SUPPORTING INFORMATION

(Organometallics)

Reactions of Conjugated Dienes with a Triruthenium Hydrido Carbonyl Cluster: Synthesis and Reactivity of Trinuclear Derivatives Having an Edge-Bridging Allyl Ligand

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Table SI-1. Atomic coordinates for structure I (DFT data)

Ru	0.443199	-1.422600	0.562700
Ru	0.445000	1.420799	0.563700
Ru	2.884700	-0.002300	0.217200
O	3.126299	3.084500	0.387999
C	3.609200	-0.002300	1.974100
C	2.588299	2.046300	0.341000
O	4.041300	-0.002200	3.040999
O	3.123999	-3.089100	0.388400
C	0.574700	-2.087300	2.345700
O	0.634700	2.459799	3.437600
O	-0.122801	-4.172100	-0.701600
C	2.587600	-2.050100	0.340800
C	0.086200	-3.134000	-0.240401
O	0.630999	-2.464300	3.435600
C	0.577700	2.083700	2.347300
N	1.748600	-0.000901	-1.765100
N	0.456500	-0.000300	-1.093400
C	1.904499	-1.197000	-2.629000
H	1.770800	-2.101601	-2.042101
H	2.905999	-1.193000	-3.064500
H	1.160700	-1.178600	-3.437600
C	1.905799	1.195200	-2.628601
H	1.772699	2.099900	-2.041600
H	1.162100	1.177699	-3.437300
H	2.907300	1.190499	-3.063901
O	-0.109500	4.172100	-0.702200
C	0.090500	3.133200	-0.238900
O	5.664900	-0.000000	-1.106100
C	4.625700	-0.001400	-0.605100
C	-1.801800	-1.297600	0.788699
H	-2.006601	-2.051200	1.549099
C	-1.800000	1.298100	0.791300
H	-2.003000	2.050499	1.553300
C	-1.611600	-0.000500	1.363900
C	-2.616901	-1.552200	-0.474700
H	-2.484500	-2.599501	-0.765601
H	-2.238901	-0.967900	-1.316000
C	-2.615500	1.556500	-0.471200
H	-2.238300	0.974100	-1.314101
H	-2.482100	2.604499	-0.759300
C	-4.569100	0.002000	0.369699
H	-5.664900	0.002499	0.430800
H	-4.220901	0.000500	1.409400
C	-4.139400	-1.308600	-0.307700
H	-4.601400	-1.378500	-1.301900
H	-4.558001	-2.138000	0.277300
C	-4.138100	1.314100	-0.304301
H	-4.555701	2.142299	0.283000
H	-4.600400	1.387000	-1.298200
H	-1.434101	-0.001600	2.435800
H	-0.283300	0.000299	-1.801900

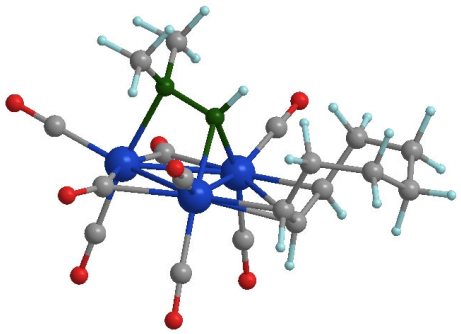


Table SI-2. Atomic coordinates for structure II (DFT data)

