100	2.42990600	-1.57360600	N	0.24959800	0.52585900	1.52299500
N	-0.19794300	1.79719500	-1.12839700	C	1.59945200	0.55534100	1.66810700
C	-1.39558400	2.44663400	-1.08456600	H	1.83484300	2.17623500	4.64397000
C	-1.49563100	3.77094700	-1.48490300	H	-0.64919700	2.06620000	4.36523100
C	-0.35917600	4.43178700	-1.93928600	H	-1.59097200	1.01688900	2.32242000
H	1.75621400	4.23355700	-2.34399800	O	-0.56313800	-0.78023800	-2.15500700
H	1.81162600	1.85438000	-1.60090900	C	1.81894100	-2.16795600	-2.31249200
H	-2.45019200	4.28559000	-1.44715300	C	-4.79236400	1.23140000	0.09319200
H	-0.42491800	5.46831500	-2.25479900	H	-5.81459100	1.56855300	0.23292600
C	-1.29670800	-4.14517700	1.27710800	C	-3.84423600	2.11387500	-0.41535300
C	-2.65845000	-4.01397600	1.50472500	H	-4.12108400	3.13261500	-0.66473100
H	1.75971000	-2.51427000	-4.15589400	O	2.16580200	-1.86436300	-3.55692100

³10(LRu^{IV}-OH)

Ru	0.32752600	0.25916800	-0.53026700	C	2.52152500	1.81358700	0.61660800
C	-4.56571600	0.58834300	-0.16556900	N	1.19706400	1.97669300	0.33342700
C	-3.78012800	-0.05231100	0.81631600	C	0.58765000	3.13732800	0.58615200
C	-2.38302700	0.00323000	0.66471700	H	0.74516700	5.12678500	1.37344200
N	-1.78399500	0.67045200	-0.36878800	H	3.16555700	4.85236500	1.95237500
C	-2.53951800	1.33316400	-1.24480200	H	4.30166400	2.70965900	1.42679500
C	-3.94825500	1.26789500	-1.18148900	H	-0.44444100	3.20746000	0.24640600
H	-5.65012700	0.54071400	-0.09589200	C	-4.34612800	-0.74269000	1.93177800
H	-4.51372000	1.77914500	-1.95471200	C	-3.55502600	-1.33239400	2.86670400
O	-2.21651900	1.98252200	-3.47376300	C	-2.13300900	-1.28025600	2.74938400
C	2.52230000	-1.63094600	-0.61024600	H	-5.42956300	-0.77767500	2.01726700
N	2.22889700	-0.35608400	-0.29374800	H	-3.98660700	-1.84892000	3.72032600
C	3.09775200	0.49957700	0.27604700	C	-1.26221600	-1.85112700	3.69791800
C	4.39853000	0.07152500	0.52147700	C	0.09901000	-1.75647300	3.52103300
H	5.12956800	0.73091300	0.97685500	C	0.59144100	-1.10387500	2.38405700
C	-0.84121500	-3.70292300	-2.11110900	N	-0.20398900	-0.55850000	1.47323600
C	-0.89069100	-2.38700900	-1.66824400	C	-1.55075700	-0.62869500	1.64172900
N	0.18826000	-1.76021400	-1.19643200	H	-1.67902000	-2.35933600	4.56442100
C	1.38724000	-2.40593200	-1.14799500	H	0.79537700	-2.18000000	4.23663900
C	1.49824000	-3.72078100	-1.57646200	H	1.66473100	-1.02871700	2.21617400
C	0.37070400	-4.37573300	-2.06079400	O	0.55207400	0.82087400	-2.20073800
H	-1.74042300	-4.17833900	-2.48730800	C	-1.91568100	2.24769700	-2.29656700
H	-1.81308700	-1.81114000	-1.69301600	C	4.74338700	-1.23328400	0.18213600
H	2.45456000	-4.23230300	-1.53842700	H	5.75304600	-1.58448400	0.37071000
H	0.44550400	-5.40456200	-2.39898700	C	3.80973900	-2.10165400	-0.37598300
C	1.26839000	4.19731200	1.17576500	H	4.08458300	-3.12432700	-0.61149100
C	2.60960600	4.04213100	1.49060800	O	-1.25203300	3.19173400	-1.81649900
C	3.24823000	2.83961100	1.20087800				

${}^4\mathbf{11}(\text{LRu}^{\text{IV}}-\text{OH}_2\bullet)$

Ru	0.29600500	-0.12163300	-0.39030500	N	0.61353800	1.90078700	-0.87486300
C	-4.64445100	-0.41320400	-0.69613900	C	-0.31620900	2.73819600	-1.31893600
C	-3.96554700	0.14991200	0.39706300	H	-0.79669500	4.70773300	-2.03219600
C	-2.54337600	0.12807400	0.36956400	H	1.56195600	5.52859700	-1.80454300
N	-1.83013000	-0.40794300	-0.64945800	H	3.30012000	3.96798900	-0.96482500
C	-2.51708500	-1.00529600	-1.63601000	H	-1.33222400	2.36234000	-1.39826500
C	-3.91973800	-0.98737600	-1.71634900	C	-4.62544200	0.72885700	1.51720400
H	-5.73010400	-0.40434800	-0.72141000	C	-3.91348100	1.22305200	2.56892900
H	-4.40107500	-1.45921000	-2.56618500	C	-2.48004000	1.18615900	2.57933100
O	-0.84304400	-2.55752000	-2.37740600	H	-5.71084900	0.75564500	1.51961600
C	2.96180900	-0.91143000	0.47693900	H	-4.42191200	1.65114300	3.42835900
N	2.26633100	0.14453900	0.01872100	C	-1.69632800	1.64660400	3.65045200
C	2.83309900	1.32844500	-0.25670000	C	-0.32117600	1.55036400	3.57544000
C	4.22745400	1.49673600	-0.05869800	C	0.27501200	1.01891500	2.43006600
H	4.70338600	2.44771600	-0.27332500	N	-0.45303300	0.58937700	1.39820700
C	0.47092900	-4.18495300	1.25389100	C	-1.80905400	0.65417600	1.46790600
C	-0.00546000	-2.94913100	0.77804700	H	-2.17714700	2.06849500	4.52864800
N	0.81348800	-1.93437100	0.53639900	H	0.31325500	1.88505100	4.38818300
C	2.16376100	-2.07827800	0.75715000	H	1.35523100	0.94251000	2.35343300
C	2.68555800	-3.28204800	1.23924000	H	0.67208000	-1.67363600	-2.54510100
C	1.82487700	-4.34839300	1.48465700	O	1.17826800	-0.90531200	-2.20046000
H	-0.23962200	-4.98260200	1.43981600	C	-1.71647700	-1.74892000	-2.66618900
H	-1.06507300	-2.79630600	0.59569000	C	4.97761700	0.42365200	0.40392200
H	3.75027600	-3.38624500	1.41708800	H	6.04573000	0.53369000	0.55314900
H	2.21578600	-5.28886000	1.85756800	C	4.36118400	-0.78998800	0.67380300
C	-0.00431400	4.05953100	-1.67470200	H	4.94358500	-1.63153800	1.03318400
C	1.29931200	4.50836000	-1.54657800	O	-2.07990800	-1.31749600	-3.80750100
C	2.27394300	3.63445700	-1.07540100	H	1.33271800	-0.30086000	-2.94204400
C	1.91403600	2.32693600	-0.74682100				

⁴¹²(^HLRu^{IV}-OH•)

Ru	-0.35725600	0.16431500	-0.48752900	N	-0.41725100	-1.88037700	-0.95908100
C	4.64243800	0.20719700	-0.31929200	C	0.61373500	-2.64852800	-1.33239600
C	3.82970400	-0.23522900	0.73917100	H	1.28782500	-4.55671000	-2.02501700
C	2.42518500	-0.10948200	0.60166500	H	-1.02596200	-5.52490200	-2.00938500
N	1.84729300	0.44464800	-0.47290400	H	-2.93126900	-4.10110200	-1.30278600
C	2.65588200	0.94472800	-1.44150500	H	1.59894400	-2.19280100	-1.33739500
C	4.03962200	0.80733500	-1.41183800	C	4.35859600	-0.78933000	1.92403100
H	5.72197200	0.10204700	-0.26291800	C	3.51369300	-1.19279500	2.98000100
H	4.62835800	1.20478100	-2.23071400	C	2.11757800	-1.07754700	2.87120400
O	1.07536400	2.51725000	-2.26417900	H	5.43511900	-0.89747400	2.02861600
C	-3.06154100	0.77617200	0.27772000	H	3.95105800	-1.59886600	3.88849700
N	-2.27937800	-0.23588700	-0.16040500	C	1.23360900	-1.45666000	3.90834800
C	-2.73104200	-1.46619500	-0.48541900	C	-0.12531800	-1.31136100	3.71547800
C	-4.08666900	-1.73104900	-0.35105400	C	-0.58660500	-0.81967900	2.49880300
H	-4.49185000	-2.70777700	-0.59114800	N	0.24044200	-0.45978200	1.49556200
C	-0.75899600	4.19637300	1.15149500	C	1.56337200	-0.56437100	1.67230500
C	-0.21406600	3.02958100	0.63609700	H	1.63188200	-1.85212600	4.83877500
N	-0.98315100	1.97191000	0.34714300	H	-0.84052500	-1.58117500	4.48327500
C	-2.33409800	2.01237500	0.57552600	H	-1.65262700	-0.71443000	2.31785400
C	-2.92473300	3.15412900	1.08670000	H	-0.59362200	1.56548500	-2.49455800
C	-2.12758800	4.25837800	1.37514100	O	-0.70670000	0.61949800	-2.25900400
H	-0.10947000	5.03684900	1.36760000	C	2.03478600	1.81417500	-2.49925800
H	0.84839500	2.93755600	0.43560600	C	-4.92369600	-0.71366700	0.10175200
H	-3.99342300	3.18483900	1.26929700	H	-5.98575300	-0.90776400	0.20992000
H	-2.57841500	5.15875800	1.77999400	C	-4.42353100	0.54551000	0.42102500
C	0.43040900	-3.96738800	-1.72071700	H	-5.08768300	1.32522400	0.77651900
C	-0.85304100	-4.49535000	-1.71308600	O	2.70046900	1.75637700	-3.62786900
C	-1.92423600	-3.69861700	-1.31781200	H	2.31901000	2.38474400	-4.26723600
C	-1.68702300	-2.38930300	-0.93863800				

⁴13(LRu^{IV}-OH•)

