

–Electronic Supporting Information–

Systematic Modulation of a Bichromic
Cyclometalated Ru(II) Scaffold Bearing a
Redox-Active Triphenylamine Constituent

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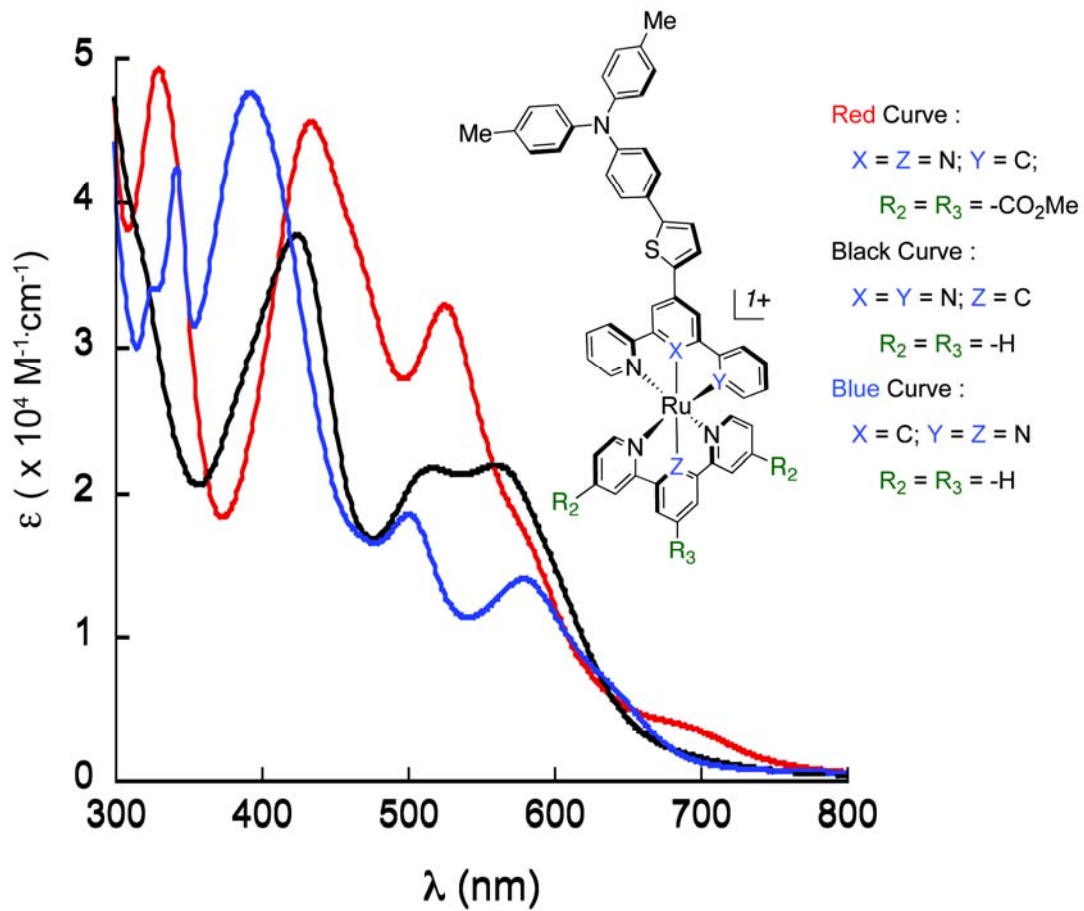
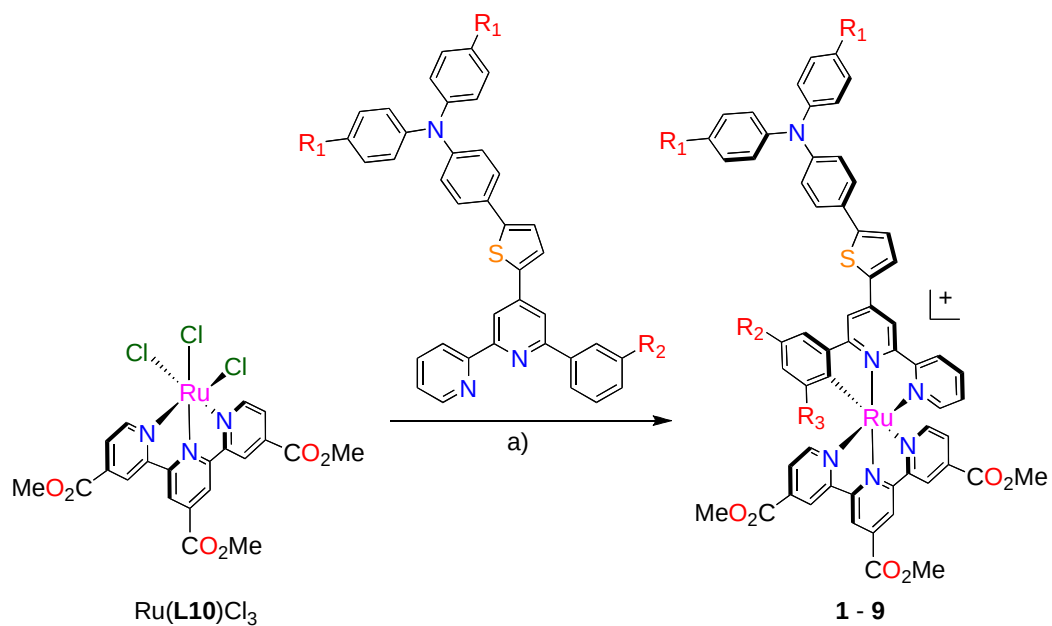


Figure S1. UV-vis absorption spectra in MeOH C = X (blue), Y (red) and Z (black) highlighting the effect that the *position* of the Ru-C bond has on the absorption profile.

Scheme S1. Assembly of Complexes **1 - 9**.^a



^aReaction conditions: a) MeOH/H₂O/THF (5:1:1 v/v/v), *N*-ethylmorpholine, 65 °C, N₂, 14 h, AgNO₃. Counterion for complexes **1 – 9** is NO₃[−].

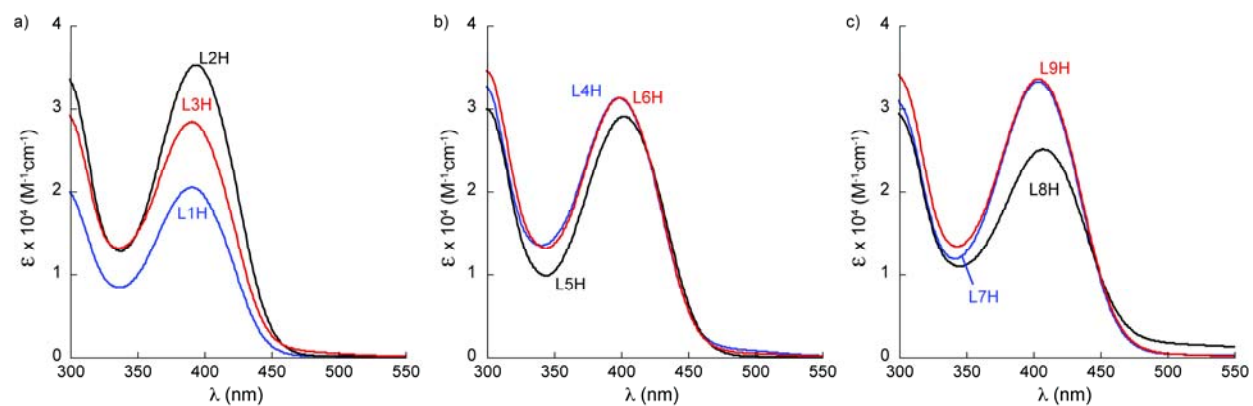


Figure S2. UV-vis absorption spectra of ligands in MeOH where: a) $-R_1 = -H$ (**L1H**, **L2H**, and **L3H**); b) $-R_1 = -Me$ (**L4H**, **L5H**, and **L6H**); and c) $-R_1 = -OMe$ (**L7H**, **L8H**, and **L9H**).

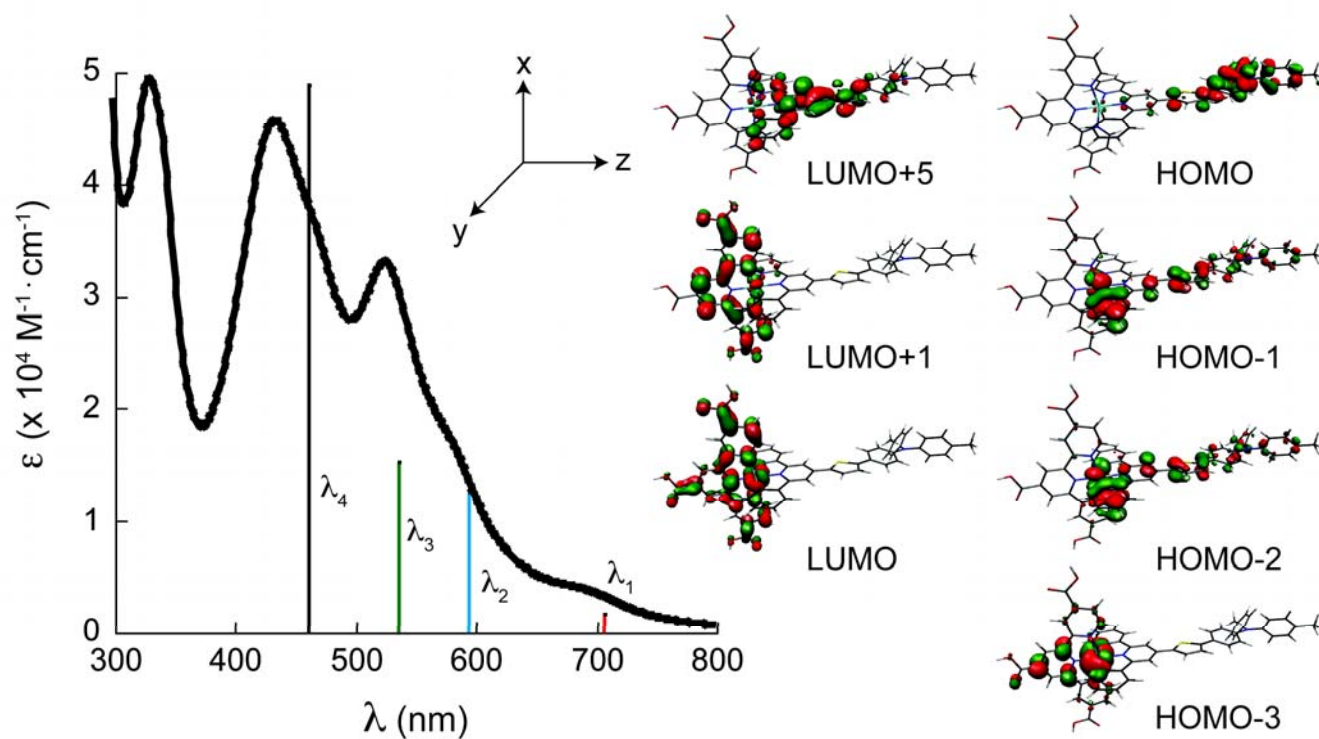


Figure S3. Experimental UV-vis absorption spectrum of **2** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >39% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (709, 0.013, 39%); λ_2 : HOMO $\rightarrow$ LUMO+1 (594, 0.092, 46%); λ_3 : HOMO-2 $\rightarrow$ LUMO (536, 0.108, 85%); λ_4 : HOMO $\rightarrow$ LUMO+5 (447, 0.343, 68%).