Ru	-0.394050	0.955800	0.511200
Ru	-0.374150	-1.782901	0.183400
Ru	-2.914450	-0.516600	0.596900
N	-2.312951	-0.177500	-1.569600
N	-0.898950	-0.204901	-1.240900
H	-0.358750	-0.080801	-2.103100
C	-2.648950	-1.227400	-2.561100
H	-3.731850	-1.251100	-2.699800
H	-2.309450	-2.198000	-2.209700
H	-2.166850	-1.008000	-3.524400
O	-3.040250	2.361800	1.423600
C	-2.473050	1.413099	1.018500
O	-3.387150	-1.207000	3.524400
O	-0.019850	3.783300	-0.635500
O	-5.922750	-0.421800	0.054600
O	-2.815050	-3.783300	0.030600
O	1.290650	-3.662000	-1.625300
O	0.290050	1.783000	3.383400
O	0.042550	-3.267500	2.842300
C	-0.175750	2.729899	-0.189400
C	-2.702150	1.129400	-2.154800
H	-2.469350	1.934300	-1.463000
H	-3.777650	1.119900	-2.344000
H	-2.170850	1.296700	-3.102600
C	-0.096150	-2.702000	1.848300
C	0.653050	-2.985600	-0.944400
C	-3.213550	-0.937301	2.415400
C	-2.104050	-2.870601	0.069700
C	-4.784250	-0.467200	0.264300
C	0.029150	1.484600	2.301200
C	1.728850	0.403900	-0.343400
H	1.433150	0.285499	-1.384100
C	1.318450	-0.561401	0.586600
C	2.907950	1.355100	-0.197000
C	2.196750	-0.777700	1.806500
H	2.699650	2.240000	-0.810100
H	3.001150	1.718500	0.831600
H	1.608250	-1.064801	2.680700
H	2.697250	0.158700	2.077900
C	4.187450	-1.654300	0.342200
H	4.936250	-2.455001	0.369100
H	3.612850	-1.823101	-0.577100
C	3.281050	-1.853301	1.569800
H	2.803150	-2.837700	1.492400
H	3.904950	-1.888700	2.472300
C	4.259850	0.768100	-0.660200
H	4.141250	0.348900	-1.669500
H	4.960950	1.606300	-0.763600
C	4.913750	-0.292200	0.246200
H	5.060050	0.125699	1.252200
H	5.922750	-0.464201	-0.147700

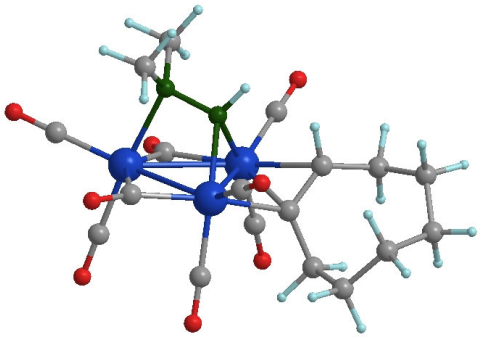


Table SI-3. Atomic coordinates for structure III (DFT data)

Ru	2.149250	-0.006751	0.257750
Ru	-0.290550	-1.429650	0.563350
Ru	-0.286450	1.422349	0.565250
O	-0.145650	-2.546750	3.411350
O	-0.944050	-4.132750	-0.760150
O	2.391550	3.083549	0.397550
C	2.830350	-0.008350	2.030150
C	-2.305350	-0.001750	1.410650
H	-2.138250	-0.002850	2.482850
O	2.383350	-3.097950	0.394750
C	-3.339850	-1.258050	-0.536350
H	-2.687550	-1.308650	-1.416450
H	-3.957650	-2.161950	-0.571050
O	3.235050	-0.009450	3.108150
C	-0.173950	2.114450	2.340150
C	-0.182950	-2.132650	2.334350
C	1.849150	2.047250	0.360150
C	1.211650	-1.199251	-2.608750
H	1.073350	-2.104950	-2.024450
H	2.217250	-1.194350	-3.034850
H	0.475650	-1.180450	-3.424550
C	-2.529950	-1.255550	0.767350
C	-0.689950	3.114250	-0.261350
C	-2.526250	1.253650	0.769350
N	-0.250850	-0.002250	-1.087150
H	-0.984950	-0.000750	-1.803650
C	1.844050	-2.059950	0.358150
C	-4.213350	0.002550	-0.650250
H	-4.756350	0.004049	-1.602450
H	-4.964850	0.002949	0.149450
O	-0.934050	4.132750	-0.746950
O	4.964850	-0.010150	-0.989350
C	3.909950	-0.008851	-0.522150
O	-0.126850	2.507849	3.424550
C	-3.336350	1.260550	-0.534250
H	-3.951750	2.166250	-0.567350
H	-2.684050	1.310850	-1.414350
C	1.215150	1.192450	-2.607150
H	1.078650	2.097650	-2.021950
H	0.479650	1.176350	-3.423450
H	2.220950	1.185550	-3.032650
N	1.047650	-0.003750	-1.745750
C	-0.697750	-3.117350	-0.269250
H	-2.779550	2.060850	1.452250
H	-2.785850	-2.062950	1.449150