Ru	0.34446000	0.03225600	-0.51505600	C	1.98214800	2.38559300	-0.01394800
C	-4.64675900	0.04294500	-0.45525500	N	0.66906900	2.08763800	-0.25534600
C	-3.86161400	-0.02761400	0.70886700	C	-0.23907500	3.06520300	-0.36159600
C	-2.44815700	-0.02431200	0.55403500	H	-0.64095700	5.16706100	-0.34759400
N	-1.84633100	0.01557300	-0.65849400	H	1.75682900	5.75515100	0.09107000
C	-2.62809500	0.02091200	-1.74436900	H	3.43236900	3.93667000	0.30345700
C	-4.03055200	0.09618500	-1.68310700	H	-1.26542300	2.76584600	-0.55296400
H	-5.72978800	0.06477900	-0.37547600	C	-4.41698600	-0.08397000	2.01853400
H	-4.59748800	0.15837000	-2.60590000	C	-3.61284700	-0.14028600	3.11549300
O	-1.41771100	-1.06198100	-3.55898300	C	-2.18572100	-0.13498000	2.98978000
C	2.90994700	-1.15340000	0.03201500	H	-5.49809500	-0.08348100	2.12049400
N	2.28028300	0.03837100	-0.04490100	H	-4.03950100	-0.18935700	4.11348500
C	2.88555200	1.23514000	0.10539900	C	-1.31550000	-0.18613300	4.09339800
C	4.24857300	1.26041300	0.36519500	C	0.04775300	-0.17169600	3.88598000
H	4.77423400	2.19900200	0.50151000	C	0.54268100	-0.10763200	2.58271100
C	0.20248200	-4.35622900	-0.41000200	N	-0.26535600	-0.05945300	1.52210100
C	-0.18115400	-3.02463100	-0.48523000	C	-1.61199400	-0.07366000	1.70998500
N	0.70912200	-2.03271100	-0.36539500	H	-1.72701300	-0.23517400	5.09786500
C	2.02911400	-2.31376400	-0.13929600	H	0.74690000	-0.20715500	4.71354400
C	2.46312000	-3.62556000	-0.05536400	H	1.61353800	-0.09180500	2.40161800
C	1.53986300	-4.65730000	-0.19735500	H	0.40084100	-0.63559800	-2.94129600
H	-0.54588200	-5.13261700	-0.52148000	O	0.68909900	0.09373100	-2.34978200
H	-1.21548100	-2.74142600	-0.65594900	C	-1.96599100	-0.07574000	-3.11511900
H	3.50982600	-3.84667700	0.12415200	C	4.93314300	0.04988400	0.44928100
H	1.86896600	-5.68952800	-0.13544400	H	5.99914000	0.05489700	0.65199600
C	0.11919400	4.40076700	-0.24666700	C	4.27537800	-1.16587800	0.28509700
C	1.44813600	4.71933100	-0.00657000	H	4.82154100	-2.09956900	0.35960200
C	2.39074900	3.70127500	0.11280300	O	-2.13246200	1.11278100	-3.54550500

$^{214}\text{(}^{\text{H}}\text{LRu}^{\text{IV}}\text{-OH}\bullet\text{)}$

Ru	0.34328600	0.27070900	-0.53857600	C	2.13879000	2.13715800	0.78087700
C	-4.60485700	0.11891600	-0.28360100	N	0.79749500	1.93480500	0.60212500
C	-3.78011700	-0.50140500	0.66844900	C	-0.09762000	2.83629500	1.03184600
C	-2.38779700	-0.31193500	0.53911700	H	-0.43403800	4.72609500	1.97288000
N	-1.84228500	0.45313700	-0.44049100	H	2.01538100	5.16221400	2.27425000
C	-2.65240800	1.08543400	-1.29594700	H	3.65857200	3.46423400	1.50726500
C	-4.04188800	0.91455300	-1.25680000	H	-1.14527500	2.60947400	0.86753900
H	-5.68165800	-0.01728300	-0.23287700	C	-4.28326800	-1.29938000	1.74237000
H	-4.65294200	1.43612000	-1.98492500	C	-3.44066400	-1.85689200	2.65043800
O	-1.11697400	2.80729700	-1.88584700	C	-2.02590300	-1.66934400	2.55131200
C	2.86694300	-1.15736000	-0.60178700	H	-5.35784300	-1.43917300	1.81858700
N	2.30684300	0.01275800	-0.22127000	H	-3.82448500	-2.45255000	3.47399600
C	2.99271400	1.03005500	0.34256400	C	-1.10699800	-2.20124200	3.47563700
C	4.36422600	0.90938100	0.50271500	C	0.24088900	-1.96754400	3.31269600
H	4.94549000	1.70605700	0.95368900	C	0.67929400	-1.22302700	2.21503000
C	-0.07722100	-3.86772800	-1.92544800	N	-0.17271600	-0.70869700	1.33021100
C	-0.36375800	-2.57396500	-1.50940200	C	-1.50646500	-0.91245800	1.48588200
N	0.60584900	-1.75453200	-1.09969800	H	-1.47053000	-2.79123700	4.31288000
C	1.90995500	-2.15066600	-1.09270500	H	0.97281800	-2.35483100	4.01246300
C	2.24754700	-3.43045700	-1.50210700	H	1.73944000	-1.04323600	2.05823900
C	1.24174300	-4.29651000	-1.92084300	O	0.24414300	0.54639100	-2.21953200
H	-0.88544800	-4.51003900	-2.25618200	C	-2.06123700	2.12211700	-2.20495900
H	-1.37632500	-2.18089400	-1.52287500	C	4.97974700	-0.26866600	0.08363600
H	3.28294900	-3.75392100	-1.49107700	H	6.05276700	-0.37963000	0.19996300
H	1.49496800	-5.30117100	-2.24368700	C	4.23931900	-1.31492300	-0.45733800
C	0.31111900	4.01341500	1.63863000	H	4.72631200	-2.23812000	-0.75110700
C	1.66902700	4.24754300	1.80372300	O	-2.74371600	2.22937100	-3.33270500
C	2.59497700	3.29789300	1.37426700	H	-2.37517600	2.96437700	-3.85264800

$^{215}(\text{LRu}^{\text{IV}}-\text{O}\bullet)$

Ru	0.31033200	-0.16533000	-0.56717900	C	2.49311000	3.56945200	-0.96499900
C	-4.38830400	-0.77136900	-1.40293200	C	2.06674800	2.28671000	-0.65189900
C	-3.98704600	0.05801200	-0.33121300	N	0.74684000	2.01158500	-0.50488200
C	-2.60686400	0.15044600	-0.10609500	C	-0.16225700	2.97236800	-0.66878800
N	-1.71544500	-0.47350200	-0.88742300	H	-0.56685900	5.03292300	-1.09228900
C	-2.09185200	-1.35850400	-1.79746800	H	1.86503200	5.58276600	-1.37808000
C	-3.44928400	-1.51141800	-2.10217600	H	3.55087400	3.78218200	-1.07984400
H	-5.44592800	-0.87264200	-1.63262100	H	-1.20720600	2.69154800	-0.56135700
H	-3.73544700	-2.23045900	-2.86330300	C	-4.84424200	0.75605600	0.58103900
O	0.12713100	-2.09529000	-1.53221200	C	-4.33203800	1.40629200	1.66530400
C	2.96783300	-1.04362400	0.43648900	C	-2.92624800	1.40057000	1.95823600
N	2.33765300	0.01123100	-0.10474200	H	-5.91649800	0.73825300	0.40692600
C	2.96914600	1.16653100	-0.37256000	H	-4.99484500	1.91663800	2.35896400
C	4.35276900	1.23699400	-0.25513000	C	-2.32704200	1.94004400	3.11301800
H	4.88406100	2.15691000	-0.47460300	C	-0.96772800	1.79416800	3.30526500
C	0.13721700	-3.70013500	2.04935800	C	-0.18961400	1.12011200	2.35311500
C	-0.19476500	-2.51118000	1.41814100	N	-0.73128600	0.61862200	1.24947600
N	0.74098500	-1.71324400	0.89761000	C	-2.06681500	0.76938200	1.04831200
C	2.04942100	-2.05852900	0.95851300	H	-2.93847100	2.45306300	3.85083800
C	2.44292000	-3.24403600	1.56220900	H	-0.48326200	2.18720500	4.19228300
C	1.47352800	-4.07497500	2.10952400	H	0.88138400	0.98788700	2.48901600
H	-0.64675700	-4.31701600	2.47396900	O	0.59650500	0.22807500	-2.24778000
H	-1.22768900	-2.18763500	1.32575300	C	-0.96174200	-2.25444600	-2.23868600
H	3.49256900	-3.51526000	1.60424800	C	5.04202800	0.11192700	0.18314300
H	1.76324900	-5.00765400	2.58309800	H	6.12284300	0.14433100	0.27378600
C	0.20157900	4.27731100	-0.97290300	C	4.35029400	-1.02960900	0.57309000
C	1.54819100	4.57493700	-1.12914200	H	4.87684200	-1.87587600	1.00083400
O	-1.12031200	-3.10483800	-3.09458600				

${}^2\mathbf{16}(\text{H}^{\text{L}}\text{Ru}^{\text{III}}\text{-OOH}+\text{H}_2\text{O})$

Ru	0.30134800	0.05457800	0.10828800	C	-0.97904100	-1.56049900	2.48019000
C	-4.44543800	1.34765500	0.27514700	H	-1.85916900	-2.63295600	4.11653100
C	-3.98726400	0.21431900	-0.42162000	H	0.19769100	-4.02695600	4.46990800
C	-2.59556800	0.00140400	-0.46773700	H	2.16298000	-3.66936200	3.00051400
N	-1.70123100	0.85567600	0.10154100	H	-1.84504700	-0.92956700	2.29403800
C	-2.16252000	1.95835900	0.68882200	C	-4.85908300	-0.71195100	-1.07635300
C	-3.53405300	2.21959800	0.82560200	C	-4.36147800	-1.77870300	-1.75537700
H	-5.51359200	1.53247700	0.35672800	C	-2.95188600	-2.01494200	-1.82302000
H	-3.85241100	3.11768000	1.34624000	H	-5.93030600	-0.53487300	-1.02560300
O	-0.49050000	3.58454000	0.26826000	H	-5.02552500	-2.47379600	-2.26291300
C	2.95340000	-0.46589300	-0.89229200	C	-2.37967100	-3.09217300	-2.52699800
N	2.07143100	-0.86305400	0.04491900	C	-1.01148700	-3.24265500	-2.54633800
C	2.32153600	-1.83526300	0.94289600	C	-0.21138200	-2.32781700	-1.85134400
C	3.55552000	-2.47435000	0.91982100	N	-0.72492300	-1.30686700	-1.17366800
H	3.79026600	-3.26286000	1.62666400	C	-2.07506000	-1.13501500	-1.16088700
C	1.33703000	2.58934800	-3.30956800	H	-3.02558900	-3.79242600	-3.05090600
C	0.64648100	2.00554300	-2.25529300	H	-0.53939400	-4.05850500	-3.08286200
N	1.18372000	1.03615300	-1.50923300	H	0.87122500	-2.43282200	-1.84311100
C	2.45016300	0.60057700	-1.77180900	C	-1.16040600	3.00401000	1.09492300
C	3.18648200	1.14574500	-2.81406000	C	4.49191600	-2.08245500	-0.03355800
C	2.62295400	2.15069300	-3.59213800	H	5.46075300	-2.57101800	-0.06381800
H	0.86498200	3.37485700	-3.88979500	C	4.20178500	-1.07802100	-0.94972900
H	-0.35200800	2.32563800	-1.97109300	H	4.93629400	-0.78234600	-1.69109200
H	4.19183100	0.79099800	-3.01797400	O	-1.15831000	3.23242700	2.39340900
H	3.18827300	2.58640100	-4.41013000	O	0.89801700	1.37685700	1.37690300
C	-0.97915900	-2.50926800	3.49496900	O	2.11707900	1.99146200	1.12060500
C	0.16029900	-3.27691200	3.68593100	H	2.01323800	2.81637700	1.65384100
C	1.26352400	-3.07802700	2.86220600	H	-0.36712500	3.79665000	2.59094100
C	1.20237100	-2.11508500	1.86503500	O	1.33899200	4.26782800	2.52171600
N	0.07743500	-1.36639000	1.68752800	H	1.40727100	5.02277500	1.92292900
H	1.77902000	4.53932100	3.33699500				