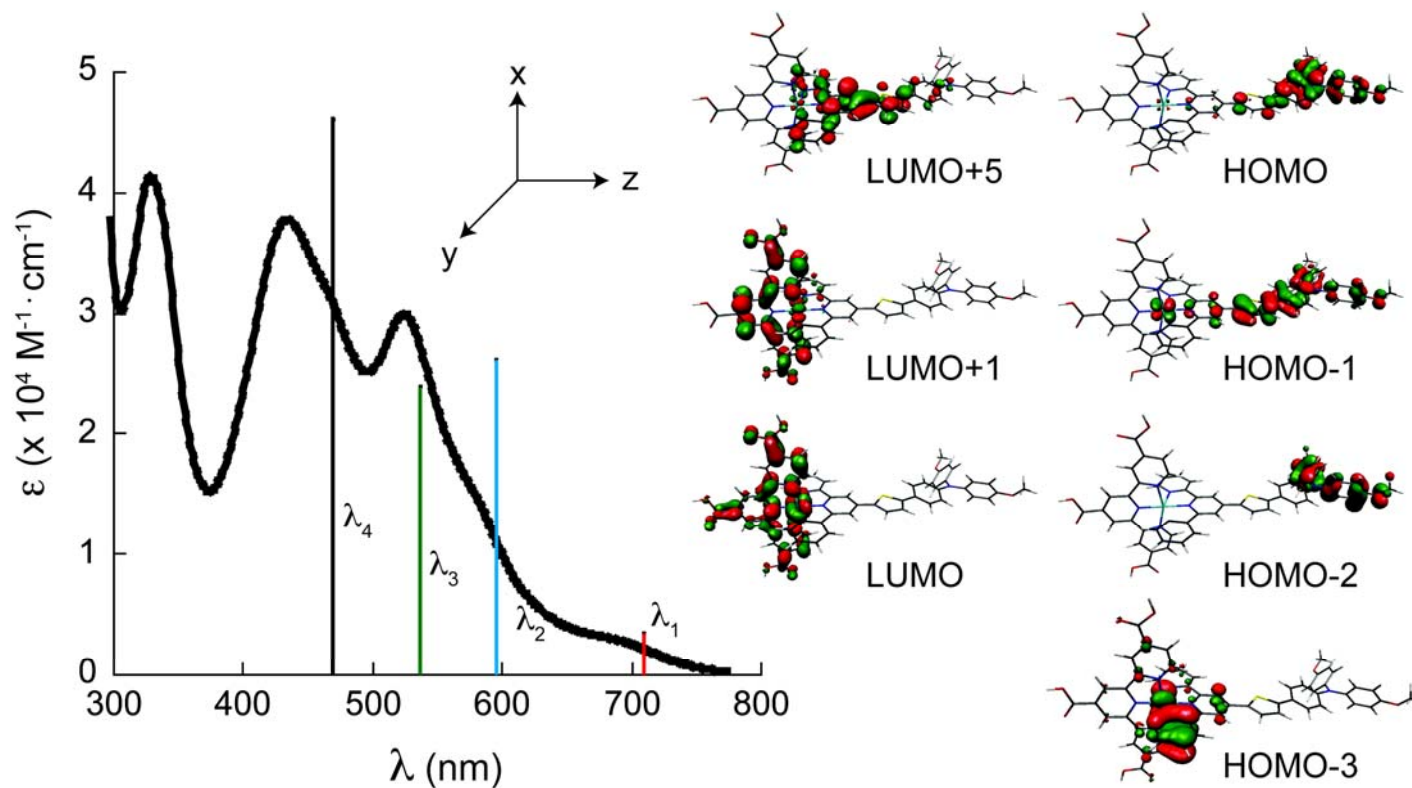


Figure S4. Experimental UV-vis absorption spectrum of **3** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >40% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (710, 0.027, 85%); λ_2 : HOMO-2 $\rightarrow$ LUMO (595, 0.210, 47%); λ_3 : HOMO-2 $\rightarrow$ LUMO+1 (537, 0.192, 74%); λ_4 : HOMO $\rightarrow$ LUMO+5 (469, 0.368, 78%).

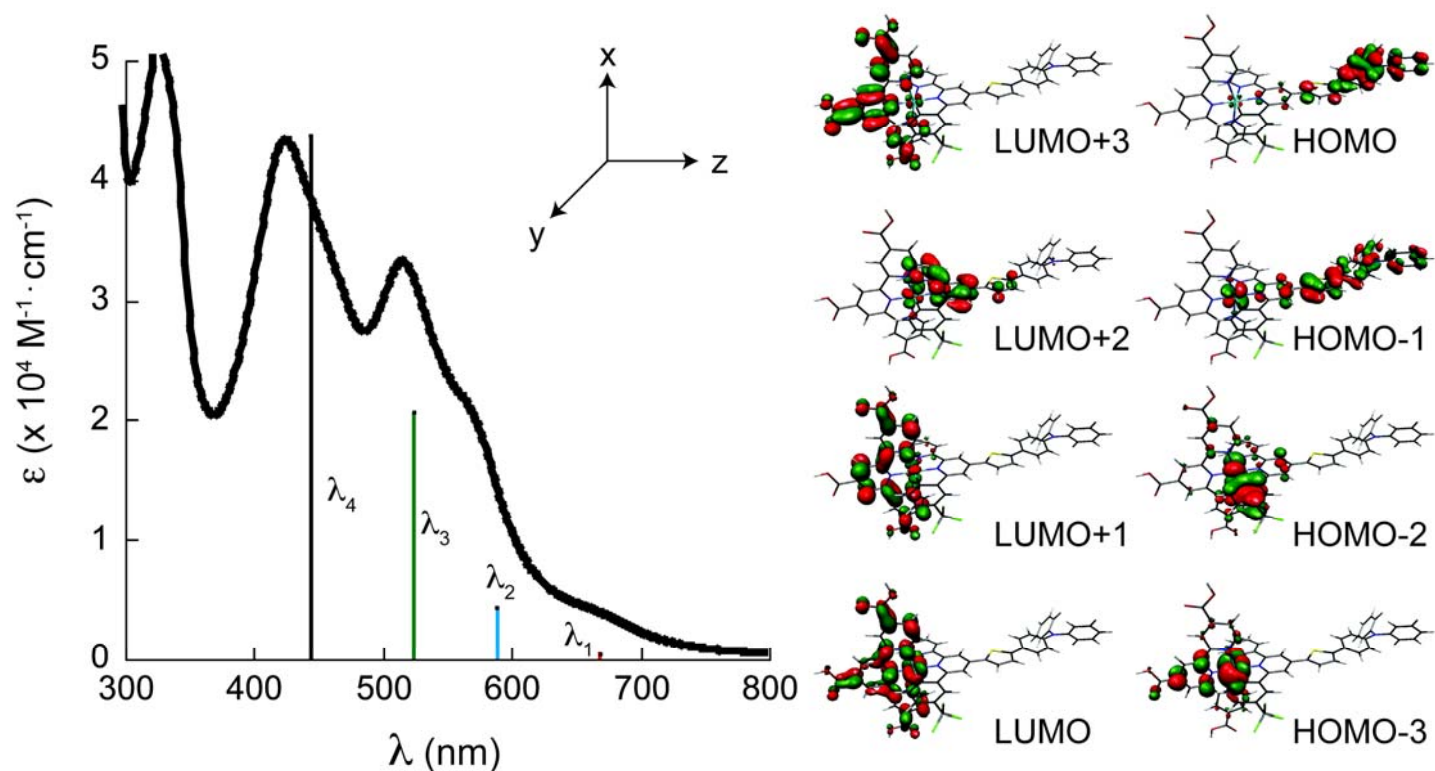


Figure S5. Experimental UV-vis absorption spectrum of **4** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >40% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (699, 0.027, 85%); λ_2 : HOMO $\rightarrow$ LUMO+1 (588, 0.027, 89%); λ_3 : HOMO-2 $\rightarrow$ LUMO+1 (524, 0.124, 88%); λ_4 : HOMO-3 $\rightarrow$ LUMO (443, 0.262, 54%).

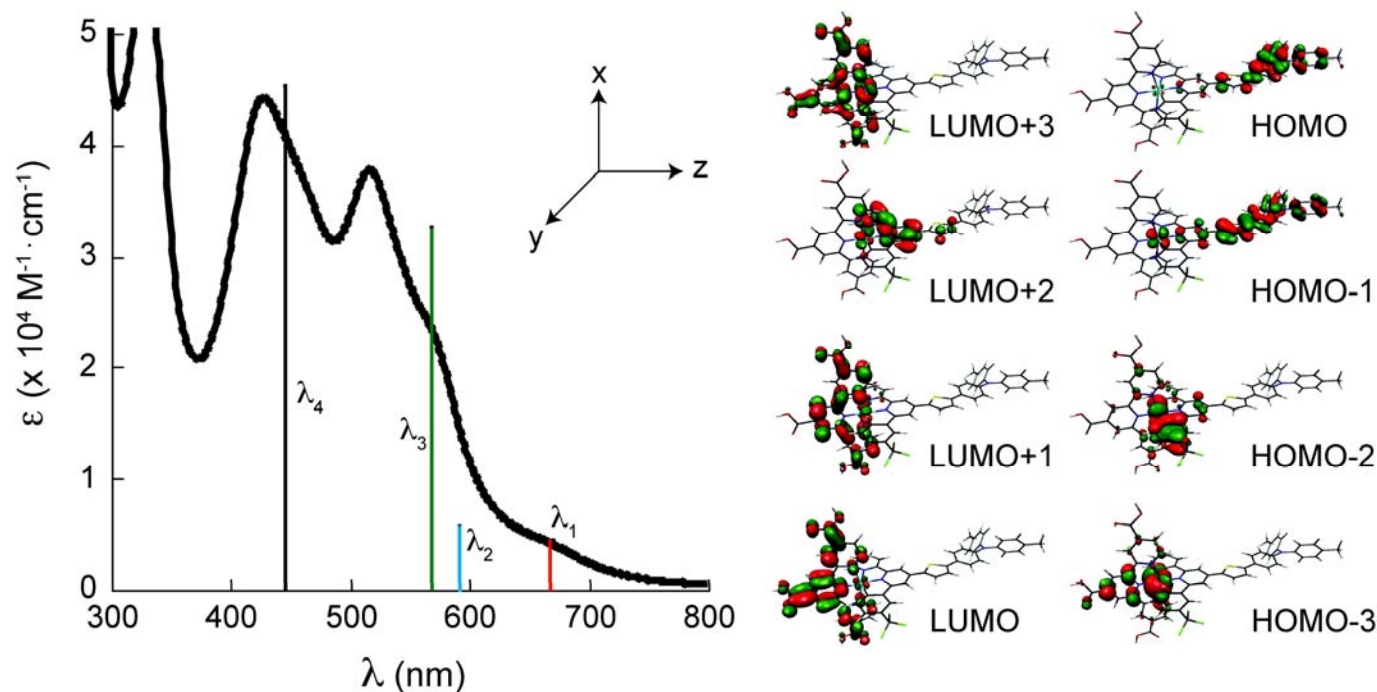


Figure S6. Experimental UV-vis absorption spectrum of **5** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >40% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (669, 0.027, 81%); λ_2 : HOMO-3 $\rightarrow$ LUMO (591, 0.035, 61%); λ_3 : HOMO-1 $\rightarrow$ LUMO+1 (567, 0.197, 32%) and HOMO-2 $\rightarrow$ LUMO (567, 0.197, 32%); λ_4 : HOMO-3 $\rightarrow$ LUMO+2 (445, 0.273, 53%).