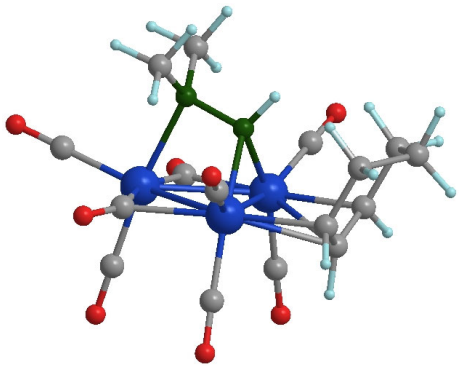


Table SI-4. Atomic coordinates for structure IV (DFT data)

Ru	1.969899	-0.255699	0.351700
Ru	-0.771300	-1.164800	-0.060299
Ru	-0.211399	1.527500	-0.215400
O	-1.870300	-1.952100	2.689000
O	-1.613800	-3.788300	-1.415899
O	2.563400	3.011700	-0.009900
C	2.157799	0.004700	2.214999
C	-2.170899	0.703600	-0.104000
H	-2.739400	0.701500	1.983200
O	1.422600	-3.130500	0.970799
C	-4.039499	-0.768699	-1.100900
H	-4.652999	-0.215000	-1.829000
H	-3.984399	-1.795999	-1.479200
O	2.266300	0.177400	3.351299
C	-0.475600	2.346200	1.505300
C	-1.458400	-1.669200	1.649600
C	1.680100	2.269500	-0.098199
C	1.717900	-1.693299	-2.511600
H	1.255400	-2.462399	-1.899100
H	2.786399	-1.900799	-2.600000
H	1.265300	-1.700800	-3.513100
C	-2.656400	-0.137300	-1.106200
C	-0.887100	2.983600	-1.317599
C	-3.115999	1.098499	1.034000
N	0.136400	-0.058199	-1.684400
H	-0.321100	-0.026100	-2.601300
C	1.101100	-2.062100	0.591799
C	-4.720099	-0.716600	0.268400
H	-5.772900	-1.004600	0.173100
H	-4.256300	-1.440899	0.949800
O	-1.332300	3.824000	-1.967200
O	4.930599	-0.970799	0.085299
C	3.811100	-0.692099	0.191600
O	-0.607999	2.835900	2.539099
C	-4.590200	0.696700	0.840099
H	-5.118200	0.787000	1.795800
H	-5.072299	1.401300	0.148699
C	2.189700	0.637700	-2.762100
H	2.028299	1.641000	-2.378000
H	1.773000	0.573399	-3.777300
H	3.261799	0.434500	-2.801699
N	1.542900	-0.362100	-1.878800
C	-1.284199	-2.815500	-0.887900
H	-3.065099	2.188099	1.140599
H	-2.203299	-0.120699	-2.093600

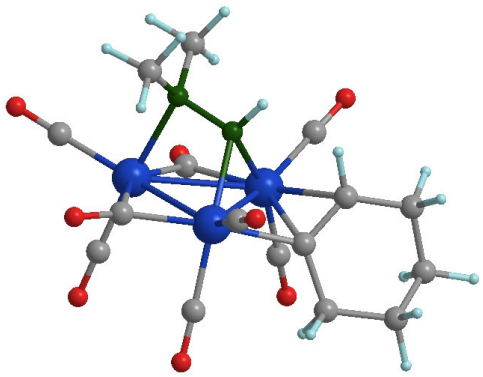


Table SI-5. Atomic coordinates for structure X (DFT data)

