Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information

(Ms. for Dalton Transactions)

Activation of two C–H bonds of NHC N–methyl groups on triosmium and triruthenium carbonyl clusters

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Table SI-1. Atomic coordinates for the DFT-optimized structure of 2a

Os	1.37472100	0.00103100	0.84717500
Os	-0.86580400	1.50565900	-0.41968200
Os	-1.15448000	-1.44702400	0.05204000
C	0.65802200	0.44478100	2.60433700
O	0.28587900	0.65736800	3.67292400
C	2.78730100	-1.03631400	1.62684000
O	3.66470700	-1.61605700	2.10859800
C	2.26601900	1.68653000	0.68941800
O	2.82771200	2.69603400	0.61636500
C	-1.63153300	1.76653100	1.36977800
O	-2.11112100	1.99414700	2.39204700
C	-0.19006800	3.31378100	-0.44635700
O	0.18219600	4.40682500	-0.48422000
C	-2.59047400	1.73169300	-1.24593400
O	-3.61759300	1.89207000	-1.74929100
C	-0.02241200	1.10896800	-2.13417300
O	0.43441400	0.96501800	-3.18433100
C	-2.06908400	-1.09924500	1.73919600
O	-2.62064100	-0.97946300	2.74506900
C	-1.15489200	-3.33716000	0.34798500
O	-1.17243700	-4.48184600	0.50587900
C	-2.75388300	-1.37698900	-0.99177700
O	-3.70275000	-1.36207200	-1.65114700
C	2.04775300	-0.71118800	-1.06273100
N	1.36146200	-1.52254500	-1.90189800
N	3.28587100	-0.58123400	-1.63493400
C	2.14728700	-1.89156200	-2.98155600
H	1.77096600	-2.52919200	-3.76497800
C	3.35481800	-1.30168400	-2.81779300
H	4.24652500	-1.32602600	-3.42351400
C	-0.05874400	-1.91318300	-1.81471000
H	-0.07036400	-2.99214800	-1.99706200
H	-0.54876200	-1.46037200	-2.68089400
H	0.46604800	-1.57557500	0.87017800
C	4.40811500	0.20122300	-1.12504700
H	4.20946600	1.27191600	-1.20148600
H	5.28886100	-0.03583600	-1.72320000
H	4.61642700	-0.05422000	-0.08570100

Table SI-2. Atomic coordinates for the DFT-optimized structure of 3a

Os	-1.43873500	-0.28850400	-0.73487200
Os	0.60589700	1.58220200	0.18312600
Os	1.48677300	-1.16072300	-0.04537100
C	-0.84713600	0.04190400	-2.56283700
O	-0.47275900	0.22217100	-3.63755400
C	-2.64378100	-1.72354800	-1.20218700
O	-3.39574400	-2.54825000	-1.50669500
C	-2.66816600	1.18056000	-0.73158800
O	-3.44022800	2.04199600	-0.71778500
C	0.48631500	2.68374300	-1.43104000
O	0.40416900	3.33669300	-2.37915300
C	-0.64433000	2.59782000	1.20381600
O	-1.40499200	3.18050700	1.85259000
C	2.17418700	2.43496800	0.89404800
O	3.11009200	2.94742400	1.33953700
C	2.00797600	-1.85331400	-1.82072200
O	2.31351300	-2.28542500	-2.84187400
C	1.31436300	-2.84640500	0.85165400
O	1.18438600	-3.84467000	1.41422600
C	3.28084200	-0.90152800	0.56384500
O	4.35513500	-0.72680500	0.94246800
C	-1.67147500	-0.58430500	1.35224200
N	-0.58831300	-0.46089600	2.15121000
N	-2.69223300	-0.94201200	2.17839500
C	-0.91128200	-0.74643500	3.46549100
H	-0.18561200	-0.69590100	4.26129700
C	-2.23770000	-1.04843100	3.48657500
H	-2.89184600	-1.31440800	4.30132700
C	0.69839000	-0.02146100	1.62471000
H	1.35828300	0.09135400	2.48499400
H	1.59672700	0.47229900	-0.88529800
H	-0.23243100	-1.60535300	-0.56536100
C	-4.06456000	-1.21284600	1.76478300
H	-4.37819200	-0.47954900	1.02160100
H	-4.71674300	-1.13126300	2.63563700
H	-4.15580600	-2.21642100	1.34062600

Table SI-3. Atomic coordinates for the DFT-optimized structure of 3c

Ru	-1.46258300	-0.52741100	-0.64994100
Ru	0.31051900	1.61368200	0.15681200
Ru	1.61050600	-0.91695500	-0.18384300
C	-1.08852600	-0.08380900	-2.52769700
O	-0.84080900	0.14889100	-3.62525500
C	-2.48425800	-2.15346100	-1.02938100
O	-3.12977200	-3.07905800	-1.25092200
C	-2.91004400	0.73636700	-0.49646200
O	-3.81134700	1.44860300	-0.40427900
C	-0.09872600	2.71406400	-1.44180900
O	-0.33930300	3.35870100	-2.36322900
C	-1.00208100	2.40103300	1.31504800
O	-1.76466100	2.85603600	2.05127000
C	1.78131000	2.70356000	0.76987600
O	2.65366600	3.34863200	1.15813900
C	2.12712300	-1.50386100	-2.02967900
O	2.41063100	-1.86079000	-3.08125000
C	1.76324200	-2.61875500	0.71573200
O	1.81206900	-3.62434400	1.27106600
C	3.37575700	-0.33810200	0.32036000
O	4.42092500	0.02601400	0.62880200
C	-1.47058800	-0.88440500	1.39726600
N	-0.39200100	-0.60391500	2.13441300
O	-2.37674200	-1.45690900	2.21379500
C	-0.60417400	-1.00683400	3.45445100
H	0.13434900	-0.87580300	4.22863900
C	-1.84486300	-1.53107400	3.48420800
H	-2.46376300	-1.96028700	4.25384500
C	0.76463100	0.05463100	1.54001600
H	1.45253000	0.26145100	2.36096100
H	1.33825800	0.66740100	-0.99989100
H	-0.01887300	-1.57759900	-0.61433000