$^{217}\text{(LRu}^{\text{III}}\text{-OOH+H}_3\text{O}^+)$

Ru	-0.21351700	-0.13560200	-0.24500100	H	-0.17126800	-4.80662400	2.14596200
C	4.62412000	-0.89958200	-0.82988000	H	-2.46871800	-4.50741100	3.09797900
C	4.08764500	-0.12907700	0.22288100	H	-3.72464000	-2.42690900	2.59954200
C	2.68710300	-0.04866400	0.31034600	H	0.76650100	-2.98870500	0.68911100
N	1.84920100	-0.69781200	-0.55368900	C	4.89545500	0.55596400	1.18185700
C	2.37548200	-1.48100600	-1.49589800	C	4.33251600	1.26953100	2.19316800
C	3.77323500	-1.55964400	-1.67639800	C	2.91214800	1.35546200	2.31754500
H	5.70324400	-0.96724900	-0.94798000	H	5.97610400	0.48531000	1.08562100
H	4.14051900	-2.16990200	-2.49554800	H	4.94857500	1.78319600	2.92664900
O	0.75154600	-3.14333500	-1.67660700	C	2.26672600	2.05707900	3.35322600
C	-2.43572700	1.72109100	-0.09575500	C	0.89114500	2.08790400	3.40514500
N	-2.04758700	0.49100200	0.29161700	C	0.15523300	1.42846800	2.41555000
C	-2.78606800	-0.31508500	1.07888800	N	0.73978500	0.75566600	1.42849100
C	-4.04269600	0.11218900	1.49077700	C	2.09833100	0.70637400	1.36671000
H	-4.66654800	-0.50723100	2.12617300	H	2.86384400	2.56757700	4.10500500
C	0.60867800	3.66744700	-2.27837300	H	0.36539400	2.61604400	4.19301200
C	0.75063600	2.39700000	-1.73706200	H	-0.93201200	1.44783700	2.42973000
N	-0.23686000	1.80368200	-1.06052100	O	-0.78213500	-0.88768500	-1.94784800
C	-1.42394900	2.45059200	-0.87582700	C	1.49378500	-2.39414300	-2.34727200
C	-1.62197500	3.72204600	-1.39377500	C	-4.48937400	1.36335600	1.07421300
C	-0.59528800	4.33499300	-2.10338600	H	-5.47017800	1.71027400	1.38396100
H	1.43154800	4.11382000	-2.82564500	C	-3.69019700	2.18458800	0.28591800
H	1.67059100	1.82855700	-1.84890500	H	-4.04040000	3.16723200	-0.01161200
H	-2.56875600	4.23248400	-1.24887400	O	1.68270900	-2.32190800	-3.57426000
H	-0.73961900	5.32876400	-2.51580700	O	-1.87984600	-0.14284100	-2.56895900
C	-0.74433700	-3.90485000	1.95957700	H	-1.66951700	-0.20964100	-3.51910700
C	-2.01693000	-3.73552300	2.48255900	O	-3.68780500	-1.48553600	-1.76893400
C	-2.72252800	-2.56691400	2.20760100	H	-3.65895600	-2.41280100	-2.05092900
C	-2.12842000	-1.58858100	1.42687500	H	-4.58224100	-1.15140000	-1.93939700
N	-0.86964400	-1.76460900	0.93073000	H	-2.83285100	-0.81744900	-2.26243400
C	-0.19906400	-2.89340700	1.17745400				

${}^3\mathbf{18}(\text{LRu}^{\text{IV}}\text{-OO-LRu}^{\text{IV}})$

Ru	2.24678000	-0.79660300	0.19130800	Ru	-2.54038300	0.39734000	-0.22438400
C	4.95570800	3.24892400	0.06742700	C	-0.23941700	3.98999400	-2.37508700
C	5.54209700	1.96576100	0.05388000	C	-1.15325700	4.28093600	-1.33759800
C	4.66735500	0.87440300	0.18858100	C	-1.79456500	3.17844000	-0.76359600
N	3.33461400	1.02163300	0.33392700	N	-1.55409900	1.92435900	-1.15880200
C	2.80807600	2.23542900	0.44795100	C	-0.80558500	1.65956000	-2.21574300
C	3.59727800	3.38151500	0.28164800	C	-0.09081600	2.68998100	-2.83803800
H	5.58637600	4.12624300	-0.05312200	H	0.30460500	4.80093900	-2.85261700
H	3.11774600	4.35275800	0.35790700	H	0.53565800	2.45502900	-3.69329500
O	1.02051400	1.10742300	1.39828100	O	-1.94890000	-0.40009300	-2.02468700
C	0.96397600	-3.34684300	0.82677200	C	-4.44888600	-1.82223200	-0.24447300
N	1.47550100	-2.63255600	-0.19237100	N	-3.49329600	-1.26130000	0.51463400
C	1.41408700	-3.02389600	-1.47960000	C	-3.11727300	-1.76603700	1.70045600
C	0.78792300	-4.22483200	-1.79146400	C	-3.59324400	-3.00851100	2.10200900
H	0.71909900	-4.56832200	-2.81798000	H	-3.28579800	-3.44535400	3.04654400
C	1.81074800	-1.47073400	4.50034900	C	-5.69974600	0.95731000	-3.14687500
C	2.10284100	-0.90319800	3.26635500	C	-4.68055900	1.20473900	-2.24148700
N	1.80376100	-1.52356900	2.12214400	N	-4.30129700	0.28176000	-1.35115500
C	1.18551200	-2.73581300	2.14395400	C	-4.90034600	-0.94134600	-1.32176300
C	0.84957200	-3.34220300	3.34691200	C	-5.91750500	-1.24303900	-2.21429600
C	1.17419000	-2.70427900	4.53869200	C	-6.31974700	-0.28585200	-3.13674300
H	2.07759200	-0.94114400	5.40885200	H	-5.98701600	1.73275900	-3.84788000
H	2.57197800	0.07208500	3.17375700	H	-4.15388300	2.15393000	-2.22596900
H	0.35549200	-4.30865700	3.35469200	H	-6.39396800	-2.21728300	-2.18330800
H	0.92931500	-3.17035100	5.48833400	H	-7.11422300	-0.51046000	-3.84097200
C	3.25334600	-0.25599800	-4.08607800	C	-1.00809800	1.19873000	3.80605100
C	2.73820600	-1.42277600	-4.63042000	C	-1.21315200	-0.01350000	4.44315000
C	2.13109400	-2.35509100	-3.79625800	C	-1.87018000	-1.04144500	3.77033300
C	2.04652200	-2.09786900	-2.43644100	C	-2.32273200	-0.82045200	2.48185300
N	2.56463600	-0.95144200	-1.91222700	N	-2.12607900	0.38692600	1.87611900
C	3.14843300	-0.05697500	-2.71599700	C	-1.46284400	1.36123800	2.50309900
H	3.73236700	0.49730400	-4.70163700	H	-0.48816100	2.01825900	4.28990900

H	2.80749500	-1.61322800	-5.69695800	H	-0.86724300	-0.16684100	5.46131100
H	1.72359400	-3.27383300	-4.20540000	H	-2.03950400	-2.00081900	4.25057400
H	3.53490400	0.84513900	-2.24852800	H	-1.27062300	2.28295800	1.95718400
C	6.94306700	1.69299300	-0.06249400	C	-1.53032100	5.57058400	-0.83934500
C	7.41593900	0.41710000	-0.00094700	C	-2.52343700	5.70238800	0.08858600
C	6.53470100	-0.69984400	0.17742700	C	-3.25038500	4.57038200	0.59469200
H	7.62595700	2.52946700	-0.18579200	H	-1.02754300	6.45117900	-1.22961200
H	8.48238800	0.22058000	-0.07402800	H	-2.81094700	6.68929600	0.44151900
C	6.95333700	-2.03781600	0.30454000	C	-4.35936800	4.61790100	1.46075200
C	6.01254100	-3.02709800	0.49818900	C	-5.00759000	3.44651700	1.80315600
C	4.65268800	-2.69762700	0.55094000	C	-4.55989300	2.21555800	1.30658700
N	4.23088100	-1.44132700	0.42885400	N	-3.50095800	2.14781900	0.50396400
C	5.15482400	-0.45579400	0.24948300	C	-2.85406900	3.29979700	0.16012300
H	8.01219500	-2.27915700	0.25627800	H	-4.70879600	5.57311500	1.84406200
H	6.30274500	-4.06635700	0.60678400	H	-5.87160500	3.45637800	2.45837300
H	3.89804400	-3.46719400	0.68871100	H	-5.05193600	1.28102700	1.56553700
O	0.32513600	-0.24729800	-0.55817800	O	-0.64872000	-0.57106600	0.20187000
C	1.36997400	2.23457900	0.91854700	C	-0.99836100	0.24587300	-2.68958000
C	0.24070400	-4.98154900	-0.75864000	C	-4.49878900	-3.66553800	1.27455800
H	-0.25567600	-5.91933200	-0.98724400	H	-4.88105900	-4.63891300	1.56482800
C	0.32570600	-4.55415500	0.56116000	C	-4.96877400	-3.06119500	0.11207600
H	-0.09528300	-5.15196000	1.36229500	H	-5.73544300	-3.54101300	-0.48710400
O	0.69583800	3.26893300	0.86777800	O	-0.41457300	-0.21907100	-3.64420100

${}^2\mathbf{19}(\text{LRu}^{\text{III}}\text{-OOH})$

Ru	0.30520400	-0.18976100	-0.33822400	N	0.08653000	1.76286500	-1.18959600
C	-4.57045000	-0.84960100	-0.38220800	C	-0.99578300	2.30674300	-1.74905800
C	-3.90517100	-0.10694900	0.61653800	H	-1.88536800	3.98714400	-2.74399500
C	-2.50013100	-0.07771400	0.56512900	H	0.24771100	5.30707100	-2.68794500
N	-1.77686800	-0.75321100	-0.37736300	H	2.26441600	4.29531200	-1.65738200
C	-2.42043700	-1.51396700	-1.26252500	H	-1.89474200	1.69399500	-1.75634700
C	-3.83169600	-1.53818000	-1.30790100	C	-4.58754700	0.59761600	1.65609400
H	-5.65781200	-0.87504000	-0.39624600	C	-3.90060300	1.27667400	2.61326600
H	-4.30250800	-2.12909400	-2.08776400	C	-2.47241500	1.31142400	2.59630800
O	-0.92023300	-3.27064500	-1.61015300	H	-5.67448000	0.56779000	1.66885900
C	3.04381000	-0.22712200	0.56600100	H	-4.42174000	1.80063900	3.41067100
N	2.14635600	0.54015600	-0.08049200	C	-1.70260000	1.97450200	3.57170200
C	2.40279800	1.78915900	-0.51289200	C	-0.32894200	1.95355500	3.48773700
C	3.66673900	2.32904200	-0.30563900	C	0.27937300	1.28298100	2.41994600
H	3.90968400	3.33294500	-0.63758400	N	-0.42149300	0.65357700	1.48357000
C	1.39028500	-3.96467000	1.59795100	C	-1.78073900	0.65137000	1.56078900
C	0.67756900	-2.97983800	0.92323200	H	-2.20473800	2.49465600	4.38414100
N	1.22401500	-1.79396600	0.63603500	H	0.29157900	2.45013200	4.22580600
C	2.52279300	-1.54158200	0.97186100	H	1.36284200	1.26492300	2.32327400
C	3.28071700	-2.49013600	1.64303400	C	-1.65759200	-2.45092700	-2.19815600
C	2.70355700	-3.71271200	1.96792100	C	4.62224100	1.55679800	0.35084100
H	0.91409900	-4.91455400	1.81725200	H	5.61294700	1.96580300	0.52254400
H	-0.32750000	-3.13724800	0.53557100	C	4.32101800	0.27525200	0.79819700
H	4.31285500	-2.28121800	1.90619500	H	5.06757100	-0.31407100	1.32035900
H	3.28322500	-4.46368200	2.49612000	O	-1.93000400	-2.32908800	-3.40666200
C	-0.98222100	3.58252100	-2.30000900	O	0.72163100	-0.83853700	-2.10210500
C	0.19942300	4.30783800	-2.26616100	O	1.94822900	-1.50046600	-2.20779600
C	1.33102500	3.74268300	-1.68730300	H	1.95301200	-1.74733900	-3.14741400
C	1.25384500	2.46445700	-1.15229700				