H	0.43974400	0.74846400	-3.85480900
C	1.13222000	0.84476500	-3.00755100
H	2.15875100	0.77395200	-3.37372200
H	0.98604900	1.81180900	-2.53512500
N	0.89474100	-0.24485600	-2.02906500
C	1.09531900	-1.53032100	-2.74199400
H	0.41190500	-1.59881500	-3.59935300
H	2.12606900	-1.57854500	-3.09931300
H	0.90858100	-2.36361200	-2.07071800
N	-0.43831600	-0.16166500	-1.45179400
H	-1.15097200	-0.27827000	-2.17863600
Ru	-0.56420300	1.43537300	0.02739700
C	-0.83853200	3.01911400	-1.03632100
O	-1.01796300	3.97188400	-1.66306100
C	1.58752900	2.00177700	-0.09650100
O	2.14037800	3.03445800	-0.12370900
C	-2.82805600	1.40571000	0.03259100
H	-3.09965100	1.27012800	-1.01298200
Ru	1.88172500	-0.04426400	0.03044800
C	3.67991200	-0.11846000	-0.65378500
O	4.75433300	-0.16006200	-1.07191100
Ru	-0.60367800	-1.38949400	0.31602200
C	-0.95141600	-3.14713100	-0.38086200
O	-1.18198600	-4.19956300	-0.79485000
C	-2.75532200	-1.11919500	0.17989600
O	-3.15341600	-1.19993800	-1.16768600
C	-4.55742500	-1.37927300	-1.33130200
H	-5.12463700	-0.52961100	-0.92753700
H	-4.89927300	-2.29933300	-0.83672700
C	1.56415900	-2.07168200	0.36122000
O	2.06944900	-3.10363800	0.56999600
C	-3.49471900	2.59948200	0.69357800
H	-3.26458000	3.53630000	0.17963400
H	-4.58579900	2.47590900	0.67295500
C	-2.68984700	0.19807800	0.75958000
H	-3.23917800	-1.87489300	0.80425300
H	-3.19742900	2.70759800	1.74053000
C	-0.51720300	2.30523200	1.72742500
H	-2.71124000	0.24590500	1.84524500
C	2.46448500	0.15028000	1.82792300
C	-0.70119900	-1.91295100	2.15399500
O	-0.47486300	2.80502000	2.76755500
O	2.80949600	0.26819700	2.91985800
O	-0.78994800	-2.20182600	3.26865200
H	-4.74574200	-1.46120600	-2.40396300

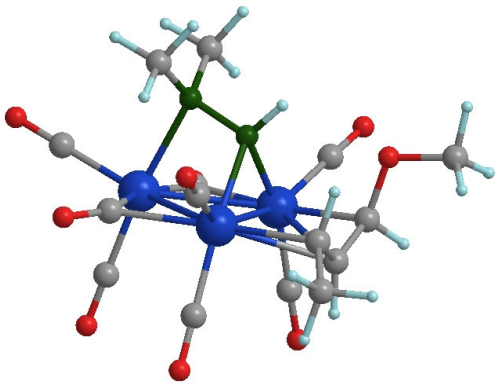


Table SI-6. Atomic coordinates for structure XI (DFT data)

H	-0.54073200	-1.13980100	-3.81421100
C	-1.00986900	-1.44934200	-2.86988800
H	-1.99500300	-1.87035500	-3.08145000
H	-0.39040200	-2.20424300	-2.39411600
N	-1.16928000	-0.27978100	-1.97153700
C	-1.99090500	0.72434500	-2.69071800
H	-1.50354000	1.00602000	-3.63443800
H	-2.96926800	0.29133400	-2.90949400
H	-2.11949700	1.61059300	-2.07587800
N	0.12322900	0.27306900	-1.58844200
H	0.61771400	0.56536300	-2.43691500
Ru	1.08262400	-0.97536400	-0.08532700
C	1.95928900	-2.34997800	-1.10753600
O	2.49761100	-3.16165100	-1.72567200
C	-0.60857300	-2.45930200	0.09042900
O	-0.64793900	-3.62525800	0.16075000
C	2.99549800	0.05415500	-0.26168700
H	3.23760900	0.20978000	-1.31763600
Ru	-1.73408300	-0.71075800	0.20212900
C	-3.46184800	-1.45228400	-0.22185100
O	-4.49651700	-1.89289400	-0.47882500
Ru	-0.08097900	1.60938600	0.12894200
C	-0.61798200	3.28832300	-0.64014200
O	-0.93066000	4.30413800	-1.09199200
C	2.01046200	2.40317100	-0.13481700
C	2.39670200	2.79473800	-1.55261900
H	1.86433900	3.69559800	-1.86789300
H	2.19077600	2.01494100	-2.29071500
H	3.47210100	3.01193600	-1.60743200
C	-2.28143400	1.27290100	0.40508700
O	-3.17250700	1.99706400	0.63421100
O	3.98358500	-0.69631000	0.39800700
C	5.28218800	-0.12134000	0.29990500
C	2.46509800	1.18540300	0.44744200
H	2.04813800	3.24717900	0.55107200
H	5.32574400	0.86749100	0.77777800
C	1.63961200	-1.65202200	1.62169100
H	2.58873800	1.15240700	1.52664900
C	-1.96700300	-0.97307300	2.06906600
C	-0.10260100	2.23187600	1.93232500
O	1.94269400	-2.04397900	2.66150100
O	-2.09922300	-1.12860300	3.20200100
O	-0.08856700	2.59746300	3.02722300
H	5.59672700	-0.02056700	-0.74945500
H	5.96655400	-0.79944500	0.81350500