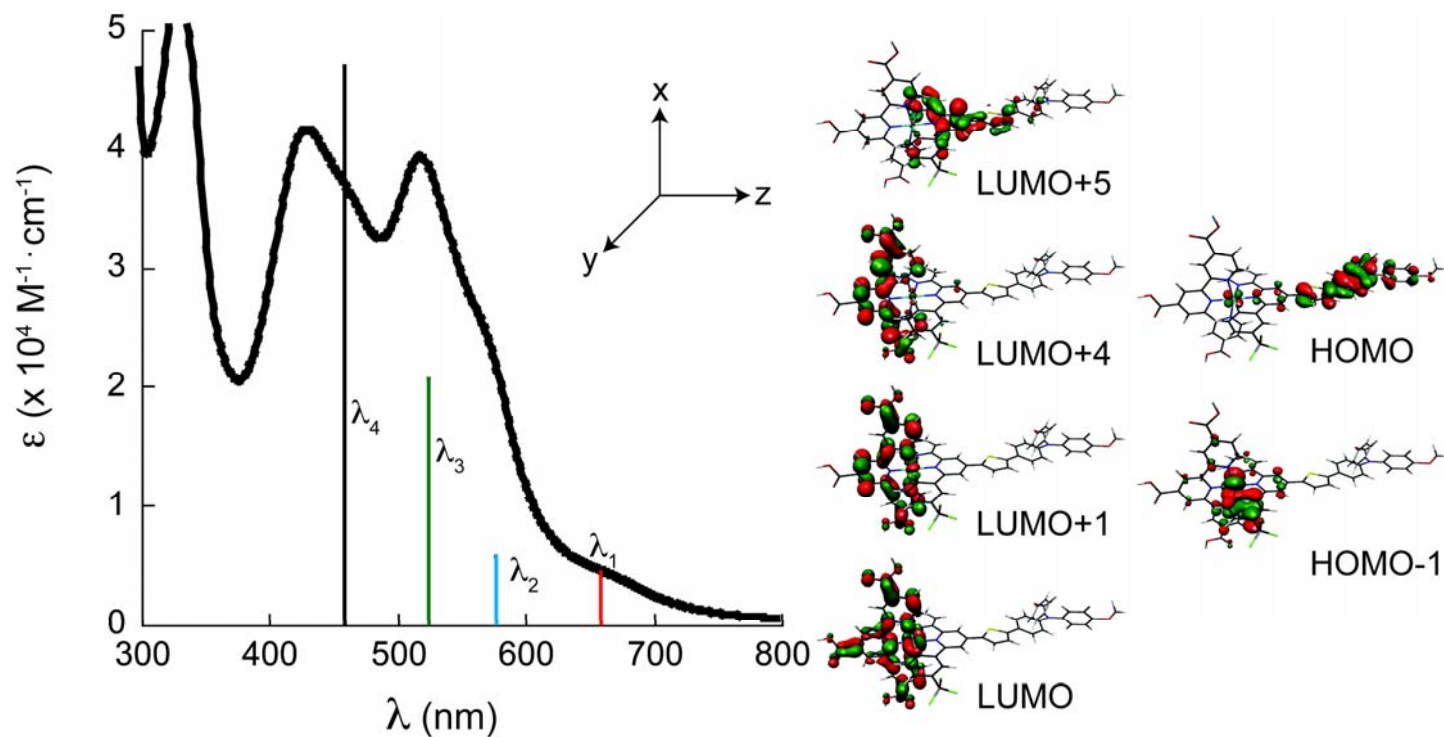


Figure S7. Experimental UV-vis absorption spectrum of **6** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >40% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (668, 0.026, 78%); λ_2 : HOMO-2 $\rightarrow$ LUMO (577, 0.035, 48%); λ_3 : HOMO-2 $\rightarrow$ LUMO+1 (524, 0.125, 83%); λ_4 : HOMO $\rightarrow$ LUMO+5 (459, 0.282, 50%).

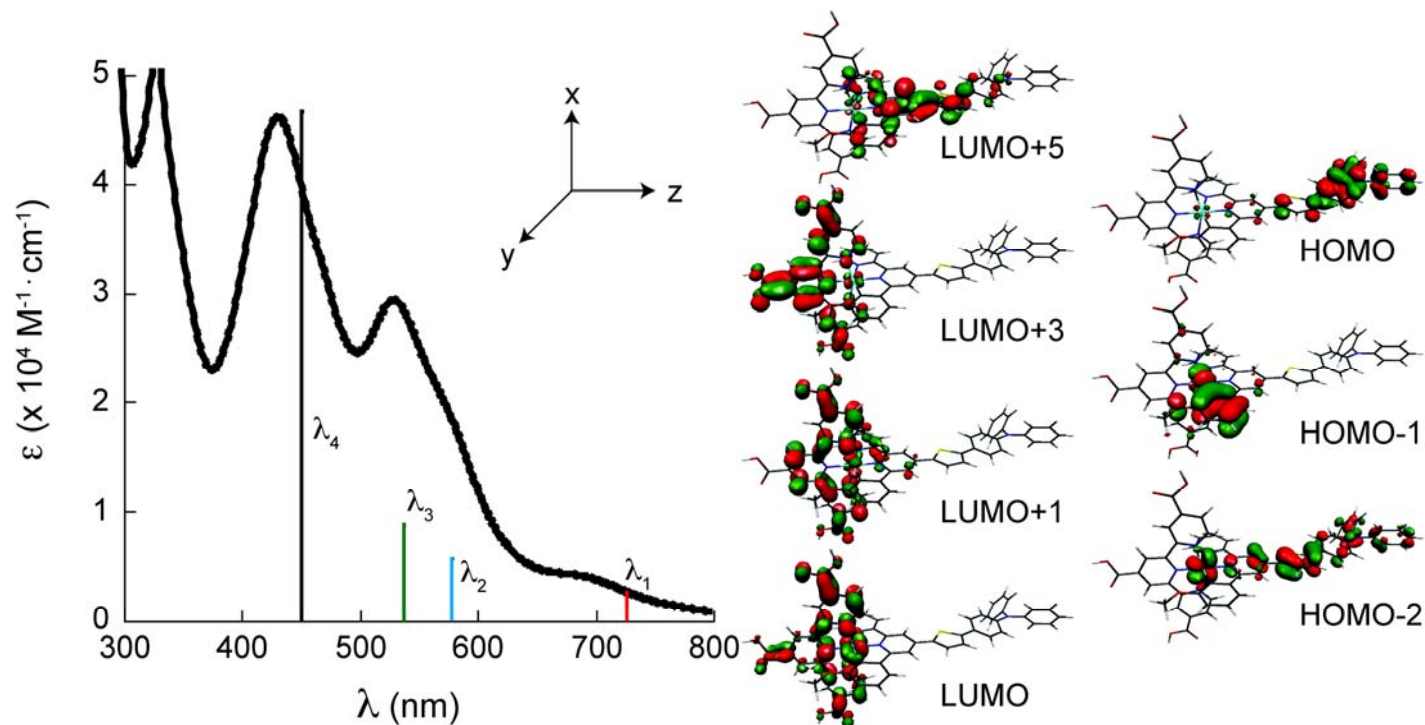


Figure S8. Experimental UV-vis absorption spectrum of **7** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >40% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (727, 0.028, 85%); λ_2 : HOMO $\rightarrow$ LUMO+1 (578, 0.058, 76%); λ_3 : HOMO-2 $\rightarrow$ LUMO+1 (536, 0.088, 84%); λ_4 : HOMO-2 $\rightarrow$ LUMO+3 (451, 0.467, 35%).

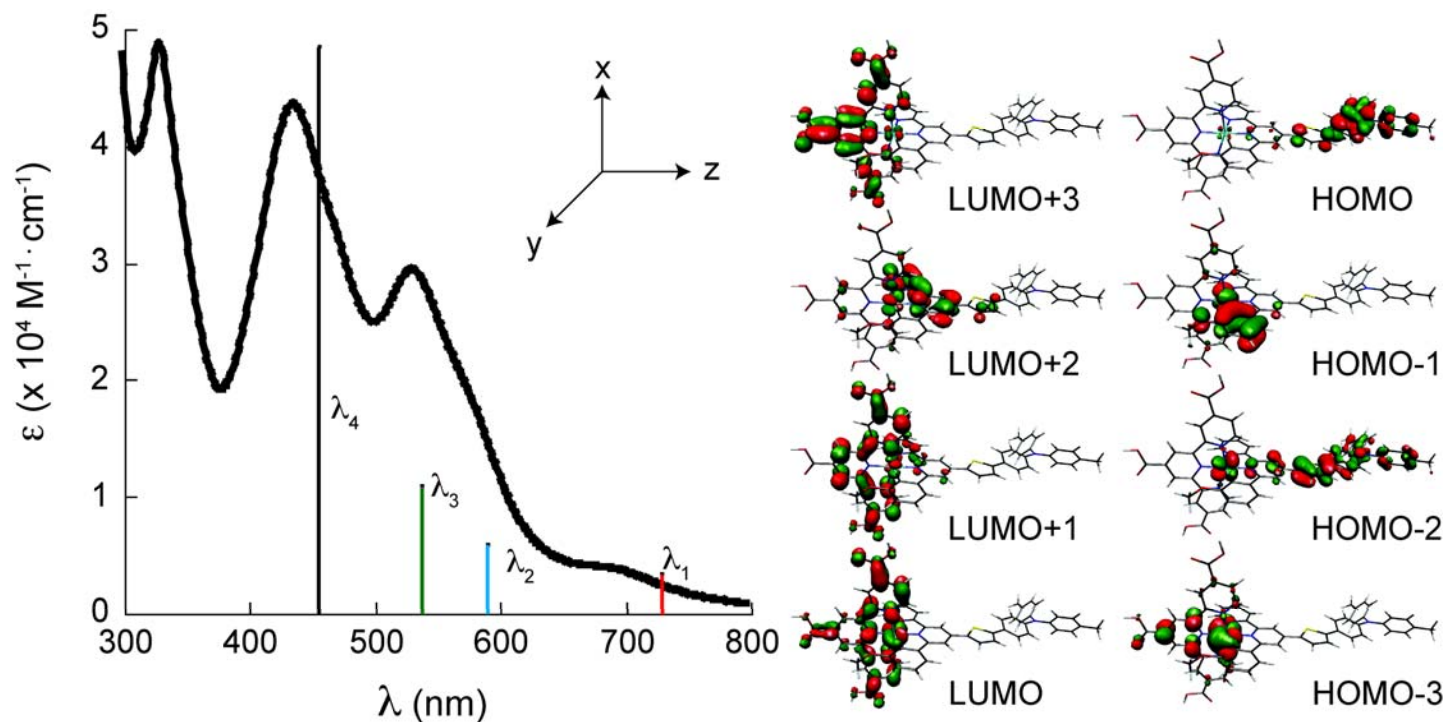


Figure S9. Experimental UV-vis absorption spectrum of **8** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >39% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (728, 0.028, 84%); λ_2 : HOMO $\rightarrow$ LUMO+1 (589, 0.048, 75%); λ_3 : HOMO-2 $\rightarrow$ LUMO+1 (537, 0.088, 83%); λ_4 : HOMO-3 $\rightarrow$ LUMO+2 (455, 0.389, 39%).