$^{220}\text{(}^{\text{H}}\text{LRu}^{\text{III}}\text{-OO)}$

Ru	0.32604700	-0.12186300	-0.25323200	N	0.16086700	1.83313100	-1.05056400
C	-4.51890900	-0.87848600	-0.70991900	C	-0.91720800	2.42861300	-1.57384000
C	-3.94715100	-0.22691400	0.39630100	H	-1.80061100	4.17295100	-2.45385200
C	-2.53972900	-0.16071800	0.45924000	H	0.34045900	5.47920400	-2.31632300
N	-1.72477100	-0.72772800	-0.47624800	H	2.35107100	4.38636700	-1.35522900
C	-2.30270200	-1.40045400	-1.47283000	H	-1.82333300	1.82805000	-1.61965800
C	-3.69388800	-1.46353300	-1.64373800	C	-4.72393400	0.36759100	1.44114200
H	-5.60029100	-0.92614500	-0.81037100	C	-4.12578200	0.98181600	2.49512000
H	-4.09596800	-1.99553400	-2.50039500	C	-2.69974700	1.06807400	2.58405000
O	-0.71193600	-3.11171600	-1.95034500	H	-5.80736200	0.30835500	1.37275200
C	3.07913900	-0.27532600	0.56675200	H	-4.71981500	1.42326700	3.29179000
N	2.16357500	0.55838700	0.02928100	C	-2.02753500	1.68482300	3.65521000
C	2.46953200	1.80408000	-0.38948400	C	-0.65025500	1.72561100	3.65513200
C	3.77114700	2.27657900	-0.25031100	C	0.05297800	1.16563300	2.58152000
H	4.04011100	3.27499000	-0.58036900	N	-0.55588900	0.57811900	1.55587800
C	1.32701500	-3.95318600	1.65164600	C	-1.91406900	0.51450500	1.55394500
C	0.63013000	-2.92893400	1.02490000	H	-2.60176800	2.12178800	4.46869200
N	1.21110100	-1.77469900	0.67993900	H	-0.10024700	2.19122300	4.46636200
C	2.53356900	-1.58492300	0.95232600	H	1.14046500	1.19765600	2.54774900
C	3.28404800	-2.57319900	1.57799200	C	-1.43884900	-2.24099100	-2.36333200
C	2.67606200	-3.77173900	1.92927600	C	4.73055000	1.44150000	0.31285900
H	0.81323900	-4.87269000	1.91260500	H	5.75103000	1.79359100	0.42748500
H	-0.42287200	-3.01938700	0.77109200	C	4.39207000	0.15649300	0.72485800
H	4.33526300	-2.40661200	1.79319700	H	5.14341900	-0.49683700	1.15719100
H	3.25057200	-4.55222400	2.41917600	O	-1.66311900	-1.98292200	-3.65153400
C	-0.89798600	3.73597300	-2.03953300	O	0.90839800	-0.70231200	-2.12062900
C	0.28832300	4.45407600	-1.96230600	O	2.00676500	-1.39496600	-2.20136300
C	1.41366800	3.84321700	-1.42491200	H	-1.13352600	-2.60643700	-4.17649200
C	1.33102800	2.53069300	-0.97376800				

²21(LRu^{III}-OO)

Ru	0.32265700	-0.15480100	-0.29565400	C	1.27874100	2.49736900	-1.07165200
C	-4.54732500	-0.92695200	-0.57072400	N	0.12169100	1.77659500	-1.13700200
C	-3.94172800	-0.20344900	0.47628700	C	-0.96089200	2.33568000	-1.69143000
C	-2.53511500	-0.13989400	0.48751700	H	-1.86392700	4.03326600	-2.64065100
N	-1.74953700	-0.76750700	-0.43913700	H	0.25377700	5.37980700	-2.52870900
C	-2.34416300	-1.51440600	-1.37207500	H	2.27192100	4.35572900	-1.50898900
C	-3.75003200	-1.56793000	-1.48380500	H	-1.85510800	1.71619400	-1.72463500
H	-5.63253100	-0.97541600	-0.63350400	C	-4.68631400	0.45510500	1.50383700
H	-4.17096100	-2.14317200	-2.30330200	C	-4.05999400	1.12651400	2.50681400
O	-0.82004100	-3.25324300	-1.69913500	C	-2.63318500	1.19990300	2.55350800
C	3.06136100	-0.22343900	0.58011100	H	-5.77203100	0.39764600	1.46726000
N	2.14074500	0.56515600	-0.01654100	H	-4.62939200	1.61736400	3.29281300
C	2.42208800	1.81400400	-0.44685900	C	-1.92744500	1.85933300	3.57759500
C	3.70139800	2.33244900	-0.26879200	C	-0.55054900	1.87702700	3.54812200
H	3.94947500	3.33342000	-0.60770500	C	0.11992900	1.24912200	2.49098900
C	1.42971200	-3.98283900	1.55826900	N	-0.51877800	0.62090000	1.50895800
C	0.71050200	-2.98461200	0.91267400	C	-1.87921700	0.58308300	1.53309600
N	1.24467800	-1.78833400	0.63835200	H	-2.47774900	2.34548600	4.38000500
C	2.54695800	-1.54617800	0.96268400	H	0.02451800	2.37273100	4.32359900
C	3.31547900	-2.50681400	1.60958400	H	1.20736700	1.25959400	2.43813500
C	2.74850500	-3.73664800	1.91874400	C	-1.52924200	-2.41513500	-2.29566300
H	0.95702200	-4.93794400	1.76463000	C	4.66454100	1.54365700	0.35183800
H	-0.29932500	-3.13694500	0.53699500	H	5.66689600	1.93342900	0.50000900
H	4.34936800	-2.29709400	1.86738100	C	4.35042900	0.25803900	0.78290800
H	3.33559500	-4.49578000	2.42741800	H	5.10346700	-0.35745700	1.26543000
C	-0.95864600	3.62611500	-2.20210500	O	-1.74774100	-2.26847000	-3.51502500
C	0.21484000	4.36726900	-2.13836100	O	0.90565500	-0.77102900	-2.14687900
C	1.34404700	3.79513300	-1.56803100	O	2.04775600	-1.39054800	-2.22150000

¹22(^HLRu^{IV}-OOH)

Ru	0.32103400	-0.20468600	-0.35445400	N	0.58192600	1.81129100	-0.83026800
C	-4.60517500	-0.25964100	-0.66183700	C	-0.39894300	2.64080600	-1.20289800
C	-3.90824600	0.35597800	0.39062400	H	-0.94694300	4.58088400	-1.91355700
C	-2.50433000	0.21892600	0.39910800	H	1.42942200	5.38845000	-1.93238800
N	-1.82624400	-0.49132100	-0.53941500	H	3.23848300	3.84213400	-1.22662500
C	-2.52312600	-1.14067600	-1.47487500	H	-1.41059000	2.24607400	-1.19844700
C	-3.91438700	-1.01657800	-1.58302000	C	-4.54595500	1.09006700	1.43914800
H	-5.68530300	-0.15988900	-0.72535600	C	-3.82121500	1.62789200	2.45478100
H	-4.42696700	-1.54650800	-2.37844400	C	-2.39774300	1.48724100	2.49773500
O	-0.85400000	-2.78574900	-1.87326800	H	-5.62702000	1.19396200	1.41109400
C	2.98034000	-0.94688300	0.55467300	H	-4.30960700	2.16954200	3.26027300
N	2.29302200	0.06353700	-0.00815600	C	-1.59701600	1.99550800	3.53740300
C	2.85201700	1.23799700	-0.35322300	C	-0.23213400	1.80741100	3.50541700
C	4.22111600	1.41372300	-0.18671600	C	0.34409100	1.13233600	2.42656100
H	4.70013100	2.34935600	-0.45378700	N	-0.39639900	0.64146400	1.43451600
C	0.30194800	-3.94198700	1.83191300	C	-1.74747700	0.79993500	1.45769400
C	-0.10572600	-2.75608000	1.24377100	H	-2.06533600	2.53030700	4.35957600
N	0.78762200	-1.85470600	0.80927900	H	0.40964800	2.17886500	4.29628300
C	2.12821200	-2.06248900	0.97799900	H	1.41979400	0.98794400	2.37166300
C	2.58614800	-3.23364100	1.55322200	C	-1.79535000	-2.15802200	-2.30030400
C	1.66177700	-4.18441600	1.97879200	C	4.96530100	0.36680800	0.34579800
H	-0.44206400	-4.65573800	2.16669000	H	6.03549900	0.48477400	0.47976600
H	-1.15501400	-2.51771700	1.10374200	C	4.35090700	-0.81955400	0.73821800
H	3.65051300	-3.40550500	1.67349700	H	4.92933900	-1.61788300	1.19034900
H	2.00879100	-5.10675600	2.43387500	O	-2.35499500	-2.32207500	-3.48873300
C	-0.12877600	3.93946300	-1.60632900	O	0.44535600	-0.47606400	-2.19906900
C	1.18895000	4.37702000	-1.62082800	O	1.52509900	0.02398400	-2.85644600
C	2.20497500	3.51251100	-1.23052800	H	1.18530500	0.15263400	-3.76544900
C	1.88371000	2.22379700	-0.83370700	H	-1.89809700	-3.04607300	-3.94988100

³23(LRu^{IV}-OOH)