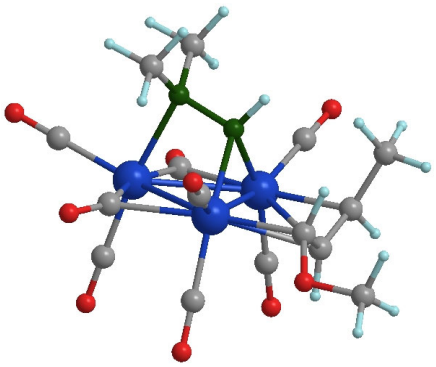


Table SI-7. Atomic coordinates for structure XII (DFT data)

H	0.37348400	1.02118600	-3.76867200
C	1.11607000	0.89512400	-2.96894600
H	2.08264000	0.64755300	-3.41306000
H	1.20379100	1.82469100	-2.41386200
N	0.70730000	-0.20498500	-2.06177000
C	0.58463400	-1.43479500	-2.88165000
H	-0.14321500	-1.28009500	-3.68993300
H	1.55875500	-1.66946300	-3.31599700
H	0.25733000	-2.26471200	-2.26202900
N	-0.54101800	0.10436600	-1.38039200
H	-1.29565500	0.20239100	-2.06692500
Ru	-0.22514200	1.55367500	0.21938600
C	-0.18847900	3.27588900	-0.64498200
O	-0.15349900	4.31847600	-1.13937800
C	1.98958100	1.66777300	-0.02755600
O	2.74828000	2.56041400	-0.02175600
C	-2.44735400	1.99793100	0.43140500
C	-3.16554100	2.41136200	-0.84377400
Ru	1.83802100	-0.39540700	-0.07636500
C	3.53264100	-0.78914300	-0.90284300
O	4.54422100	-1.02096400	-1.40664200
Ru	-0.84984800	-1.21611300	0.30980800
C	-1.60960100	-2.80652000	-0.46665500
O	-2.08062500	-3.75549500	-0.92445000
C	-2.93655100	-0.53337300	0.40044600
O	-3.48266700	-0.50512000	-0.89100600
C	-4.89185500	-0.70362200	-0.92045300
H	-5.42615900	0.10310000	-0.40036200
H	-5.16674100	-1.66417500	-0.46231000
C	1.11077300	-2.33140700	0.11854100
O	1.39706100	-3.46139200	0.19997000
H	-2.46134600	2.78814900	1.17997100
H	-2.95836900	1.75484300	-1.68769400
H	-2.89011600	3.43290700	-1.11850000
C	-2.53900900	0.70420200	1.01263700
H	-3.46557600	-1.22164300	1.06374600
H	-4.25215300	2.40103700	-0.68366200
C	0.07287500	2.22159900	1.98165400
H	-2.40936300	0.64582400	2.08898600
C	2.55843400	-0.48895000	1.67894000
C	-0.90912900	-1.85675300	2.10959000
O	0.22691600	2.60375500	3.06030300
O	2.98848400	-0.54273800	2.74548600
O	-0.96562600	-2.21376600	3.20668300
H	-5.18988000	-0.71334700	-1.97085200