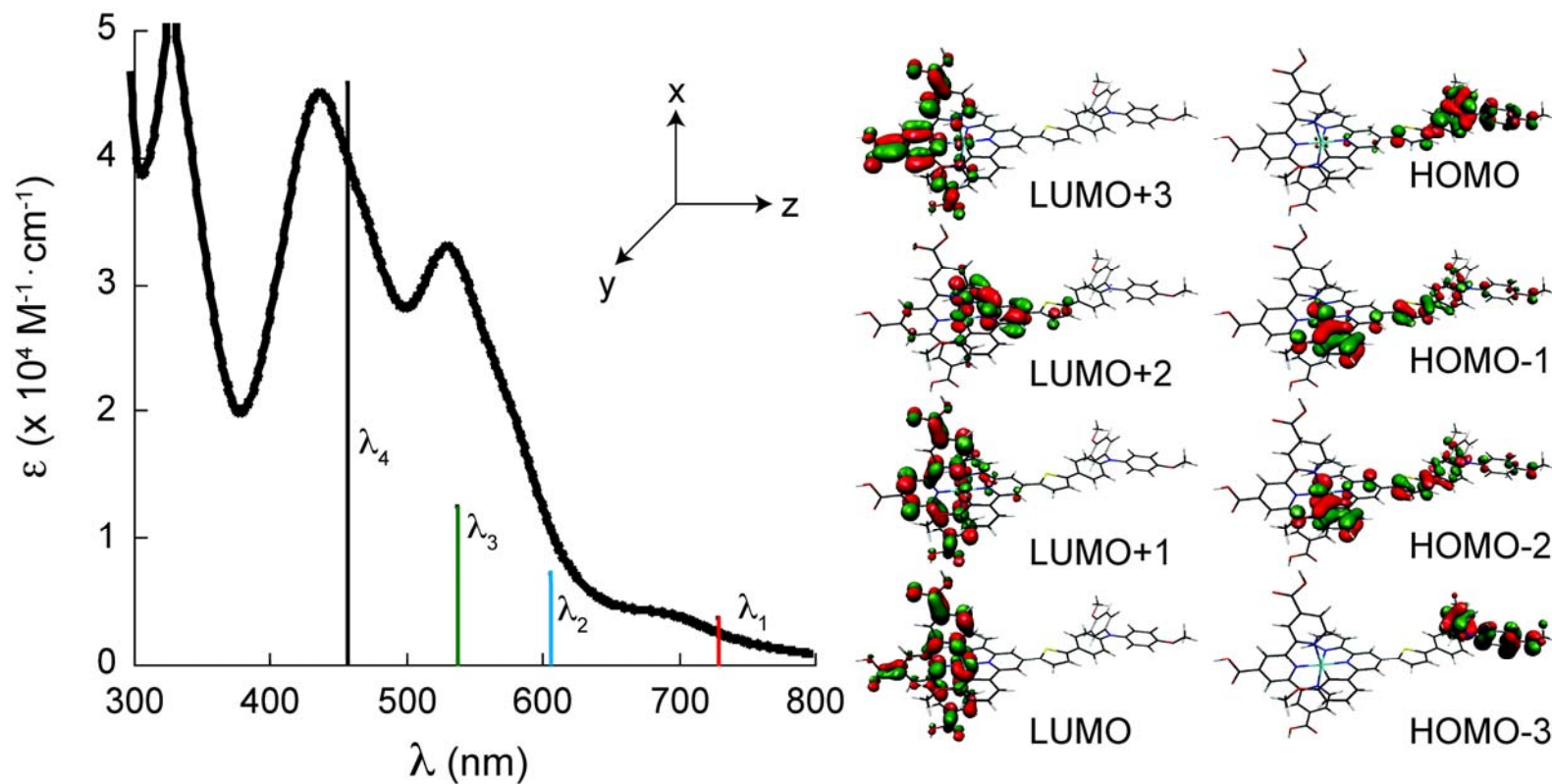


Figure S10. Experimental UV-vis absorption spectrum of **9** overlaid with calculated transitions represented by vertical bars (only the transitions with contributions >40% are shown). Details of calculated transitions (theoretical wavelength in nm, oscillator strength, % contribution to transition): λ_1 : HOMO-1 $\rightarrow$ LUMO (729, 0.027, 82%); λ_2 : HOMO-1 $\rightarrow$ LUMO+1 (605, 0.051, 41%); λ_3 : HOMO-2 $\rightarrow$ LUMO+1 (537, 0.087, 84%); λ_4 : HOMO-3 $\rightarrow$ LUMO+2 (457, 0.322, 45%).

Optimized Cartesian Coordinates for (1):

Ru	-3.721417000	-0.010298000	-0.002952000
C	-3.727970000	-0.269072000	-2.051320000
N	-1.700447000	-0.096221000	-0.395932000
N	-2.771069000	0.216237000	1.956613000
C	-4.832904000	-0.364208000	-2.917011000
H	-5.841259000	-0.299312000	-2.518274000
C	-4.664455000	-0.542490000	-4.297114000
H	-5.535759000	-0.612409000	-4.941673000
C	-3.379651000	-0.630943000	-4.850363000
H	-3.252708000	-0.768803000	-5.918606000
C	-2.263095000	-0.540530000	-4.019646000
H	-1.270885000	-0.610763000	-4.455902000
C	-2.422868000	-0.361130000	-2.632952000
C	-1.296415000	-0.259231000	-1.699215000
C	0.066346000	-0.304386000	-1.997987000
H	0.374005000	-0.419777000	-3.028091000
C	1.043322000	-0.192137000	-0.980133000
C	0.578463000	-0.026774000	0.349217000
H	1.291074000	0.060565000	1.158375000
C	-0.786732000	0.019269000	0.611874000
C	-1.396226000	0.190869000	1.942169000
C	-0.669952000	0.323253000	3.133476000

H	0.412206000	0.302217000	3.114254000
C	-1.344789000	0.482561000	4.344117000
H	-0.789116000	0.585644000	5.268890000
C	-2.744533000	0.507745000	4.347397000
H	-3.303032000	0.630230000	5.267320000
C	-3.420488000	0.371884000	3.136863000
H	-4.501892000	0.385562000	3.088566000
N	-4.151094000	-2.023977000	0.283506000
N	-5.654743000	0.068752000	0.287964000
N	-4.059711000	2.028350000	-0.220915000
C	-3.283449000	-3.070244000	0.236565000
H	-2.252283000	-2.818493000	0.031839000
C	-3.687295000	-4.385583000	0.427667000
H	-2.970376000	-5.194067000	0.381116000
C	-5.044160000	-4.650023000	0.677690000
C	-5.946837000	-3.584904000	0.720111000
H	-6.992982000	-3.795386000	0.906016000
C	-5.494638000	-2.279083000	0.518972000
C	-6.353781000	-1.096334000	0.523677000
C	-7.732570000	-1.057109000	0.722075000
H	-8.301453000	-1.958290000	0.907409000
C	-8.398372000	0.178692000	0.675296000
C	-7.674560000	1.356277000	0.422749000

H	-8.212920000	2.295311000	0.383088000
C	-6.298781000	1.287925000	0.227287000
C	-5.387507000	2.394317000	-0.061316000
C	-5.782216000	3.730303000	-0.184176000
H	-6.818135000	4.015760000	-0.058724000
C	-4.829992000	4.709145000	-0.477018000
C	-3.488210000	4.328252000	-0.646661000
H	-2.741621000	5.076536000	-0.881573000
C	-3.143663000	2.991000000	-0.513729000
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C	-9.857377000	0.291289000	0.879265000
O	-10.491420000	1.352928000	0.849246000
O	-10.455663000	-0.924582000	1.112627000
H	-11.422563000	-0.817614000	1.239514000
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O	-6.528354000	6.371039000	-0.435423000
H	-6.738356000	7.323762000	-0.539911000
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O	-6.752243000	-6.289040000	1.117681000
O	-4.585198000	-6.976241000	0.824015000
H	-4.958630000	-7.872412000	0.966689000
C	3.080691000	-0.481628000	-2.496366000

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C	4.496695000	-0.470808000	-2.457769000
H	2.534767000	-0.685078000	-3.409819000
H	5.103481000	-0.674502000	-3.330347000
C	6.442732000	-0.135208000	-0.823441000
C	6.850797000	-0.168565000	0.529349000
C	7.459970000	-0.020566000	-1.801752000
C	8.189493000	-0.104191000	0.889526000
C	8.800487000	0.046497000	-1.452165000
C	9.199752000	0.002962000	-0.094904000
H	6.107502000	-0.279655000	1.312607000
H	7.192698000	0.048170000	-2.850630000
H	8.465589000	-0.153865000	1.935288000
H	9.550474000	0.150727000	-2.226100000
N	10.558369000	0.063820000	0.261734000
C	11.580144000	-0.395255000	-0.640939000
C	11.480412000	-1.660131000	-1.245810000
C	12.699450000	0.412491000	-0.900849000
C	12.484596000	-2.101465000	-2.111987000
C	13.706407000	-0.042567000	-1.756667000
C	13.602025000	-1.297448000	-2.369126000

H	10.624107000	-2.290265000	-1.031566000
H	12.774835000	1.387048000	-0.431596000
H	12.400937000	-3.080132000	-2.573406000
H	14.567925000	0.587772000	-1.951181000
H	14.383444000	-1.646137000	-3.035798000
C	10.965625000	0.575583000	1.542393000
C	10.479534000	1.811129000	2.004063000
C	11.877022000	-0.149032000	2.328312000
C	10.892117000	2.304738000	3.244872000
C	12.295625000	0.358591000	3.561346000
C	11.802676000	1.583623000	4.027249000
H	9.789564000	2.378636000	1.389145000
H	12.252713000	-1.100562000	1.969086000
H	10.514568000	3.261095000	3.592208000
H	13.001045000	-0.207476000	4.160817000
H	12.127513000	1.973944000	4.985834000

Optimized Cartesian Coordinates for (2):

Ru	-4.123120000	-0.016243000	-0.003582000
C	-4.143984000	-0.568408000	-1.992769000
N	-2.106058000	-0.202127000	-0.382376000
N	-3.159782000	0.476537000	1.899399000

C	-5.253623000	-0.757257000	-2.836701000
H	-6.258612000	-0.609933000	-2.451748000
C	-5.094263000	-1.133164000	-4.177718000
H	-5.969178000	-1.271783000	-4.806092000
C	-3.814093000	-1.330602000	-4.712959000
C	-2.692897000	-1.151005000	-3.903156000
H	-1.704067000	-1.305286000	-4.325208000
C	-2.843594000	-0.773972000	-2.555764000
C	-1.710973000	-0.565406000	-1.647179000
C	-0.350841000	-0.687275000	-1.936367000
H	-0.048763000	-0.955533000	-2.939345000
C	0.632460000	-0.448960000	-0.946211000
C	0.176490000	-0.076810000	0.344070000
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C	-1.786061000	0.420414000	1.887592000
C	-1.052333000	0.714586000	3.044930000
H	0.029081000	0.668905000	3.027648000
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C	-3.117914000	1.121135000	4.219656000
H	-3.670038000	1.390913000	5.111601000
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H	-4.882473000	0.848227000	2.994699000

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N	-6.055510000	0.138458000	0.264165000
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H	-3.453437000	-5.086244000	1.183883000
C	-5.521705000	-4.475296000	1.369716000
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C	-8.055613000	1.460598000	0.181832000
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C	-5.149362000	4.604258000	-1.161739000
C	-3.813229000	4.181667000	-1.264129000