Ru	0.28018600	-0.21923800	-0.36925500	N	-0.12641900	1.76929200	-1.03769400
C	-4.53206800	-1.02151700	-0.54251200	C	-1.26284100	2.24036300	-1.55875000
C	-3.93187300	-0.30778200	0.51566400	H	-2.31512500	3.88424100	-2.44363200
C	-2.52908100	-0.22395500	0.50693300	H	-0.31883600	5.39841700	-2.30707500
N	-1.76748300	-0.79138700	-0.45516800	H	1.79599800	4.51952000	-1.35251400
C	-2.34197500	-1.54550900	-1.38450300	H	-2.10201400	1.55144500	-1.60753400
C	-3.73647800	-1.65593500	-1.47314600	C	-4.63916200	0.30246700	1.59995900
H	-5.61540300	-1.09848200	-0.59122000	C	-3.97038800	0.90606300	2.62104300
H	-4.14993800	-2.27091500	-2.26626300	C	-2.53856100	0.95522000	2.64754200
O	-0.18502000	-2.34975600	-1.79309600	H	-5.72492700	0.25744600	1.60024100
C	3.05573900	-0.04292200	0.52168600	H	-4.51348400	1.35176700	3.45037300
N	2.06493100	0.67427000	-0.04189900	C	-1.77990400	1.50198200	3.69965500
C	2.18592400	1.97063600	-0.38683200	C	-0.40392900	1.45778600	3.63620900
C	3.39617000	2.61657100	-0.16683000	C	0.22451100	0.89327600	2.52006500
H	3.52713400	3.66130500	-0.42684300	N	-0.46833000	0.38445300	1.50400000
C	1.71925700	-3.91817300	1.48508000	C	-1.82922100	0.40528200	1.56816600
C	0.91855300	-2.96427000	0.87053800	H	-2.28406500	1.94540700	4.55458400
N	1.38387900	-1.75031600	0.56464700	H	0.21067500	1.85816900	4.43484100
C	2.67078600	-1.41929800	0.86018100	H	1.30839600	0.86291800	2.45368200
C	3.52054100	-2.33542300	1.46220100	C	-1.39473000	-2.37355900	-2.21602200
C	3.03793300	-3.60029500	1.77764100	C	4.44329300	1.89885200	0.40424300
H	1.30538400	-4.89309800	1.71831900	H	5.39409200	2.39102600	0.58241500
H	-0.11065200	-3.16750800	0.59177800	C	4.28455900	0.56405600	0.75825800
H	4.54773500	-2.06614900	1.68509000	H	5.10028600	0.01562300	1.21689300
H	3.69082700	-4.32772000	2.24962900	O	-1.83287900	-3.05010100	-3.14390500
C	-1.37361400	3.54278400	-2.02787200	O	0.98342400	-0.34479200	-2.34061600
C	-0.26728800	4.37462800	-1.95034800	O	2.16851300	-0.93113800	-2.45412200
C	0.91859200	3.88441700	-1.41316300	H	2.35685800	-0.90472300	-3.41557200
C	0.97034000	2.57423200	-0.96229700				

$^{324}(\text{HLRu}^{\text{IV}}\text{-OO})$

Ru	0.30419900	-0.16168200	-0.33059500	N	0.25478600	1.84256200	-1.02529700
C	-4.62775100	-0.51889000	-0.34815100	C	-0.79298400	2.52636300	-1.49363700
C	-3.88705900	0.06900000	0.69017600	H	-1.56008900	4.35525600	-2.30853200
C	-2.48062500	0.01378000	0.59542400	H	0.68277000	5.47778000	-2.22779600
N	-1.82466800	-0.60176400	-0.42561200	H	2.63419700	4.20885300	-1.36674600
C	-2.56088600	-1.20675900	-1.35967500	H	-1.74421500	2.00034600	-1.51802200
C	-3.96331000	-1.15754200	-1.36973000	C	-4.49209300	0.70933200	1.81703800
H	-5.71349000	-0.47895800	-0.32714400	C	-3.73176000	1.24751600	2.80535500
H	-4.50050800	-1.64776700	-2.17441400	C	-2.30296200	1.20423500	2.73937300
O	-0.91427100	-2.78079800	-2.05672100	H	-5.57710100	0.74561200	1.86679100
C	3.05611700	-0.53570500	0.45164000	H	-4.19302200	1.72287600	3.66709600
N	2.20956100	0.36987400	-0.07830200	C	-1.46666400	1.73148400	3.74074900
C	2.58267700	1.60641500	-0.45842400	C	-0.09925800	1.65111000	3.59714000
C	3.91414500	1.98509600	-0.31994600	C	0.43776000	1.06675300	2.44641700
H	4.24801700	2.97296300	-0.61935800	N	-0.33423400	0.56052500	1.48652900
C	1.03761500	-4.07860300	1.54634500	C	-1.68795400	0.60821500	1.62316300
C	0.41006300	-3.00240900	0.93157300	H	-1.90934100	2.19651300	4.61802300
N	1.07707700	-1.89766500	0.58813300	H	0.57418600	2.04329100	4.35118900
C	2.41445100	-1.80406700	0.84198300	H	1.51261600	1.01335000	2.29872200
C	3.09561700	-2.85004100	1.44734400	C	-1.85567900	-2.08124000	-2.34731300
C	2.39835600	-3.99983600	1.80338000	C	4.81547100	1.06856000	0.21102900
H	0.45981200	-4.95734000	1.81185800	H	5.85863800	1.34631800	0.32350500
H	-0.64862200	-3.01560700	0.68845400	C	4.39633800	-0.19836900	0.60599600
H	4.15989500	-2.77165500	1.64475800	H	5.10597900	-0.90304600	1.02641300
H	2.91918700	-4.82387700	2.28126600	O	-2.43572600	-2.04221800	-3.54285900
C	-0.68252600	3.83801800	-1.93628100	O	0.69608700	-0.41537800	-2.43418100
C	0.56004000	4.45346300	-1.88990200	O	1.51321700	-1.35521700	-2.35094500
C	1.65433600	3.74404600	-1.40846200	H	-1.98935400	-2.68561100	-4.11895600
C	1.48245100	2.43488300	-0.98117500				

³25(LRu^{IV}-OO)

Ru	0.29070400	-0.14049900	-0.34982100	N	0.32433900	1.88546700	-0.96466700
C	-4.60709400	-0.54172400	-0.47784300	C	-0.69100500	2.61128800	-1.44088200
C	-3.90465000	0.03782400	0.60020000	H	-1.38101100	4.48220000	-2.23045000
C	-2.50190800	0.02495900	0.52665000	H	0.89212500	5.53160900	-2.06842300
N	-1.81170100	-0.53641400	-0.50783800	H	2.78061600	4.18623500	-1.18401900
C	-2.49116400	-1.14035700	-1.48098800	H	-1.65527500	2.11109900	-1.49802500
C	-3.90280800	-1.11578000	-1.50471900	C	-4.53944000	0.62242700	1.73964200
H	-5.69467500	-0.53324500	-0.47535300	C	-3.80831700	1.14402400	2.76158100
H	-4.40432800	-1.57729900	-2.35026200	C	-2.37969200	1.12805900	2.71993400
O	-1.03393000	-2.85370500	-2.08867300	H	-5.62618700	0.63191700	1.77469300
C	3.00113900	-0.61370100	0.53487500	H	-4.29425200	1.57812200	3.63173700
N	2.20706200	0.32489300	-0.01776000	C	-1.56348300	1.62368400	3.75420100
C	2.62529200	1.56623100	-0.33003100	C	-0.19313400	1.55838200	3.63217600
C	3.95296100	1.91276500	-0.09999100	C	0.37006300	1.01490000	2.47291500
H	4.32406900	2.90363200	-0.34007800	N	-0.37908700	0.53958200	1.48059500
C	0.87751400	-4.18512400	1.28614000	C	-1.73772600	0.58231000	1.59082700
C	0.29855500	-3.06288000	0.70497600	H	-2.02395800	2.05180400	4.64135900
N	0.99331300	-1.94128400	0.50033700	H	0.46325200	1.92761600	4.41262400
C	2.31402500	-1.88441000	0.83514500	H	1.44844000	0.96861100	2.34726200
C	2.94564000	-2.97581300	1.41380000	C	-1.74500300	-1.93479500	-2.54745900
C	2.21551300	-4.13659600	1.64872100	C	4.80208100	0.96069200	0.45453500
H	0.28141300	-5.07787100	1.44230700	H	5.84090800	1.21392700	0.64157400
H	-0.72597000	-3.05284900	0.34356600	C	4.33545000	-0.30866600	0.78344500
H	3.99716300	-2.92671000	1.67815300	H	5.00496900	-1.03830500	1.22656600
H	2.69680900	-4.99601700	2.10569800	O	-1.97890500	-1.59841700	-3.72328100
C	-0.52969600	3.92898400	-1.84895200	O	0.67294600	-0.34422500	-2.45110100
C	0.72989300	4.50427900	-1.75713000	O	1.41156200	-1.35070200	-2.38334400
C	1.78901900	3.75193600	-1.26259000	C	1.56698400	2.43846200	-0.87089200

$^{226}\text{(}^{\text{H}}\text{LRu}^{\text{IV}}\text{-OOH}\bullet\text{)}$

Ru	-0.33186100	0.17982200	-0.34227200	N	-0.61511100	-1.83937300	-0.78602000
C	4.62263300	0.25105100	-0.77351500	C	0.35032400	-2.68134400	-1.17348900
C	3.94401200	-0.31556500	0.32438000	H	0.86646300	-4.63013600	-1.88038000
C	2.53211300	-0.20070000	0.35944300	H	-1.51567500	-5.42104300	-1.83493400
N	1.83206700	0.44499600	-0.58015600	H	-3.29717800	-3.85244200	-1.10816100
C	2.51383900	1.06267100	-1.57392100	H	1.36519100	-2.29815200	-1.20754800
C	3.89345900	0.94751600	-1.72183800	C	4.60091900	-0.98107300	1.37745000
H	5.70216300	0.16087800	-0.85204400	C	3.87782300	-1.50106700	2.47273400
H	4.37796000	1.43797800	-2.55904800	C	2.47612600	-1.38853600	2.53613400
O	0.86909300	2.72150400	-1.92936400	H	5.68201700	-1.08831600	1.35125400
C	-2.97025700	0.96861500	0.57621800	H	4.41183800	-1.99305400	3.28174100
N	-2.29452100	-0.06649900	0.04246900	C	1.71146300	-1.87172700	3.62163100
C	-2.87086800	-1.24131100	-0.27842000	C	0.33988800	-1.70509200	3.60244900
C	-4.24130400	-1.39507100	-0.10267600	C	-0.25389300	-1.08554100	2.50828600
H	-4.73206600	-2.33060100	-0.34738300	N	0.46118200	-0.62168000	1.46192000
C	-0.25755900	3.97078100	1.75054100	C	1.79454000	-0.75664500	1.47003800
C	0.13607900	2.76494500	1.19598800	H	2.20810200	-2.36298600	4.45367000
N	-0.76876700	1.85987900	0.78891500	H	-0.28466400	-2.05121000	4.41751300
C	-2.10731000	2.08664300	0.96075600	H	-1.33128700	-0.95417400	2.46614900
C	-2.55007500	3.27901600	1.50173200	C	1.74556200	2.04624900	-2.41293000
C	-1.61419900	4.23235600	1.89519700	C	-4.97123000	-0.32720200	0.40658300
H	0.49634100	4.68531100	2.06037400	H	-6.04229100	-0.42878000	0.54616400
H	1.18388300	2.51808100	1.06415100	C	-4.34130100	0.86154400	0.76555800
H	-3.61199700	3.46548700	1.62103500	H	-4.90867400	1.67899000	1.19684600
H	-1.94959200	5.17101500	2.32477700	O	2.20465200	2.10439500	-3.64552300
C	0.06030700	-3.98111100	-1.55794600	O	-0.52676900	0.46263800	-2.17124600
C	-1.26083800	-4.40855500	-1.53883300	O	-1.62100500	-0.02795600	-2.79652300
C	-2.26130900	-3.53174600	-1.13632600	H	-1.33052800	-0.09024100	-3.73107000
C	-1.92168500	-2.24247300	-0.75846200	H	1.73656900	2.80553800	-4.13237700