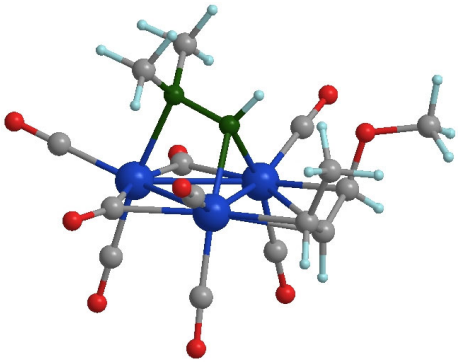


Table SI-8. Atomic coordinates for structure XIII (DFT data)

H	0.79375800	-1.45209900	-3.70893200
C	1.24868500	-1.63101200	-2.72492800
H	2.27475300	-1.97848900	-2.86347400
H	0.67892700	-2.39320000	-2.20081300
N	1.26866600	-0.37478800	-1.93552800
C	2.02981100	0.62918300	-2.71889300
H	1.55815000	0.78040800	-3.69979600
H	3.04895700	0.26510000	-2.86472700
H	2.06080900	1.57614100	-2.18741500
N	-0.08145700	0.08837300	-1.64599400
H	-0.56864000	0.26373800	-2.53139000
Ru	-0.98960800	-1.10239900	-0.07050600
C	-1.68227300	-2.64848800	-0.98194800
O	-2.11327200	-3.56444500	-1.53500700
C	0.81289400	-2.40526300	0.31548100
O	0.94685000	-3.55056100	0.50517700
C	-2.94313800	-0.26249500	-0.46886400
H	-3.09977900	-0.20939200	-1.55385900
Ru	1.78521900	-0.56280600	0.28631700
C	3.57904500	-1.18647200	-0.03253800
O	4.65281400	-1.55744300	-0.23335800
Ru	-0.07562000	1.58607600	-0.05595400
C	0.37383600	3.21116300	-0.97959800
O	0.62632300	4.19213000	-1.53452400
C	-2.18216000	2.15455400	-0.53502400
H	-2.25472800	2.07812900	-1.62262400
C	2.14551200	1.46877200	0.32634400
O	2.95431400	2.29314100	0.51770500
O	-3.92828400	-1.03261400	0.16945500
C	-5.25314900	-0.58209500	-0.09350100
H	-5.47361500	-0.59658500	-1.17116200
C	-2.57777200	0.97843000	0.16099600
C	-2.64457600	3.50325800	-0.00698200
H	-5.41981200	0.43552700	0.28662900
C	-1.58629900	-1.65430000	1.66703700
H	-2.82449400	1.06383400	1.21757300
C	1.98736600	-0.63999200	2.17415200
C	-0.17208600	2.36467800	1.68328600
O	-1.92300000	-1.96261500	2.72467300
O	2.10290200	-0.68439800	3.31849200
O	-0.23354800	2.81265700	2.74581600
H	-2.07741600	4.33050100	-0.44130800
H	-2.55262000	3.56616700	1.08106400
H	-3.70179600	3.66231400	-0.25825100
H	-5.92749100	-1.27182100	0.41782700

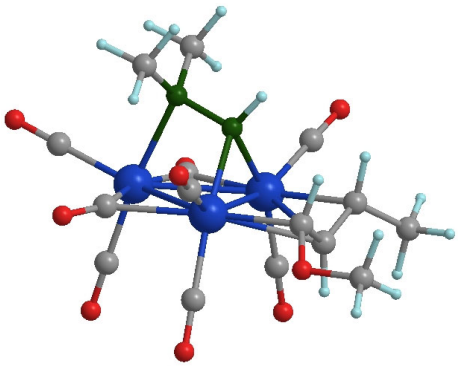


Table SI-9. Atomic coordinates for structure XIV (DFT data)