H	-3.052876000	4.876296000	-1.598604000
C	-3.491829000	2.872161000	-0.937837000
H	-2.479365000	2.500806000	-1.011533000
C	-10.259967000	0.506266000	0.761048000
O	-10.876036000	1.561179000	0.566662000
O	-10.881096000	-0.652820000	1.162764000
H	-11.847332000	-0.513614000	1.259722000
C	-5.481548000	6.005750000	-1.512004000
O	-4.658365000	6.846364000	-1.887449000
O	-6.820090000	6.281443000	-1.372879000
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O	-5.100265000	-6.758166000	1.873985000
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C	2.042250000	-0.572787000	-1.243500000
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C	4.635711000	-0.553575000	-1.185938000
C	4.074874000	-1.046208000	-2.351903000
H	2.105986000	-1.433607000	-3.232990000
H	4.675424000	-1.422280000	-3.169754000
C	6.030920000	-0.393119000	-0.827430000

C	6.444983000	-0.135092000	0.499690000
C	7.045045000	-0.485647000	-1.811803000
C	7.783318000	0.016731000	0.831236000
C	8.385762000	-0.335414000	-1.491373000
C	8.790742000	-0.079436000	-0.158553000
H	5.705179000	-0.080637000	1.292278000
H	6.774828000	-0.645978000	-2.849908000
H	8.063241000	0.195265000	1.861669000
H	9.132159000	-0.394143000	-2.273438000
N	10.146808000	0.075127000	0.168072000
C	11.174505000	-0.524874000	-0.641911000
C	11.130155000	-1.892741000	-0.957114000
C	12.252224000	0.248864000	-1.099529000
C	12.141157000	-2.466654000	-1.730800000
C	13.264497000	-0.339675000	-1.860403000
C	13.226475000	-1.704008000	-2.197228000
H	10.310597000	-2.501217000	-0.590010000
H	12.295642000	1.303914000	-0.852462000
H	12.095963000	-3.527023000	-1.961992000
H	14.094254000	0.271418000	-2.203333000
C	10.553398000	0.836200000	1.318708000
C	10.051596000	2.129168000	1.538807000
C	11.482985000	0.300367000	2.224750000

C	10.464178000	2.861187000	2.654728000
C	11.898383000	1.047670000	3.328020000
C	11.397714000	2.339928000	3.566775000
H	9.343803000	2.557266000	0.837132000
H	11.874596000	-0.697469000	2.060759000
H	10.066024000	3.859594000	2.811146000
H	12.616322000	0.617353000	4.020314000
H	-1.157581000	1.295784000	5.117146000
C	11.871003000	3.150983000	4.752151000
H	12.820921000	3.657816000	4.534399000
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C	14.308078000	-2.327841000	-3.050168000
H	14.060130000	-2.263177000	-4.118513000
H	15.269971000	-1.824029000	-2.909519000
H	14.444125000	-3.388094000	-2.812370000
H	-3.694244000	-1.621030000	-5.751077000

Optimized Cartesian Coordinates for (3):

Ru	-4.513546000	-0.031849000	-0.016289000
C	-4.541776000	-0.878271000	-1.898850000
N	-2.498161000	-0.249912000	-0.380113000

N	-3.544774000	0.745249000	1.785980000
C	-5.655941000	-1.211239000	-2.690421000
H	-6.659547000	-1.022086000	-2.320407000
C	-5.502534000	-1.787526000	-3.958991000
H	-6.380703000	-2.034035000	-4.548601000
C	-4.224061000	-2.047636000	-4.471108000
C	-3.098602000	-1.730127000	-3.711028000
H	-2.111073000	-1.935325000	-4.114005000
C	-3.243163000	-1.151026000	-2.436603000
C	-2.106840000	-0.791020000	-1.581235000
C	-0.747798000	-0.934271000	-1.863237000
H	-0.450731000	-1.354129000	-2.814349000
C	0.240361000	-0.530793000	-0.932694000
C	-0.212040000	0.019413000	0.293973000
H	0.508671000	0.339248000	1.034503000
C	-1.574142000	0.147811000	0.543164000
C	-2.170301000	0.704770000	1.770056000
C	-1.432885000	1.171797000	2.866587000
H	-0.351082000	1.136287000	2.847642000
C	-2.096177000	1.682472000	3.982705000
C	-3.495663000	1.718987000	3.988155000
H	-4.045188000	2.108500000	4.836377000
C	-4.183033000	1.242152000	2.874252000

H	-5.264731000	1.249228000	2.830882000
N	-4.962928000	-1.869223000	0.845120000
N	-6.440965000	0.159351000	0.261001000
N	-4.833270000	1.854896000	-0.828358000
C	-4.111084000	-2.902293000	1.084063000
H	-3.081078000	-2.740520000	0.798063000
C	-4.528307000	-4.099058000	1.652770000
H	-3.823558000	-4.900816000	1.826993000
C	-5.882179000	-4.253316000	1.994746000
C	-6.769041000	-3.203331000	1.745564000
H	-7.813244000	-3.330551000	2.003862000
C	-6.304239000	-2.019933000	1.168093000
C	-7.148550000	-0.871728000	0.842222000
C	-8.522083000	-0.750785000	1.044391000
H	-9.097577000	-1.546537000	1.497968000
C	-9.173838000	0.428053000	0.646332000
C	-8.441548000	1.465369000	0.044447000
H	-8.968941000	2.360521000	-0.261525000
C	-7.071377000	1.317557000	-0.145959000
C	-6.153972000	2.272319000	-0.766373000
C	-6.538243000	3.514200000	-1.282060000
H	-7.568876000	3.839377000	-1.233630000
C	-5.582575000	4.343718000	-1.872962000

C	-4.248216000	3.908626000	-1.940678000
H	-3.499138000	4.538855000	-2.403525000
C	-3.914011000	2.669502000	-1.413928000
H	-2.901982000	2.291275000	-1.450681000
C	-10.626334000	0.622775000	0.833165000
O	-11.247440000	1.640042000	0.502048000
O	-11.235144000	-0.458619000	1.425349000
H	-12.197479000	-0.300446000	1.531581000
C	-5.929327000	5.669461000	-2.437958000
O	-5.119927000	6.437814000	-2.966819000
O	-7.264841000	5.964883000	-2.309101000
H	-7.467717000	6.844374000	-2.693809000
C	-6.418180000	-5.491565000	2.608025000
O	-7.601502000	-5.660685000	2.922608000
O	-5.452424000	-6.447823000	2.797199000
H	-5.835336000	-7.256561000	3.199950000
C	2.263839000	-1.206098000	-2.340960000
C	1.648962000	-0.666180000	-1.227531000
S	2.921572000	-0.074570000	-0.059299000
C	4.243322000	-0.623040000	-1.187905000
C	3.679077000	-1.185645000	-2.320652000
H	1.709806000	-1.629450000	-3.170310000
H	4.277809000	-1.600604000	-3.120862000

C	5.638808000	-0.431001000	-0.849998000
C	6.061512000	-0.095592000	0.457074000
C	6.646384000	-0.567555000	-1.836498000
C	7.400416000	0.089844000	0.767530000
C	7.987596000	-0.384828000	-1.537736000
C	8.401676000	-0.048360000	-0.224826000
H	5.327770000	-0.005013000	1.252052000
H	6.369183000	-0.788369000	-2.861628000
H	7.686166000	0.328526000	1.784044000
H	8.727546000	-0.478610000	-2.322413000
N	9.755970000	0.144117000	0.079160000
C	10.789762000	-0.447729000	-0.730090000
C	10.807368000	-1.827709000	-0.973516000
C	11.815419000	0.355822000	-1.262508000
C	11.819068000	-2.404327000	-1.750119000
C	12.832420000	-0.212382000	-2.021635000
C	12.836992000	-1.594632000	-2.272716000
H	10.027680000	-2.455004000	-0.554846000
H	11.809778000	1.423311000	-1.072826000
H	11.809131000	-3.473106000	-1.923985000
H	13.629903000	0.391084000	-2.438213000
C	10.161438000	0.943328000	1.205116000
C	9.657847000	2.247382000	1.379732000

C	11.097160000	0.446628000	2.121650000
C	10.069872000	3.023093000	2.458074000
C	11.529529000	1.228302000	3.198545000
C	11.009890000	2.518248000	3.371776000
H	8.947561000	2.647703000	0.664696000
H	11.495085000	-0.553292000	1.989091000
H	9.694636000	4.028835000	2.605010000
H	12.257806000	0.820848000	3.888498000
O	13.891183000	-2.057615000	-3.045806000
C	13.979494000	-3.477611000	-3.341424000
H	14.083410000	-4.068198000	-2.423783000
H	13.104293000	-3.821034000	-3.905266000
H	14.875159000	-3.585200000	-3.951327000
O	11.360170000	3.375401000	4.405109000
C	12.349712000	2.938578000	5.375949000
H	12.006138000	2.051861000	5.921293000
H	13.310795000	2.726444000	4.893533000
H	12.460037000	3.774599000	6.064949000
H	-1.531715000	2.045780000	4.833588000
H	-4.108671000	-2.493447000	-5.453047000

Optimized Cartesian Coordinates for (4):

Ru	-3.521157000	-0.348456000	-0.334388000
C	-3.596379000	1.124298000	1.101089000
N	-1.516408000	0.002774000	-0.033665000
N	-2.514682000	-1.731481000	-1.700726000
C	-4.726472000	1.712379000	1.702185000
H	-5.722093000	1.387217000	1.416781000
C	-4.605085000	2.713924000	2.669263000
H	-5.489728000	3.147302000	3.123012000
C	-3.334115000	3.152619000	3.069135000
C	-2.189565000	2.594954000	2.496616000
H	-1.216702000	2.942920000	2.825222000
C	-2.309473000	1.590677000	1.526191000
C	-1.150464000	0.953633000	0.886728000
C	0.199538000	1.211251000	1.119345000
H	0.475013000	1.956012000	1.853385000
C	1.209143000	0.508170000	0.416417000
C	0.783644000	-0.464992000	-0.523726000
H	1.521087000	-1.023830000	-1.084078000
C	-0.572156000	-0.697285000	-0.728514000
C	-1.140652000	-1.676748000	-1.671364000
C	-0.377713000	-2.513329000	-2.497199000
H	0.703358000	-2.465169000	-2.468256000
C	-1.014899000	-3.409196000	-3.356339000

C	-2.413693000	-3.456783000	-3.378282000
H	-2.943228000	-4.139323000	-4.031638000
C	-3.127050000	-2.604639000	-2.538015000
H	-4.209444000	-2.605451000	-2.519346000
N	-3.940399000	1.036038000	-1.832121000
N	-5.446254000	-0.633701000	-0.566845000
N	-3.870650000	-1.820641000	1.096690000
C	-3.074349000	1.896733000	-2.430347000
H	-2.049273000	1.848892000	-2.090157000
C	-3.471869000	2.793945000	-3.414226000
H	-2.756568000	3.467104000	-3.867049000
C	-4.819649000	2.816330000	-3.808007000
C	-5.720491000	1.941107000	-3.196738000
H	-6.759893000	1.967408000	-3.500390000
C	-5.274982000	1.058788000	-2.210397000
C	-6.134594000	0.114517000	-1.497053000
C	-7.506448000	-0.067221000	-1.665096000
H	-8.067674000	0.509742000	-2.387838000
C	-8.174654000	-1.016754000	-0.875298000
C	-7.461028000	-1.765867000	0.075000000
H	-8.000959000	-2.486341000	0.677089000
C	-6.092198000	-1.562371000	0.221830000
C	-5.192865000	-2.230943000	1.162102000