⁴²⁷(LRu^{IV}-OOH•)

Ru	0.29041000	-0.13899900	-0.32614700	N	0.30197500	1.86196400	-0.97550100
C	-4.58549000	-0.69594800	-0.75991100	C	-0.76466100	2.52608200	-1.43737400
C	-3.97699200	-0.02687300	0.31431800	H	-1.54039100	4.32764400	-2.29095000
C	-2.56430000	-0.02559700	0.36391300	H	0.69753000	5.46073000	-2.25686400
N	-1.79084100	-0.65751400	-0.55751700	H	2.66413500	4.22999500	-1.37599200
C	-2.41077300	-1.35191600	-1.52261900	H	-1.71452400	1.99993900	-1.44338500
C	-3.79853800	-1.36979300	-1.67138400	C	-4.70994300	0.63563400	1.34678200
H	-5.66819000	-0.70411900	-0.84929700	C	-4.06728500	1.23951600	2.38164700
H	-4.23305400	-1.94378000	-2.48415800	C	-2.63822000	1.24730000	2.46001900
O	-0.51887600	-2.75631900	-2.00891600	H	-5.79448200	0.63392800	1.28969700
C	3.03540900	-0.47100600	0.60676800	H	-4.62778900	1.72857000	3.17363400
N	2.20449400	0.42746500	0.04315100	C	-1.91623100	1.83315800	3.51734400
C	2.60549700	1.64024500	-0.38465100	C	-0.53973600	1.78153300	3.51311700
C	3.94161500	1.99858400	-0.25290800	C	0.12535700	1.16953200	2.44559800
H	4.29284500	2.96794600	-0.58913300	N	-0.53925100	0.61803800	1.43394700
C	0.86126200	-3.84345400	1.88615400	C	-1.89874500	0.63508400	1.43527700
C	0.28240600	-2.76463000	1.23517700	H	-2.45243700	2.31826500	4.32866000
N	1.02377200	-1.73569800	0.80129000	H	0.04525800	2.21571500	4.31594600
C	2.36629900	-1.70076600	1.03889800	H	1.21067600	1.13546800	2.41110500
C	2.99313400	-2.75167100	1.68578900	C	-1.59616600	-2.24343500	-2.37623600
C	2.23179800	-3.83882300	2.10478200	C	4.82417900	1.08702500	0.31610400
H	0.23550800	-4.66624200	2.21289300	H	5.87154600	1.34973800	0.42272300
H	-0.78688000	-2.72069200	1.05047100	C	4.37911100	-0.15442500	0.75837400
H	4.06141200	-2.72290800	1.87192900	H	5.06881600	-0.85663300	1.21365600
H	2.71068500	-4.66920200	2.61383800	O	-1.97666600	-2.63269000	-3.51431500
C	-0.65742800	3.82440500	-1.91352400	O	1.01476900	-0.65202800	-2.14736400
C	0.58417300	4.44393600	-1.89476400	O	2.04685300	-1.49008800	-2.13871200
C	1.68894700	3.75546200	-1.40441900	H	2.31642700	-1.54398900	-3.08094500
C	1.52785600	2.45830900	-0.94668900				

⁴²⁸(^HLRu^V-OO)

Ru	0.15789100	-0.01026700	-0.19955200	N	0.61533300	1.98334400	0.25836800
C	-4.24443300	0.26427800	-1.98265800	C	-0.23340600	3.01313800	0.13248500
C	-4.04545100	0.18104700	-0.58936900	H	-0.54297700	5.12691200	0.23671200
C	-2.70987300	0.10839100	-0.15592100	H	1.83168600	5.56867900	0.91882000
N	-1.68765700	0.11339700	-1.02090200	H	3.38744100	3.65620300	1.19278100
C	-1.87449500	0.18353000	-2.33812200	H	-1.25122600	2.77958700	-0.16679300
C	-3.16597900	0.26483800	-2.86147400	C	-5.05904300	0.15826200	0.42123700
H	-5.25635100	0.32442700	-2.37387400	C	-4.72340400	0.06981600	1.74022200
H	-3.31280900	0.32312300	-3.93492600	C	-3.35699700	-0.00415000	2.18320400
O	0.49924800	0.04735700	-2.43230900	H	-6.10136400	0.21058400	0.12070600
C	2.60157600	-1.36863500	0.66924600	H	-5.50192400	0.05218900	2.49829600
N	2.05126600	-0.14747900	0.54532700	C	-2.94190600	-0.09746600	3.52633600
C	2.71706400	0.98877900	0.81950000	C	-1.59478200	-0.16403200	3.81677600
C	4.04228800	0.92399600	1.23475900	C	-0.64546300	-0.14231500	2.78540500
H	4.60013100	1.82468900	1.46731100	N	-1.01254100	-0.05499700	1.51072700
C	-0.25602600	-4.35667300	-0.15749000	C	-2.34867300	0.01590900	1.21292600
C	-0.52955600	-3.00000800	-0.22953900	H	-3.68185000	-0.11755300	4.32195200
N	0.41429300	-2.07858500	0.00755900	H	-1.24638100	-0.23527300	4.84112000
C	1.67532300	-2.46361800	0.36210200	H	0.42009100	-0.19655500	2.99356400
C	2.00221400	-3.80779200	0.44602000	C	-0.57187900	0.14652500	-3.05451900
C	1.02785600	-4.76338000	0.17983600	C	4.64159300	-0.32582200	1.35210100
H	-1.04357400	-5.07223100	-0.36490200	H	5.67620300	-0.39616600	1.67155500
H	-1.51840500	-2.63818400	-0.49623200	C	3.92596200	-1.48626700	1.07766800
H	3.00751900	-4.10770300	0.72282300	H	4.39238300	-2.45954600	1.18655600
H	1.27286000	-5.81882000	0.24302300	O	-0.64980700	0.21832800	-4.34750600
C	0.17044200	4.31962600	0.35788200	O	3.22132300	1.01970400	-2.21223000
C	1.48549100	4.55662200	0.73461400	O	3.61572900	-0.11907000	-2.25441500
C	2.36063900	3.48652400	0.88623200	H	0.23822200	0.18356600	-4.74929000
C	1.90530100	2.19946200	0.64974500				

⁴²⁹(LRu^V-OO)

Ru	0.16614500	-0.04250200	-0.16706600	C	1.76250100	2.21370700	0.80131800
C	-4.13431500	0.46567200	-2.12307200	N	0.51496800	1.99943800	0.28743100
C	-4.02843500	0.26209600	-0.72782900	C	-0.32284300	3.02867200	0.12104700
C	-2.73027700	0.10000100	-0.22307700	H	-0.67400900	5.13564200	0.29304500
N	-1.65875100	0.13445300	-1.02577800	H	1.61353000	5.56558600	1.22988100
C	-1.74823000	0.29945500	-2.33497600	H	3.16503200	3.65500100	1.55396800
C	-3.00436500	0.47948100	-2.92662000	H	-1.30378900	2.79854000	-0.28697300
H	-5.11785000	0.60036300	-2.56633800	C	-5.10382300	0.18950000	0.21534700
H	-3.07077200	0.61776200	-4.00119200	C	-4.85616900	-0.04229100	1.53694400
O	0.59055000	-0.05405600	-2.16945100	C	-3.52456400	-0.22358400	2.04632800
C	2.63811900	-1.33268100	0.64353300	H	-6.12293900	0.31503000	-0.14015700
N	2.02582100	-0.13530500	0.60532100	H	-5.68070100	-0.10207800	2.24282700
C	2.61917600	1.02148500	0.95614300	C	-3.20167000	-0.49414200	3.39039200
C	3.93913800	0.99888100	1.38495300	C	-1.88048800	-0.66796300	3.74712900
H	4.45332600	1.90995600	1.67166200	C	-0.87007600	-0.57288100	2.77941300
C	0.02281900	-4.39861800	-0.60413400	N	-1.14320200	-0.30665400	1.50510200
C	-0.32660400	-3.05528700	-0.59564600	C	-2.45370900	-0.13929200	1.14678600
N	0.52674300	-2.10674300	-0.19867700	H	-3.99178800	-0.57078400	4.13316200
C	1.78166300	-2.44776700	0.21480700	H	-1.60156100	-0.88116400	4.77337300
C	2.18399900	-3.77616300	0.22901900	H	0.17572600	-0.70915000	3.04397800
C	1.29575900	-4.76099400	-0.18607700	C	-0.39557300	0.23579500	-3.00165900
H	-0.69769500	-5.13727500	-0.93772800	C	4.60399400	-0.22590100	1.42999300
H	-1.30925800	-2.72033300	-0.91916500	H	5.63915600	-0.25844700	1.75447400
H	3.18178200	-4.04060700	0.56373400	C	3.96437900	-1.40350700	1.06129500
H	1.59905800	-5.80315100	-0.18055300	H	4.49399900	-2.34960700	1.09415900
C	0.03516700	4.32971500	0.44520300	O	-0.25764900	0.41053100	-4.19446900
C	1.30131600	4.56069400	0.96303200	O	3.11078600	1.44881600	-1.98948900
C	2.17367600	3.49157100	1.14390800	O	3.76080500	0.43652700	-2.06984800

²TS1

Ru	-0.29238800	-0.14068800	0.19467000	H	1.65365100	3.25727000	3.73421900
C	4.42367600	-1.54308400	0.72664000	H	-0.24270900	4.86979100	3.43549400
C	4.03607800	-0.43266300	-0.05300200	H	-2.04838700	4.32636700	1.82240800
C	2.65934700	-0.18920800	-0.19368600	H	1.65455200	1.15184900	2.39009300
N	1.70988500	-0.96953500	0.40846700	C	4.97454000	0.41586700	-0.71623700
C	2.09971100	-2.05764300	1.07378500	C	4.55510600	1.42980200	-1.51852900
C	3.46273700	-2.36202200	1.25784900	C	3.16168500	1.67101500	-1.71566600
H	5.48103600	-1.75427200	0.86723000	H	6.03424400	0.21795000	-0.57640500
H	3.72502300	-3.25457000	1.81787200	H	5.26824300	2.06498600	-2.03712400
O	0.82284600	-3.92955800	0.65655300	C	2.66794900	2.66814000	-2.57892100
C	-2.71037000	0.33633000	-1.30586800	C	1.31033600	2.81782500	-2.74221200
N	-1.93264500	0.87412200	-0.34689600	C	0.44140400	1.98930600	-2.02323200
C	-2.17486000	2.05055200	0.26371000	N	0.87811500	1.04965900	-1.19120500
C	-3.31144700	2.76366600	-0.09905800	C	2.21914500	0.87152600	-1.03817900
H	-3.54670100	3.71675100	0.36212100	H	3.36847200	3.30353600	-3.11517600
C	-1.11657400	-3.29426400	-2.74958000	H	0.89716000	3.56550500	-3.41000200
C	-0.51013100	-2.54728900	-1.74546100	H	-0.63445700	2.10082900	-2.13282900
N	-1.03810300	-1.39790100	-1.31481900	C	1.03733200	-3.04865900	1.49989800
C	-2.20728700	-0.93650700	-1.85075400	C	-4.14602000	2.23282500	-1.07870100
C	-2.85129100	-1.64096600	-2.85361800	H	-5.03595500	2.78101700	-1.37128100
C	-2.29678300	-2.83332800	-3.31062200	C	-3.85587600	1.01949700	-1.69617400
H	-0.65888800	-4.22203200	-3.07481900	H	-4.51133000	0.62434300	-2.46450400
H	0.39386700	-2.88676500	-1.24475400	O	0.46460500	-2.84967700	2.60521500
H	-3.77779500	-1.26830400	-3.27795500	O	-1.15817000	-0.82844900	1.62331600
H	-2.79200400	-3.39243800	-4.09834700	O	-1.79663500	-2.45393500	1.61770300
C	0.84852300	3.05911300	3.03546400	H	-2.55630000	-2.25068200	2.25152800
C	-0.20383200	3.94602600	2.86696600	H	-0.98756900	-2.80256300	2.15523800
C	-1.21774800	3.64283400	1.96345600	O	-3.75482600	-1.72920400	3.18977500
C	-1.15429400	2.45726700	1.24668300	H	-3.48445400	-1.64632500	4.11165300
N	-0.10946100	1.60013600	1.41927100	H	-4.51761500	-2.31884300	3.20449700
C	0.85993000	1.88705800	2.28856800				