Ru	-0.68583700	-1.22705000	0.20853900
Ru	-0.33342600	1.46791900	-0.26755400
Ru	2.01352100	-0.12686200	0.21815700
N	1.35663900	-0.47932400	-1.93054100
N	-0.03986700	-0.24011100	-1.60868000
H	-0.58782400	-0.32437800	-2.47127100
C	1.83161900	0.46451500	-2.97024700
H	2.90608200	0.32822700	-3.10885100
H	1.63513000	1.48890200	-2.66577300
H	1.31742400	0.27077700	-3.92260800
O	1.72889200	-2.94802500	1.16946200
C	1.29131900	-1.94872400	0.72407400
O	2.57677700	0.61823500	3.11529100
O	-1.36933700	-4.06279800	-0.75015000
O	4.97237600	-0.70327300	-0.29672000
O	2.35010900	3.09850100	-0.53596500
O	-1.76454200	3.47622800	-2.14490300
O	-1.47657700	-1.81531900	3.11139800
O	-0.54187900	3.08825500	2.33745300
C	-1.14032000	-2.99031700	-0.38169300
C	1.55245500	-1.85404200	-2.45351700
H	1.21316700	-2.58280100	-1.72290800
H	2.61635100	-2.00780700	-2.64606400
H	0.99416700	-1.98833000	-3.39104500
C	-0.47836100	2.47701500	1.36387800
C	-1.21425900	2.74720300	-1.44356400
C	2.36893100	0.32803700	2.01721800
C	1.50139600	2.31698700	-0.44509000
C	3.85380000	-0.47521900	-0.09848700
C	-1.17592500	-1.60300900	2.01978300
C	-2.77571100	-0.33322000	-0.73723900
H	-2.45795800	-0.40120700	-1.77539200
C	-2.18477800	0.51924300	0.19093600
O	-4.01422700	-0.85841700	-0.51054100
C	-3.03938400	0.88409800	1.39813000
H	-2.41465200	1.11012700	2.26499500
H	-3.66348900	0.02689300	1.67263000
C	-3.96578200	2.07802900	1.10323700
H	-3.39531600	2.97603700	0.84513400
H	-4.57709800	2.31113300	1.98077100
C	-4.42124700	-1.89458200	-1.39743400
H	-4.63930200	1.85118000	0.27146400
H	-3.84239600	-2.80871700	-1.22386200
H	-4.30931500	-1.58670800	-2.44597600
H	-5.47499000	-2.08674400	-1.19148300

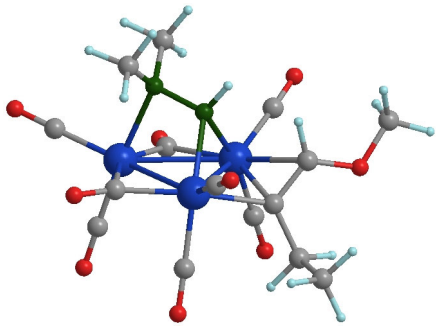


Table SI-10. Atomic coordinates for structure XV (DFT data)

Ru	-0.64919500	-1.26591500	0.12211200
Ru	-0.33558900	1.45925100	-0.22395300
Ru	2.03039600	-0.11344000	0.21599400
N	1.40382700	-0.37859000	-1.95335300
N	0.00130500	-0.17803300	-1.63431900
H	-0.54489000	-0.23515400	-2.50021500
C	1.87526200	0.62319500	-2.93919800
H	2.95258100	0.50702000	-3.07416400
H	1.66369500	1.62848900	-2.58450400
H	1.37175800	0.47203400	-3.90475700
O	1.79307800	-2.97629600	1.05508800
C	1.34749600	-1.96661900	0.64393500
O	2.57035400	0.51841000	3.14528300
O	-1.36412800	-4.03630800	-0.99717500
O	5.00320200	-0.59683900	-0.31071900
O	2.32521000	3.15955000	-0.31953400
O	-1.73819700	3.56302500	-2.01026800
O	-1.46627800	-1.98223000	2.99318000
O	-0.70847200	2.87402100	2.48620600
C	-1.07195200	-3.00746700	-0.56186100
C	1.62909400	-1.72341200	-2.53844500
H	1.29343500	-2.49151700	-1.84701200
H	2.69768600	-1.85053100	-2.72422700
H	1.08406000	-1.82216100	-3.48792000
C	-0.57055500	2.34978100	1.47235700
C	-1.19767100	2.79447800	-1.34256200
C	2.36981400	0.27072700	2.03585000
C	1.50118900	2.34742900	-0.30012800
C	3.87935900	-0.40354000	-0.10565500
C	-1.15978500	-1.72093000	1.91553600
C	-2.72653500	-0.49074300	-0.69972500
H	-2.44059200	-0.46329600	-1.74820300
C	-2.14152700	0.45290000	0.15929500
C	-4.01454800	-1.24768200	-0.43078600
O	-2.77984100	0.71297900	1.36286500
H	-3.85026900	-2.31666700	-0.60755700
H	-4.28717100	-1.14583600	0.62352400
C	-3.88084000	1.62022900	1.29141500
H	-3.55129800	2.60220100	0.92743500
H	-4.25757100	1.72328900	2.31022400
C	-5.16818600	-0.78822400	-1.34023600
H	-4.68044400	1.24853400	0.64246600
H	-4.92017900	-0.94042600	-2.39668800
H	-5.39958400	0.27360900	-1.20779200
H	-6.07714300	-1.35989300	-1.12777500