C	-5.595989000	-3.207324000	2.078645000
H	-6.628153000	-3.527060000	2.130589000
C	-4.656616000	-3.774844000	2.942457000
C	-3.320093000	-3.348234000	2.874479000
H	-2.583647000	-3.775234000	3.543740000
C	-2.967355000	-2.376835000	1.948325000
H	-1.952962000	-2.012184000	1.867060000
C	-9.627345000	-1.261618000	-1.001859000
O	-10.259590000	-2.087121000	-0.332537000
O	-10.217050000	-0.467057000	-1.955126000
H	-11.179775000	-0.646755000	-2.013473000
C	-5.023585000	-4.813462000	3.935746000
O	-4.227427000	-5.346240000	4.714525000
O	-6.359648000	-5.127924000	3.898940000
H	-6.578829000	-5.811643000	4.567730000
C	-5.336241000	3.737686000	-4.849200000
O	-6.513995000	3.779751000	-5.220777000
O	-4.359052000	4.548854000	-5.366139000
H	-4.726538000	5.152554000	-6.046947000
C	3.198809000	1.721487000	1.465209000
C	2.610089000	0.771109000	0.652562000
S	3.908569000	-0.209830000	-0.174570000
C	5.203389000	0.770661000	0.650781000

C	4.614269000	1.723850000	1.464399000
H	2.626019000	2.430722000	2.050756000
H	5.194544000	2.436156000	2.036032000
C	6.607386000	0.495839000	0.418822000
C	7.051012000	-0.312459000	-0.652972000
C	7.599397000	1.036759000	1.272943000
C	8.398206000	-0.562626000	-0.869339000
C	8.948582000	0.791689000	1.066166000
C	9.383101000	-0.015018000	-0.013256000
H	6.328147000	-0.727301000	-1.348472000
H	7.305324000	1.631871000	2.130597000
H	8.701741000	-1.169663000	-1.712847000
H	9.678300000	1.206097000	1.750296000
N	10.748831000	-0.265288000	-0.226507000
C	11.750690000	0.665536000	0.221145000
C	11.643221000	2.031805000	-0.090546000
C	12.858797000	0.204334000	0.950642000
C	12.628351000	2.925650000	0.338511000
C	13.846737000	1.102616000	1.363479000
C	13.734347000	2.465910000	1.064213000
H	10.796161000	2.384360000	-0.668876000
H	12.941225000	-0.850583000	1.187230000
H	12.539014000	3.978697000	0.092087000

H	14.699639000	0.737670000	1.926222000
C	11.186487000	-1.459560000	-0.898342000
C	10.710017000	-2.718904000	-0.494931000
C	12.118391000	-1.372414000	-1.945702000
C	11.152749000	-3.874398000	-1.144809000
C	12.566761000	-2.533888000	-2.580802000
C	12.083926000	-3.788009000	-2.187276000
H	10.004437000	-2.786497000	0.325909000
H	12.486976000	-0.400022000	-2.252599000
H	10.782652000	-4.843085000	-0.824799000
H	13.287837000	-2.457433000	-3.388010000
H	-0.430859000	-4.059240000	-3.997357000
H	12.432470000	-4.687342000	-2.683694000
H	14.500952000	3.161113000	1.389180000
C	-3.205501000	4.271866000	4.043530000
F	-3.254066000	5.525608000	3.425949000
F	-4.226218000	4.267689000	4.989262000
F	-1.995782000	4.230620000	4.735935000

Optimized Cartesian Coordinates for (5):

Ru	3.911963000	-0.405889000	0.247405000
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C	3.991126000	1.359540000	-0.807848000
N	1.907322000	0.016945000	0.048034000
N	2.899891000	-2.061946000	1.263455000
C	5.122754000	2.065405000	-1.261408000
H	6.117290000	1.678536000	-1.062655000
C	5.004169000	3.263525000	-1.970840000
H	5.889970000	3.785108000	-2.316814000
C	3.734419000	3.789077000	-2.252442000
C	2.588684000	3.120399000	-1.817829000
H	1.616838000	3.540080000	-2.051851000
C	2.705842000	1.918306000	-1.106669000
C	1.544909000	1.156205000	-0.627497000
C	0.196501000	1.465465000	-0.793372000
H	-0.076271000	2.359321000	-1.337315000
C	-0.816533000	0.622789000	-0.271172000
C	-0.394597000	-0.542381000	0.420022000
H	-1.134547000	-1.212032000	0.837470000
C	0.960440000	-0.820846000	0.563927000
C	1.526077000	-1.994306000	1.253037000
C	0.760642000	-2.995167000	1.866368000
H	-0.320209000	-2.936051000	1.853873000
C	1.394764000	-4.068616000	2.492893000
C	2.793338000	-4.127105000	2.498231000

H	3.320666000	-4.944551000	2.974507000
C	3.509304000	-3.107431000	1.874710000
H	4.591653000	-3.108517000	1.852180000
N	4.350898000	0.593860000	2.018876000
N	5.834937000	-0.752704000	0.394480000
N	4.239960000	-1.508185000	-1.487401000
C	3.496065000	1.305209000	2.801170000
H	2.469606000	1.345014000	2.463942000
C	3.906516000	1.952660000	3.960115000
H	3.200197000	2.513139000	4.557464000
C	5.255748000	1.871506000	4.341324000
C	6.145182000	1.148466000	3.542846000
H	7.185709000	1.095284000	3.839146000
C	5.687057000	0.517321000	2.384542000
C	6.534058000	-0.246707000	1.468977000
C	7.903666000	-0.478694000	1.584023000
H	8.473713000	-0.091119000	2.417623000
C	8.558267000	-1.228898000	0.593629000
C	7.833929000	-1.730044000	-0.500796000
H	8.363895000	-2.298936000	-1.254838000
C	6.467489000	-1.481981000	-0.590315000
C	5.557218000	-1.906022000	-1.654108000
C	5.945566000	-2.648285000	-2.773915000

H	6.973509000	-2.959217000	-2.903913000
C	4.996858000	-2.989793000	-3.740336000
C	3.665970000	-2.574882000	-3.568260000
H	2.922494000	-2.826532000	-4.314253000
C	3.327701000	-1.840841000	-2.440185000
H	2.318277000	-1.492625000	-2.271207000
C	10.007663000	-1.514367000	0.655134000
O	10.629352000	-2.170459000	-0.188835000
O	10.608083000	-0.968906000	1.764295000
H	11.568423000	-1.169266000	1.775967000
C	5.348338000	-3.774969000	-4.948507000
O	4.543727000	-4.105012000	-5.824851000
O	6.680695000	-4.104353000	-4.992748000
H	6.889558000	-4.617407000	-5.802654000
C	5.785320000	2.528144000	5.561177000
O	6.964460000	2.473507000	5.926784000
O	4.818308000	3.210736000	6.253442000
H	5.194171000	3.640903000	7.051348000
C	-2.795724000	2.055830000	-1.014629000
C	-2.214749000	0.938701000	-0.443592000
S	-3.522448000	-0.202217000	0.123923000
C	-4.809279000	0.949552000	-0.459035000
C	-4.210077000	2.064575000	-1.022623000

H	-2.217009000	2.879505000	-1.415446000
H	-4.783006000	2.892807000	-1.418262000
C	-6.214879000	0.635777000	-0.308866000
C	-6.669863000	-0.424248000	0.509345000
C	-7.201010000	1.392983000	-0.988632000
C	-8.019110000	-0.711232000	0.650340000
C	-8.552341000	1.115251000	-0.854488000
C	-8.998468000	0.053891000	-0.028759000
H	-5.953039000	-1.017381000	1.068656000
H	-6.900632000	2.193580000	-1.655756000
H	-8.329748000	-1.519099000	1.300549000
H	-9.276314000	1.704640000	-1.402667000
N	-10.364242000	-0.230278000	0.110191000
C	-11.361246000	0.785010000	-0.106717000
C	-11.269313000	2.029513000	0.537833000
C	-12.459633000	0.525548000	-0.941023000
C	-12.253422000	2.998925000	0.333238000
C	-13.444594000	1.497817000	-1.125901000
C	-13.358510000	2.754152000	-0.500800000
H	-10.434847000	2.230253000	1.201214000
H	-12.540867000	-0.436641000	-1.434528000
H	-12.171091000	3.954615000	0.842829000
H	-14.290738000	1.279783000	-1.770893000

C	-10.814513000	-1.547300000	0.476815000
C	-10.373280000	-2.677926000	-0.228824000
C	-11.725258000	-1.711152000	1.532737000
C	-10.828323000	-3.949253000	0.129317000
C	-12.183178000	-2.985308000	1.872056000
C	-11.744867000	-4.128289000	1.179637000
H	-9.679773000	-2.558504000	-1.054347000
H	-12.069397000	-0.841288000	2.081306000
H	-10.477735000	-4.814474000	-0.425885000
H	-12.885937000	-3.095504000	2.692914000
H	0.808434000	-4.846095000	2.968625000
C	3.609838000	5.102127000	-2.944390000
F	3.686752000	6.182330000	-2.059547000
F	4.617903000	5.300623000	-3.883254000
F	2.390872000	5.233795000	-3.608516000
C	-12.266091000	-5.501802000	1.537917000
H	-13.236423000	-5.696032000	1.061104000
H	-11.579299000	-6.289184000	1.211169000
H	-12.411221000	-5.606338000	2.618714000
C	-14.410537000	3.815293000	-0.732393000
H	-14.157412000	4.445563000	-1.595927000
H	-15.391109000	3.370872000	-0.931822000
H	-14.509262000	4.477027000	0.134437000

Optimized Cartesian Coordinates for (6):

Ru	4.315958000	-0.414811000	0.234099000
C	4.411922000	1.388348000	-0.753816000
N	2.315247000	0.030840000	0.045222000
N	3.288078000	-2.099926000	1.184373000
C	5.550326000	2.101908000	-1.177387000
H	6.541245000	1.700099000	-0.990566000
C	5.443128000	3.326724000	-1.841602000
H	6.333968000	3.854013000	-2.165271000
C	4.178325000	3.872372000	-2.106760000
C	3.026158000	3.196793000	-1.700764000
H	2.058287000	3.632537000	-1.921532000
C	3.131893000	1.967954000	-1.034975000
C	1.963674000	1.197468000	-0.588004000
C	0.618198000	1.523248000	-0.745865000
H	0.353972000	2.439009000	-1.256575000
C	-0.402880000	0.669477000	-0.258515000
C	0.007968000	-0.524093000	0.389555000
H	-0.738383000	-1.203161000	0.779487000
C	1.360377000	-0.818330000	0.526637000
C	1.914863000	-2.021227000	1.172709000
C	1.139882000	-3.038422000	1.745864000
H	0.059561000	-2.970448000	1.732613000

C	1.763811000	-4.139565000	2.333344000
C	3.161871000	-4.209121000	2.340345000
H	3.681439000	-5.047973000	2.787012000
C	3.887561000	-3.172359000	1.757577000
H	4.969933000	-3.181041000	1.738014000
N	4.757155000	0.514217000	2.043111000
N	6.235750000	-0.781892000	0.373343000
N	4.640764000	-1.453675000	-1.540006000
C	3.905431000	1.202311000	2.849234000
H	2.880344000	1.262762000	2.510906000
C	4.317307000	1.802536000	4.032833000
H	3.613496000	2.345663000	4.648879000
C	5.664705000	1.696598000	4.414447000
C	6.550988000	0.997160000	3.591807000
H	7.590166000	0.924770000	3.888771000
C	6.091564000	0.413576000	2.409330000
C	6.935458000	-0.322091000	1.468031000
C	8.302885000	-0.568906000	1.578054000
H	8.873347000	-0.217381000	2.427207000
C	8.954719000	-1.286449000	0.561967000
C	8.229895000	-1.740459000	-0.552521000
H	8.757770000	-2.284732000	-1.325952000
C	6.865681000	-1.478562000	-0.636422000