²TS2

Ru	0.02947300	-0.13688800	-0.18102300	H	0.65764800	-3.16240400	0.40567800
C	4.75704600	-1.14747200	-1.16596600	C	5.26975600	0.09189100	0.93984700
C	4.34980500	-0.45393600	-0.00731600	C	4.83144400	0.73246400	2.05587300
C	2.96746700	-0.30701100	0.20240700	C	3.43280600	0.88254000	2.30358000
N	2.03121000	-0.82889500	-0.64608800	H	6.33345500	-0.02750400	0.74877200
C	2.43539000	-1.54208300	-1.69769300	H	5.53281300	1.13749900	2.78078600
C	3.80710700	-1.67781400	-1.99792000	C	2.91371300	1.51175200	3.45119200
H	5.81810500	-1.25996200	-1.37673600	C	1.55084000	1.61035700	3.62021500
H	4.07334100	-2.22533100	-2.89655100	C	0.70257100	1.09579600	2.63446300
O	0.67957200	-3.06252000	-1.90589100	N	1.16550400	0.49968600	1.53992600
C	-1.87455200	1.98396200	0.30828900	C	2.50889100	0.37764100	1.36617300
N	-1.66002900	0.67487400	0.53617700	H	3.59848600	1.91174800	4.19509900
C	-2.45370700	-0.09689000	1.30477600	H	1.12022000	2.08351500	4.49584700
C	-3.58759100	0.46657500	1.87680400	H	-0.37689000	1.17504500	2.74116500
H	-4.25378000	-0.12548400	2.49434200	O	-0.61685800	-0.71818600	-1.78146700
C	1.21786000	3.68338300	-2.00952300	C	1.43437500	-2.30922300	-2.56031600
C	1.22406800	2.36314800	-1.58355400	C	-3.85189700	1.81330400	1.64032700
N	0.22739400	1.85609200	-0.85099000	H	-4.73253700	2.26909600	2.08194000
C	-0.83568300	2.63594800	-0.50533900	C	-2.99883100	2.58709100	0.86181500
C	-0.89739600	3.96170000	-0.90857900	H	-3.20602900	3.63787600	0.69310900
C	0.14192600	4.49036800	-1.66470100	O	1.54496600	-2.13581800	-3.78556700
H	2.04350900	4.05940700	-2.60340400	O	-2.08746500	-0.02785200	-2.31852300
H	2.03722500	1.68751300	-1.83530300	H	-1.92267700	-0.15504000	-3.26873500
H	-1.75448500	4.57216600	-0.64552200	O	-3.32165500	-1.85801500	-1.39030900
H	0.10595900	5.52685100	-1.98524900	H	-3.46234500	-2.60183500	-1.98999800
C	-0.92955800	-4.01732500	1.62998600	H	-4.18459500	-1.64976200	-0.92049200
C	-2.15011900	-3.74216400	2.22857600	H	-2.76363000	-0.93168400	-1.91925700
C	-2.68515600	-2.46024000	2.14077400	O	-5.42001400	-1.30682400	0.06203400
C	-1.97601400	-1.48029900	1.46579900	H	-6.05744700	-2.02644900	0.13995900
N	-0.77209000	-1.76511300	0.89056600	H	-5.93433600	-0.54398600	-0.22755700
C	-0.26470100	-2.99916500	0.95684700	O	-3.52503000	2.63368100	-2.19321200
H	-0.49115000	-5.00854400	1.66868000	H	-3.14354600	1.75033400	-2.28701900

H -2.69354800 -4.52062900 2.75526100

H -3.20088900 3.10673200 -2.96585500

H -3.65087200 -2.23411900 2.58136400

1-closedTS3

Ru	2.39684000	-0.28490900	0.33010200	Ru	2.94502200	-0.38920000	-0.05158400
C	3.93767200	4.02062800	-1.52256300	C	0.21620400	0.82581700	3.72229100
C	4.68381500	2.85444200	-1.78008000	C	0.84005700	1.84820100	2.97063900
C	4.13372100	1.62443700	-1.36660900	C	1.60344200	1.44257500	1.86583000
N	2.93366600	1.54449600	-0.74972100	N	1.70944800	0.14986800	1.50329800
C	2.21977500	2.65569400	-0.56691500	C	1.25431200	-0.81251600	2.30910900
C	2.69583300	3.91551600	-0.93393500	C	0.47556200	-0.49863800	3.42665400
H	4.33982400	4.98967100	-1.80712400	H	0.39359100	1.09243800	4.58198300
H	2.05934400	4.77407700	-0.74327100	H	0.08789400	-1.31355200	4.03030700
O	0.64700000	1.16435500	0.21979100	O	2.90431300	-2.09941900	1.23350200
C	2.34712500	-3.15270100	0.22335500	C	5.59203900	-1.38202300	-1.00588600
N	3.05422900	-2.14599200	0.77029100	N	4.43919700	-0.85593600	-1.44160900
C	4.01780100	-2.27985200	1.69317500	C	4.16902800	-0.68058500	-2.74684000
C	4.34991500	-3.56537600	2.10937000	C	5.05571200	-1.16383100	-3.70141600
H	5.12646100	-3.73298000	2.84773300	H	4.88602400	-0.98430000	-4.75785000
C	0.02038000	-1.75246100	-2.96599700	C	6.14660100	-0.39516800	3.04107500
C	0.56380700	-0.90721900	-2.03221500	C	4.99145500	-0.10558800	2.33084200
N	1.21094200	-1.38600700	-0.96827700	N	4.84081300	-0.48085400	1.05884500
C	1.38046500	-2.73584300	-0.80824400	C	5.82310400	-1.16255700	0.42519900
C	0.78675800	-3.62057100	-1.69329900	C	6.99923500	-1.49170300	1.08570400
C	0.07897700	-3.12298100	-2.78469200	C	7.15880500	-1.10746700	2.41095400
H	0.54709100	-1.32545400	-3.81335300	H	6.23623300	-0.06948200	4.07142000
H	0.45296000	0.17308200	-2.07925500	H	4.16562100	0.42593200	2.79513900
H	0.89839900	-4.69031300	-1.55164800	H	7.78398200	-2.03226500	0.56699700
H	0.37775700	-3.80893600	-3.49099300	H	8.07341300	-1.35334300	2.94135000
C	5.48225600	1.44576000	3.02869400	C	1.15616500	2.19693900	-3.26711500
C	5.99605200	0.29636300	3.60805600	C	1.59121700	1.52121300	-4.40045300
C	5.53503700	-0.94671600	3.18357600	C	2.54467400	0.51578000	-4.27071100
C	4.58575000	-1.01130400	2.17666700	C	3.01983500	0.19733800	-3.00511000
N	4.10728400	0.12876900	1.59461400	N	2.51727400	0.80544400	-1.90232700
C	4.52196300	1.31950800	2.03230200	C	1.63871000	1.80076600	-2.02354400
H	5.80051500	2.43413800	3.34063100	H	0.44859400	3.01871400	-3.32629200

H	6.74317500	0.35846800	4.39276400	H	1.19903200	1.77557900	-5.38025700
H	5.91457400	-1.85619600	3.63741200	H	2.91154000	-0.01619800	-5.14323900
H	4.07076500	2.19751300	1.57722300	H	1.30264300	2.29896100	-1.11277000
C	5.94793000	2.84410200	-2.44821500	C	0.82583000	3.24062200	3.29140200
C	6.58112800	1.67268700	-2.72308800	C	1.61724700	4.12707000	2.61862500
C	6.00738200	0.41463400	-2.35055800	C	2.51490500	3.69154500	1.59284900
H	6.38148300	3.79528400	-2.74502000	H	0.19807500	3.57680800	4.11237000
H	7.53346300	1.66709100	-3.24669300	H	1.61909800	5.17846400	2.89366900
C	6.56261700	-0.83158800	-2.69469200	C	3.47741000	4.50053200	0.96106900
C	5.89510900	-1.98063000	-2.33957100	C	4.36864100	3.93143500	0.07202700
C	4.70847000	-1.89078300	-1.59979200	C	4.32079100	2.55461700	-0.17814400
N	4.17008500	-0.73298300	-1.23323900	N	3.40974100	1.77616000	0.39671000
C	4.79744900	0.40341800	-1.63421100	C	2.49975100	2.33480700	1.22973400
H	7.49885000	-0.87362100	-3.24528100	H	3.52632300	5.56140800	1.19297400
H	6.26949200	-2.96165100	-2.61033300	H	5.12497800	4.52890600	-0.42481000
H	4.20171000	-2.80597000	-1.31003900	H	5.02833700	2.08295800	-0.85613300
O	1.41991200	-0.59043100	1.72911200	O	1.89139100	-1.45990000	-0.92504700
C	0.85371800	2.40923500	-0.00922000	C	1.91086200	-2.14655900	2.07915200
C	3.64623000	-4.63982900	1.57349600	C	6.19161900	-1.84246600	-3.27124100
H	3.88498900	-5.64712800	1.89898000	H	6.88094800	-2.25553600	-4.00058000
C	2.63601900	-4.44984800	0.63253500	C	6.48569100	-1.93624100	-1.91554000
H	2.09760600	-5.29992200	0.22800000	H	7.40532500	-2.40418000	-1.58088300
O	0.03180800	3.31367900	0.11101100	O	1.59343100	-3.13006500	2.72352000