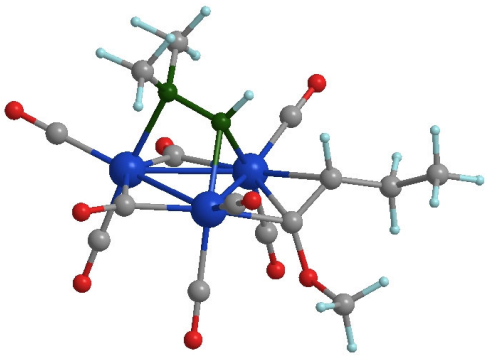


Table SI-11. Atomic coordinates for the structure of the cation of compound 6 (DFT data)

Ru	-0.32411900	-1.45690700	0.30132300
Ru	-0.32411400	1.45694700	0.30133200
Ru	2.16415900	0.00004500	-0.05776700
O	2.39920700	3.10310700	0.07113700
C	3.03938900	0.00003100	1.66099100
C	1.88697600	2.06066000	0.04637600
O	3.55273500	0.00000000	2.68306000
O	2.39911500	-3.10299800	0.07128600
C	-0.27497500	-2.39442100	1.98617100
O	-0.25074200	2.92175900	3.00357800
O	-0.89210200	-4.06190200	-1.22394900
C	1.88678600	-2.06059000	0.04653100
C	-0.69031200	-3.08502400	-0.65689800
O	-0.25098400	-2.92175800	3.00357700
C	-0.27487000	2.39449200	1.98613400
N	1.01084100	-0.00001200	-2.00173600
N	-0.27815800	-0.00001500	-1.31673500
C	1.15745400	-1.19550400	-2.87938000
H	1.04802500	-2.10904200	-2.30316400
H	2.14792200	-1.17809000	-3.33705600
H	0.39836400	-1.17321200	-3.67079400
C	1.15742000	1.19547900	-2.87938200
H	1.04794200	2.10901800	-2.30317800
H	0.39834600	1.17315200	-3.67081200
H	2.14789600	1.17811400	-3.33704400
O	-0.89186100	4.06183600	-1.22404400
C	-0.69018100	3.08494800	-0.65694700
O	4.85878800	-0.00050000	-1.50515000
C	3.85973600	-0.00024900	-0.94262400
C	-2.62222700	-1.29309700	0.50116200
H	-2.80373900	-2.05222900	1.26102300
C	-2.62219100	1.29311600	0.50113800
H	-2.80370000	2.05225100	1.26099400
C	-2.45028200	0.00000900	1.07579800
C	-3.41160100	-1.55845700	-0.77346800
H	-3.27948400	-2.60708300	-1.05585800
H	-3.02678300	-0.97476400	-1.61192300
C	-3.41154900	1.55847400	-0.77350300
H	-3.02673800	0.97475500	-1.61194300
H	-3.27939900	2.60709200	-1.05590900
C	-5.37199900	0.00005000	0.05531100
H	-6.46720600	0.00006900	0.09837900
H	-5.04911000	0.00006100	1.10407000
C	-4.93719100	-1.31258700	-0.61415800
H	-5.38423700	-1.38595300	-1.61334300
H	-5.35929400	-2.14139100	-0.03325800
C	-4.93714700	1.31265200	-0.61419800
H	-5.35922800	2.14148600	-0.03332500
H	-5.38418400	1.38600300	-1.61338800
H	-2.23169000	0.00001200	2.14154300
H	-1.02444500	-0.00000300	-2.01684600
H	0.30858800	-0.00003400	1.20576300