C	5.955427000	-1.855226000	-1.717914000
C	6.341473000	-2.557901000	-2.863756000
H	7.367387000	-2.871733000	-3.002513000
C	5.393121000	-2.855453000	-3.844947000
C	4.064943000	-2.436937000	-3.661068000
H	3.321834000	-2.654580000	-4.418043000
C	3.728887000	-1.743180000	-2.507136000
H	2.721658000	-1.393698000	-2.327974000
C	10.401684000	-1.585318000	0.616697000
O	11.020883000	-2.214064000	-0.249620000
O	11.002891000	-1.086614000	1.747234000
H	11.961622000	-1.294752000	1.754018000
C	5.742240000	-3.597401000	-5.080805000
O	4.937793000	-3.888005000	-5.971154000
O	7.072154000	-3.935267000	-5.133719000
H	7.279538000	-4.419143000	-5.961760000
C	6.195582000	2.302785000	5.659583000
O	7.373145000	2.225258000	6.026133000
O	5.231736000	2.966401000	6.374350000
H	5.608456000	3.363339000	7.188900000
C	-2.368709000	2.144834000	-0.953046000
C	-1.798090000	1.002541000	-0.422803000
S	-3.116255000	-0.148657000	0.097802000

C	-4.392402000	1.034206000	-0.444999000
C	-3.782921000	2.164906000	-0.964615000
H	-1.782452000	2.978446000	-1.321014000
H	-4.348251000	3.011862000	-1.330422000
C	-5.800826000	0.725986000	-0.310617000
C	-6.266446000	-0.360454000	0.465899000
C	-6.779022000	1.515872000	-0.964151000
C	-7.618285000	-0.641998000	0.592278000
C	-8.132854000	1.243847000	-0.844276000
C	-8.589651000	0.155721000	-0.060274000
H	-5.555918000	-0.979762000	1.004490000
H	-6.470460000	2.338605000	-1.599868000
H	-7.937112000	-1.471280000	1.210791000
H	-8.850595000	1.859050000	-1.371902000
N	-9.957988000	-0.122803000	0.064122000
C	-10.946483000	0.907669000	-0.117209000
C	-10.846946000	2.126316000	0.573934000
C	-12.044279000	0.688326000	-0.963715000
C	-11.822936000	3.110383000	0.403218000
C	-13.021159000	1.674514000	-1.114624000
C	-12.927321000	2.905760000	-0.442486000
H	-10.012991000	2.295464000	1.246699000
H	-12.131408000	-0.253974000	-1.493276000

H	-11.734810000	4.045575000	0.948611000
H	-13.866982000	1.487484000	-1.769695000
C	-10.419498000	-1.449117000	0.379722000
C	-9.984822000	-2.555838000	-0.366704000
C	-11.334701000	-1.645417000	1.426213000
C	-10.450726000	-3.836135000	-0.057876000
C	-11.803447000	-2.927811000	1.716118000
C	-11.371827000	-4.047353000	0.982430000
H	-9.287895000	-2.410897000	-1.185231000
H	-11.673814000	-0.794121000	2.006145000
H	-10.105109000	-4.682592000	-0.644244000
H	-12.509540000	-3.063287000	2.530305000
H	1.170067000	-4.929770000	2.777891000
C	4.065962000	5.211423000	-2.749200000
F	4.148485000	6.256988000	-1.824167000
F	5.078385000	5.437179000	-3.677153000
F	2.850077000	5.377457000	-3.411269000
C	-13.309361000	-5.614178000	0.764105000
H	-13.703364000	-6.634918000	0.989113000
H	-13.995909000	-4.865043000	1.228352000
H	-13.331067000	-5.468141000	-0.343268000
C	-15.325480000	3.545857000	-0.133045000
H	-16.096369000	4.341433000	-0.276442000

H	-15.662992000	2.630776000	-0.677830000
H	-15.272479000	3.303748000	0.956289000
O	-13.989693000	4.002917000	-0.640510000
O	-11.914513000	-5.454707000	1.292989000

Optimized Cartesian Coordinates for (7):

Ru	3.519238000	-0.002069000	-0.058238000
C	3.544184000	-0.285312000	2.000269000
N	1.508968000	-0.089121000	0.360141000
N	2.562439000	0.242025000	-1.998284000
C	4.647246000	-0.396038000	2.874653000
C	4.480575000	-0.588070000	4.252094000
H	5.335928000	-0.671240000	4.911325000
C	3.191113000	-0.675932000	4.798034000
C	2.075797000	-0.573288000	3.976172000
H	1.083415000	-0.643445000	4.409085000
C	2.248339000	-0.379657000	2.589509000
C	1.115132000	-0.264400000	1.663313000
C	-0.245484000	-0.310327000	1.972689000
H	-0.545977000	-0.438751000	3.003162000
C	-1.229865000	-0.183513000	0.963658000
C	-0.774875000	-0.006415000	-0.366998000
H	-1.493162000	0.092576000	-1.169691000

C	0.588100000	0.037918000	-0.640160000
C	1.187012000	0.219665000	-1.972914000
C	0.451467000	0.363462000	-3.157070000
H	-0.630520000	0.344692000	-3.128669000
C	1.115981000	0.530774000	-4.372165000
C	2.515709000	0.552309000	-4.386701000
H	3.066921000	0.680412000	-5.310268000
C	3.201667000	0.405342000	-3.183440000
H	4.283425000	0.415564000	-3.145000000
N	3.946681000	-2.011498000	-0.366217000
N	5.426904000	0.094274000	-0.487656000
N	3.864903000	2.032915000	0.179030000
C	3.100170000	-3.066684000	-0.229674000
H	2.088173000	-2.824514000	0.063228000
C	3.502618000	-4.379515000	-0.440969000
H	2.803346000	-5.195919000	-0.321591000
C	4.834942000	-4.630085000	-0.808462000
C	5.716338000	-3.554141000	-0.942621000
H	6.744916000	-3.754214000	-1.216841000
C	5.267102000	-2.252067000	-0.715520000
C	6.108175000	-1.059047000	-0.797010000
C	7.461777000	-1.007068000	-1.122350000
H	8.017376000	-1.900968000	-1.372018000

C	8.119291000	0.233965000	-1.121857000
C	7.411067000	1.401755000	-0.792362000
H	7.941017000	2.346320000	-0.793370000
C	6.059840000	1.315581000	-0.473369000
C	5.171719000	2.410404000	-0.085841000
C	5.569937000	3.744919000	0.036453000
H	6.589516000	4.039972000	-0.172319000
C	4.643611000	4.709934000	0.439554000
C	3.324375000	4.315839000	0.718998000
H	2.598639000	5.052371000	1.040432000
C	2.974725000	2.980394000	0.579650000
H	1.974323000	2.629573000	0.790922000
C	9.551901000	0.362575000	-1.458008000
O	10.179412000	1.428794000	-1.470499000
O	10.137224000	-0.844401000	-1.763144000
H	11.086207000	-0.723967000	-1.980745000
C	5.006294000	6.139128000	0.587711000
O	4.223062000	7.027382000	0.938568000
O	6.325157000	6.383211000	0.288834000
H	6.537914000	7.334829000	0.397570000
C	5.353756000	-5.996065000	-1.055149000
O	6.518754000	-6.255052000	-1.377325000
O	4.394483000	-6.963412000	-0.888343000

H	4.766169000	-7.856239000	-1.054373000
C	-3.261595000	-0.449532000	2.494277000
C	-2.641452000	-0.228551000	1.280472000
S	-3.906369000	0.022357000	-0.011218000
C	-5.234017000	-0.209093000	1.214482000
C	-4.678280000	-0.440629000	2.460087000
H	-2.712434000	-0.634470000	3.409753000
H	-5.282115000	-0.628730000	3.338267000
C	-6.629286000	-0.133034000	0.824628000
C	-7.038643000	-0.194323000	-0.526726000
C	-7.645181000	0.005764000	1.800931000
C	-8.377302000	-0.132246000	-0.887325000
C	-8.985989000	0.070101000	1.450884000
C	-9.386363000	-0.000055000	0.095145000
H	-6.296439000	-0.324969000	-1.307974000
H	-7.376726000	0.096278000	2.847889000
H	-8.654244000	-0.203097000	-1.931644000
H	-9.734818000	0.193889000	2.223068000
N	-10.744701000	0.060479000	-0.263092000
C	-11.770129000	-0.373258000	0.647689000
C	-11.677542000	-1.624491000	1.281454000
C	-12.886735000	0.444898000	0.886221000
C	-12.686280000	-2.042036000	2.154141000

C	-13.898187000	0.013466000	1.748881000
C	-13.801113000	-1.227865000	2.389541000
H	-10.823263000	-2.262853000	1.084170000
H	-12.956555000	1.408821000	0.394754000
H	-12.608121000	-3.010355000	2.637816000
H	-14.757577000	0.651639000	1.926551000
C	-11.147913000	0.549773000	-1.553866000
C	-10.660770000	1.777598000	-2.034614000
C	-12.055748000	-0.188826000	-2.330784000
C	-11.069352000	2.250080000	-3.284934000
C	-12.470244000	0.297644000	-3.573736000
C	-11.976593000	1.515147000	-4.058247000
H	-9.973047000	2.355549000	-1.426938000
H	-12.431967000	-1.134462000	-1.956777000
H	-10.691186000	3.200685000	-3.647087000
H	-13.172953000	-0.278987000	-4.166297000
H	0.552787000	0.642550000	-5.291331000
H	-14.586075000	-1.558234000	3.061375000
H	-12.298236000	1.888949000	-5.024472000
H	3.072353000	-0.824510000	5.865757000
O	5.918243000	-0.303526000	2.284745000
C	7.092224000	-0.397660000	3.139220000
H	7.108445000	0.406706000	3.883361000

H	7.139967000	-1.368503000	3.645400000
H	7.943500000	-0.292384000	2.467709000

Optimized Cartesian Coordinates for (8):

Ru	-3.919387000	0.007959000	0.043763000
C	-3.954014000	-0.540377000	-1.960692000
N	-1.910532000	-0.112476000	-0.376087000
N	-2.952998000	0.537826000	1.919732000
C	-5.060723000	-0.758005000	-2.810446000
C	-4.900098000	-1.129437000	-4.151278000
H	-5.758368000	-1.295155000	-4.790969000
C	-3.612999000	-1.291592000	-4.685564000
C	-2.494073000	-1.083846000	-3.888844000
H	-1.503354000	-1.208985000	-4.312977000
C	-2.660562000	-0.711302000	-2.538572000
C	-1.522551000	-0.470177000	-1.642836000
C	-0.163619000	-0.563575000	-1.948157000
H	0.131831000	-0.841499000	-2.950198000
C	0.826031000	-0.295620000	-0.971875000
C	0.376665000	0.071099000	0.321881000
H	1.098667000	0.283687000	1.098794000
C	-0.984869000	0.155056000	0.591769000