1-openⁿTS3

Ru	-2.07276900	-0.27268900	-0.07308000	Ru	2.51328300	-0.13277900	0.21436400
C	-4.60682700	3.61234700	-1.61202700	C	0.53831900	3.98614300	1.72797000
C	-5.29351800	2.44809700	-1.21559000	C	1.45749200	4.01268600	0.65578200
C	-4.51859500	1.32176500	-0.87983500	C	2.02648100	2.78174200	0.30548600
N	-3.17079300	1.33801200	-0.92657000	N	1.68669500	1.63486100	0.90475200
C	-2.54316200	2.43007200	-1.35459200	C	0.93909600	1.62970200	1.99394300
C	-3.23067000	3.59350600	-1.70252200	C	0.32225200	2.80889700	2.42748100
H	-5.17037100	4.50547400	-1.86887700	H	0.05567700	4.90770500	2.04377100
H	-2.65227400	4.44750200	-2.04138600	H	-0.29039200	2.77592000	3.32427400
O	-0.73747500	1.02666400	-1.10824700	O	1.90731600	-0.49428400	2.23375500
C	-1.79432400	-3.10839800	0.39049100	C	4.31239500	-2.46387100	0.53396900
N	-2.20237600	-1.98517600	1.00869100	N	3.45135100	-1.91059200	-0.33368700
C	-2.45452300	-1.87691500	2.32231800	C	3.17744900	-2.46937200	-1.52227200
C	-2.37890000	-3.02539400	3.10311200	C	3.62808600	-3.75494100	-1.80204200
H	-2.58842200	-2.99488400	4.16656000	H	3.40294400	-4.22993000	-2.75102400
C	-1.12913800	-2.47229000	-3.72716900	C	5.61491800	0.47540700	3.24142800
C	-1.39131900	-1.44258200	-2.83056300	C	4.68564300	0.70992900	2.24044500
N	-1.58465300	-1.68585500	-1.53538700	N	4.28010400	-0.26530800	1.42162000
C	-1.51792800	-2.95585300	-1.04866500	C	4.75671700	-1.52667800	1.56743900
C	-1.23340300	-4.01760500	-1.89250200	C	5.67552100	-1.82548700	2.56364300
C	-1.03877600	-3.77077000	-3.24870700	C	6.10686600	-0.81292200	3.41043400
H	-0.99966200	-2.24559400	-4.78017600	H	5.93233100	1.29484500	3.87664800
H	-1.44637100	-0.40129500	-3.13877600	H	4.25524300	1.69568000	2.08956400
H	-1.17961400	-5.02916800	-1.50357700	H	6.05297700	-2.83702900	2.67172300
H	-0.82608700	-4.59357600	-3.92384700	H	6.82540500	-1.02928900	4.19462800
C	-3.20470000	2.09586500	3.53173200	C	1.47721900	0.39293600	-4.09158900
C	-3.31960800	1.09049600	4.47928500	C	1.70995500	-0.87443500	-4.60690900
C	-3.08870900	-0.22813200	4.10348300	C	2.22915800	-1.86201500	-3.77784300
C	-2.75026400	-0.51143500	2.78916900	C	2.52431200	-1.54958300	-2.45775100
N	-2.65247500	0.48427600	1.86425700	N	2.31976200	-0.29654100	-1.97804400
C	-2.86450000	1.74978100	2.22918200	C	1.78947300	0.64431500	-2.76149900
H	-3.36974200	3.13825200	3.78204300	H	1.05920300	1.18907500	-4.69855700

H	-3.58501900	1.32462100	5.50538100	H	1.48434300	-1.10008600	-5.64509900
H	-3.17319100	-1.02656700	4.83310000	H	2.40723400	-2.86355400	-4.15669800
H	-2.75191200	2.50875100	1.45813000	H	1.59189700	1.61972300	-2.32101000
C	-6.71728200	2.32178900	-1.16038600	C	1.91790000	5.16626600	-0.05953700
C	-7.29919900	1.13352200	-0.84420500	C	2.93623200	5.07109500	-0.96266800
C	-6.51378000	-0.02889300	-0.55261900	C	3.61429500	3.82923700	-1.21199900
H	-7.32271900	3.19207100	-1.39819400	H	1.45895500	6.12897600	0.14895400
H	-8.38142800	1.03653400	-0.82482100	H	3.28829100	5.95707300	-1.48451200
C	-7.05193400	-1.30332000	-0.29944600	C	4.76148000	3.66269000	-2.01070500
C	-6.19250400	-2.35590900	-0.08648000	C	5.36380100	2.42153100	-2.08524600
C	-4.80829700	-2.13949000	-0.08441700	C	4.82995600	1.33298300	-1.38263100
N	-4.26434300	-0.94348100	-0.29190100	N	3.73345200	1.46211300	-0.64236500
C	-5.11417700	0.08849100	-0.54404800	C	3.13159400	2.68048000	-0.57043400
H	-8.12910700	-1.44639500	-0.29099200	H	5.17639800	4.51160000	-2.54800300
H	-6.55970600	-3.36108800	0.08830500	H	6.25817500	2.26844200	-2.67915000
H	-4.14905300	-2.98061900	0.09687200	H	5.29119400	0.34902500	-1.42680200
O	-0.43082100	-0.39708700	0.83430400	O	0.89555900	-1.01924600	-0.09457700
C	-1.07509200	2.22459000	-1.47310200	C	0.99954200	0.31555300	2.72022300
C	-2.00668800	-4.22118500	2.49524400	C	4.40418300	-4.40747800	-0.85013200
H	-1.94054300	-5.12413400	3.09361200	H	4.75720800	-5.41567500	-1.04161600
C	-1.69703700	-4.27526900	1.13891400	C	4.79415000	-3.74866800	0.31095000
H	-1.37992100	-5.20718500	0.68361400	H	5.47852400	-4.21702900	1.01013200
O	-0.30436300	3.06779000	-1.90385700	O	0.32254500	0.09717600	3.70959900

³TS3

Ru	-2.27477300	-0.37685900	-0.05547000	O	-0.21164400	3.38016300	-1.55663300
C	-4.35515200	3.98755600	-0.72794600	Ru	2.47592600	-0.09326400	0.22630600
C	-5.12303200	2.81650000	-0.57771700	C	0.78653100	4.18318400	1.62535000
C	-4.42562500	1.59290500	-0.52484700	C	1.77491900	4.13181900	0.61817000
N	-3.07863300	1.52529500	-0.63292000	C	2.26198900	2.85758400	0.30127300
C	-2.38451000	2.63366800	-0.88885400	N	1.79885100	1.74818200	0.88805200
C	-2.98975300	3.89386400	-0.90534200	C	0.98956300	1.80774700	1.93261100
H	-4.85170800	4.95423100	-0.74813000	C	0.43149400	3.03343500	2.31470400
H	-2.37009100	4.76317500	-1.10190600	H	0.35516300	5.14151200	1.90357700
O	-0.65327500	1.21981800	-1.63292700	H	-0.23855900	3.06301300	3.16828100
C	-1.41008800	-3.15871800	-0.15143500	O	1.77625600	-0.38874200	2.22223000
N	-1.88097700	-2.21580700	0.68632700	C	3.99970600	-2.59987600	0.59750000
C	-2.01705600	-2.39309700	2.01493300	N	3.22220200	-1.96292600	-0.29097800
C	-1.64412000	-3.61164100	2.57013000	C	2.87349800	-2.50600300	-1.46789000
H	-1.73562000	-3.79160300	3.63562500	C	3.16459700	-3.84199400	-1.72043300
C	-1.65553900	-1.85041000	-4.14465700	H	2.88611600	-4.30705400	-2.66015700
C	-1.89163800	-1.02121300	-3.05542300	C	5.55677200	0.19374600	3.32878000
N	-1.77367000	-1.46503400	-1.80026100	C	4.67456700	0.52369800	2.31200300
C	-1.41043200	-2.75530300	-1.56270800	N	4.18693000	-0.40325600	1.48222300
C	-1.13897400	-3.62158600	-2.61141900	C	4.52838000	-1.70793600	1.63244700
C	-1.26975300	-3.16390800	-3.91837400	C	5.39407600	-2.10003400	2.64344000
H	-1.77223400	-1.45652500	-5.14871800	C	5.91182900	-1.13827900	3.50122900
H	-2.17471500	0.01944200	-3.17760100	H	5.94339000	0.97423500	3.97454200
H	-0.85197200	-4.64922300	-2.41344400	H	4.34609600	1.54724900	2.15727000
H	-1.07270100	-3.83351600	-4.74999900	H	5.66341200	-3.14497200	2.75605400
C	-3.50748900	1.04787400	3.95207500	H	6.58884300	-1.42952600	4.29806100
C	-3.28166100	-0.08500700	4.71864500	C	1.49820900	0.48238400	-4.09112100
C	-2.79464200	-1.23620300	4.10935800	C	1.50716100	-0.82387300	-4.55518000
C	-2.55931000	-1.23440100	2.74316100	C	1.92455700	-1.84671600	-3.70918400
N	-2.81692900	-0.12405400	1.99858600	C	2.32240200	-1.53423500	-2.41842000
C	-3.25699300	0.99045700	2.58749100	N	2.31495900	-0.24837600	-1.98052700
H	-3.87027200	1.97096100	4.39043300	C	1.90472700	0.73033300	-2.78530000

H	-3.47257700	-0.07652600	5.78701000	H	1.17862500	1.30906500	-4.71610800
H	-2.59800400	-2.12522700	4.69889100	H	1.19196000	-1.05348400	-5.56894400
H	-3.39804300	1.86138100	1.95257500	H	1.93820200	-2.87711400	-4.05202700
C	-6.55079100	2.79744600	-0.49403000	H	1.88223500	1.73848100	-2.37817000
C	-7.22826900	1.62127700	-0.40433800	C	2.36120000	5.24061300	-0.07453000
C	-6.53708300	0.36676700	-0.37528600	C	3.40836100	5.05815200	-0.92987400
H	-7.08275300	3.74467900	-0.52097100	C	3.98626200	3.76248900	-1.15625600
H	-8.31409000	1.61015100	-0.36016600	H	1.97110300	6.23776500	0.11096200
C	-7.18204000	-0.88446200	-0.32014500	H	3.85587400	5.91003400	-1.43509200
C	-6.42904100	-2.03779600	-0.30742200	C	5.13740100	3.49782400	-1.92301500
C	-5.03102300	-1.94966700	-0.32782000	C	5.62598000	2.20787300	-1.99338400
N	-4.39822200	-0.78221800	-0.37633900	C	4.97477600	1.16748200	-1.31655100
C	-5.13361800	0.36085300	-0.40994400	N	3.87604700	1.39073200	-0.60356000
H	-8.26774200	-0.92777000	-0.29188200	C	3.38565100	2.65897800	-0.53520100
H	-6.89577400	-3.01600900	-0.27250800	H	5.64171700	4.30949700	-2.44137800
H	-4.41725200	-2.84705000	-0.29987400	H	6.51808400	1.97815500	-2.56581900
O	-0.63971400	0.18430300	0.53365700	H	5.34325600	0.14489100	-1.35802300
C	-0.96969300	2.43816400	-1.34376700	O	0.82139300	-0.79643500	-0.09395300
C	-1.13815500	-4.60150100	1.73306000	C	0.92970000	0.50078300	2.67693100
H	-0.83450800	-5.55415000	2.15517600	C	3.85665900	-4.56357700	-0.75328700
C	-1.02113200	-4.38933900	0.36358200	H	4.08457700	-5.61066200	-0.92528700
H	-0.63266400	-5.16785000	-0.28411500	C	4.31989800	-3.93853600	0.39964500
O	0.23187700	0.34810400	3.66349800	H	4.93332200	-4.48056200	1.11138100