C	-1.577686000	0.525896000	1.887642000
C	-0.837355000	0.853863000	3.031446000
H	0.244600000	0.843072000	2.998166000
C	-1.497119000	1.195821000	4.212084000
C	-2.896943000	1.205892000	4.233171000
H	-3.444406000	1.466923000	5.130593000
C	-3.587820000	0.872334000	3.070664000
H	-4.669843000	0.866872000	3.037192000
N	-4.294728000	-1.949863000	0.627756000
N	-5.825414000	0.118203000	0.475452000
N	-4.313552000	1.986233000	-0.457034000
C	-3.421276000	-2.991965000	0.637462000
H	-2.416729000	-2.768145000	0.306565000
C	-3.788551000	-4.270698000	1.037165000
H	-3.068400000	-5.077618000	1.031004000
C	-5.112539000	-4.499904000	1.446831000
C	-6.021139000	-3.438455000	1.432763000
H	-7.042560000	-3.622697000	1.742446000
C	-5.607192000	-2.171334000	1.018172000
C	-6.477528000	-0.999305000	0.940263000
C	-7.831102000	-0.936336000	1.264078000
H	-8.364440000	-1.802133000	1.632857000
C	-8.518054000	0.278169000	1.104211000

C	-7.838868000	1.408433000	0.618731000
H	-8.391199000	2.332363000	0.498839000
C	-6.487537000	1.311750000	0.303679000
C	-5.627610000	2.365434000	-0.233656000
C	-6.057713000	3.662551000	-0.528691000
H	-7.083348000	3.959162000	-0.354592000
C	-5.155893000	4.586888000	-1.061694000
C	-3.828461000	4.190304000	-1.294798000
H	-3.121315000	4.894625000	-1.714742000
C	-3.447173000	2.892869000	-0.983905000
H	-2.439615000	2.540109000	-1.153745000
C	-9.951951000	0.416877000	1.430065000
O	-10.604577000	1.460819000	1.306762000
O	-10.507604000	-0.752646000	1.894952000
H	-11.458346000	-0.626280000	2.101205000
C	-5.553118000	5.974786000	-1.396528000
O	-4.791974000	6.826807000	-1.865855000
O	-6.877217000	6.225207000	-1.127251000
H	-7.112851000	7.148495000	-1.361137000
C	-5.594508000	-5.828352000	1.892185000
O	-6.750366000	-6.066695000	2.260211000
O	-4.612076000	-6.786192000	1.856150000
H	-4.960018000	-7.654619000	2.152157000

C	2.849435000	-0.767026000	-2.462695000
C	2.235298000	-0.388988000	-1.284690000
S	3.507745000	0.019743000	-0.041022000
C	4.829116000	-0.371526000	-1.233045000
C	4.265648000	-0.760217000	-2.436050000
H	2.295051000	-1.063470000	-3.345218000
H	4.864389000	-1.062255000	-3.285351000
C	6.225584000	-0.249347000	-0.863378000
C	6.642360000	-0.126158000	0.481988000
C	7.237908000	-0.249887000	-1.853789000
C	7.982345000	-0.018838000	0.824846000
C	8.580162000	-0.143485000	-1.522041000
C	8.988227000	-0.026408000	-0.170911000
H	5.903639000	-0.145166000	1.277189000
H	6.965026000	-0.303457000	-2.902218000
H	8.264334000	0.055178000	1.867514000
H	9.325552000	-0.130067000	-2.307169000
N	10.346111000	0.081499000	0.168394000
C	11.369429000	-0.451435000	-0.691286000
C	11.295357000	-1.773053000	-1.160219000
C	12.475211000	0.338505000	-1.043694000
C	12.303902000	-2.283431000	-1.980632000
C	13.484667000	-0.188343000	-1.851381000

C	13.416722000	-1.504345000	-2.342001000
H	10.454948000	-2.396977000	-0.875589000
H	12.541957000	1.357572000	-0.678886000
H	12.234738000	-3.309110000	-2.331360000
H	14.335821000	0.434665000	-2.110473000
C	10.757554000	0.725462000	1.387299000
C	10.280806000	2.003717000	1.720061000
C	11.666597000	0.089338000	2.247716000
C	10.698894000	2.623003000	2.900231000
C	12.088566000	0.725006000	3.416660000
C	11.614101000	2.001471000	3.767306000
H	9.588121000	2.507839000	1.054715000
H	12.037947000	-0.898076000	1.996663000
H	10.320080000	3.611461000	3.143912000
H	12.790851000	0.218385000	4.072371000
H	-0.930070000	1.450865000	5.099765000
C	12.096100000	2.693481000	5.022445000
H	13.038087000	3.229967000	4.844557000
H	11.366979000	3.427202000	5.381365000
H	12.280335000	1.976790000	5.830083000
C	14.497436000	-2.056638000	-3.243999000
H	14.316412000	-1.788211000	-4.293829000
H	15.483805000	-1.663640000	-2.975420000

H	14.543507000	-3.149210000	-3.190709000
H	-3.498591000	-1.578666000	-5.725180000
O	-6.328866000	-0.578396000	-2.235622000
C	-7.506516000	-0.776466000	-3.066563000
H	-7.517326000	-0.080701000	-3.913344000
H	-7.564708000	-1.806615000	-3.435837000
H	-8.354618000	-0.572563000	-2.413920000

Optimized Cartesian Coordinates for (9):

Ru	-4.304909000	0.001026000	0.040675000
C	-4.340542000	-0.946270000	-1.808535000
N	-2.296471000	-0.218119000	-0.336489000
N	-3.337040000	0.880548000	1.781636000
C	-5.446789000	-1.334157000	-2.595430000
C	-5.286289000	-1.970768000	-3.832699000
H	-6.144953000	-2.262294000	-4.424838000
C	-3.999522000	-2.239971000	-4.322361000
C	-2.880986000	-1.875584000	-3.583455000
H	-1.890329000	-2.087988000	-3.971453000
C	-3.047531000	-1.233862000	-2.338311000
C	-1.909639000	-0.818303000	-1.508815000
C	-0.551568000	-0.966063000	-1.793319000

H	-0.257368000	-1.435291000	-2.721665000
C	0.439766000	-0.508337000	-0.891980000
C	-0.008049000	0.101695000	0.307138000
H	0.715146000	0.466060000	1.024300000
C	-1.369476000	0.234686000	0.558412000
C	-1.961595000	0.852416000	1.756780000
C	-1.220607000	1.386056000	2.819894000
H	-0.138685000	1.360435000	2.793211000
C	-1.879584000	1.950108000	3.912450000
C	-3.279271000	1.972657000	3.927795000
H	-3.826096000	2.401718000	4.758524000
C	-3.970842000	1.429732000	2.847573000
H	-5.052842000	1.423357000	2.814503000
N	-4.721753000	-1.788831000	1.009812000
N	-6.209944000	0.232895000	0.428095000
N	-4.660717000	1.838656000	-0.863067000
C	-3.871608000	-2.826399000	1.233570000
H	-2.862138000	-2.697016000	0.868816000
C	-4.266508000	-3.989292000	1.883169000
H	-3.564157000	-4.796145000	2.042896000
C	-5.594514000	-4.101663000	2.326840000
C	-6.479378000	-3.045501000	2.094762000
H	-7.504366000	-3.140973000	2.431571000

C	-6.038207000	-1.898315000	1.432961000
C	-6.884119000	-0.749669000	1.113596000
C	-8.235251000	-0.592470000	1.414928000
H	-8.785358000	-1.350998000	1.955331000
C	-8.897491000	0.575809000	1.003698000
C	-8.196295000	1.565624000	0.294606000
H	-8.729550000	2.455391000	-0.016677000
C	-6.847777000	1.377987000	0.010193000
C	-5.967574000	2.279957000	-0.730920000
C	-6.373751000	3.493670000	-1.293460000
H	-7.393844000	3.838368000	-1.189767000
C	-5.454884000	4.269122000	-2.004968000
C	-4.134864000	3.808467000	-2.143397000
H	-3.414425000	4.396221000	-2.698382000
C	-3.777478000	2.599105000	-1.564705000
H	-2.775706000	2.202240000	-1.651325000
C	-10.327536000	0.809016000	1.290161000
O	-10.958983000	1.817028000	0.949411000
O	-10.906099000	-0.225560000	1.988468000
H	-11.853687000	-0.039416000	2.161208000
C	-5.826699000	5.562844000	-2.624583000
O	-5.050695000	6.283984000	-3.259670000
O	-7.145853000	5.888076000	-2.417581000

H	-7.364262000	6.746342000	-2.839857000
C	-6.105587000	-5.301152000	3.030658000
O	-7.265891000	-5.433871000	3.436149000
O	-5.145338000	-6.268464000	3.192445000
H	-5.512824000	-7.050440000	3.657509000
C	2.457044000	-1.217319000	-2.292690000
C	1.847657000	-0.650887000	-1.189781000
S	3.125820000	-0.033568000	-0.041080000
C	4.441956000	-0.610892000	-1.161671000
C	3.872784000	-1.197958000	-2.278866000
H	1.899120000	-1.657868000	-3.110368000
H	4.468315000	-1.632952000	-3.070878000
C	5.839694000	-0.415989000	-0.833264000
C	6.271793000	-0.088276000	0.472444000
C	6.839359000	-0.544687000	-1.828483000
C	7.613311000	0.094428000	0.774112000
C	8.182868000	-0.363097000	-1.538868000
C	8.607070000	-0.037383000	-0.226524000
H	5.543789000	-0.003751000	1.273359000
H	6.553481000	-0.757237000	-2.853041000
H	7.906524000	0.325525000	1.790230000
H	8.916455000	-0.449814000	-2.330279000
N	9.963975000	0.151801000	0.068960000

C	10.992161000	-0.427586000	-0.756159000
C	11.007381000	-1.803236000	-1.023291000
C	12.015537000	0.384028000	-1.280790000
C	12.013712000	-2.367106000	-1.816092000
C	13.027371000	-0.171762000	-2.055858000
C	13.029018000	-1.549351000	-2.331079000
H	10.229835000	-2.437230000	-0.610811000
H	12.011980000	1.448109000	-1.072807000
H	12.001560000	-3.432692000	-2.008464000
H	13.822808000	0.438237000	-2.466809000
C	10.377922000	0.932643000	1.204814000
C	9.884898000	2.237975000	1.398469000
C	11.310633000	0.415570000	2.113072000
C	10.304215000	2.994990000	2.487297000
C	11.750354000	1.178262000	3.200540000
C	11.241046000	2.469641000	3.392673000
H	9.176528000	2.653674000	0.690319000
H	11.700266000	-0.585553000	1.965672000
H	9.936888000	4.001348000	2.649248000
H	12.475946000	0.755180000	3.883899000
O	14.077676000	-1.999665000	-3.119288000
C	14.162316000	-3.414218000	-3.440515000
H	14.271178000	-4.021264000	-2.534242000

H	13.283175000	-3.746575000	-4.004907000
H	15.054042000	-3.512069000	-4.057810000
O	11.598751000	3.308869000	4.438195000
C	12.585649000	2.849998000	5.401480000
H	12.234697000	1.959128000	5.935254000
H	13.544095000	2.635542000	4.914835000
H	12.704627000	3.675545000	6.101585000
H	-1.311981000	2.364759000	4.737352000
H	-3.885256000	-2.733679000	-5.281226000
O	-6.715222000	-1.046089000	-2.067215000
C	-7.892987000	-1.407707000	-2.841214000
H	-7.907349000	-0.893038000	-3.808714000
H	-7.949236000	-2.490685000	-2.999717000
H	-8.740596000	-1.080938000	-2.239963000