Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

Reactivity of a Trinuclear Ruthenium Complex Involving C-H Activation and Insertion of Alkene

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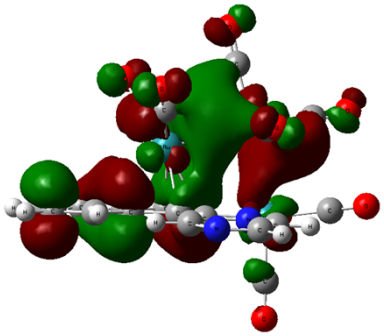

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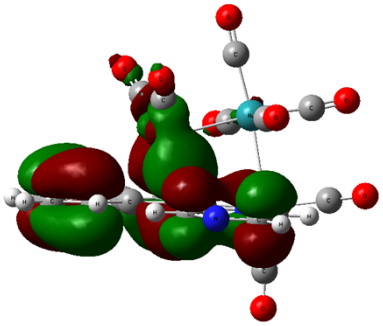

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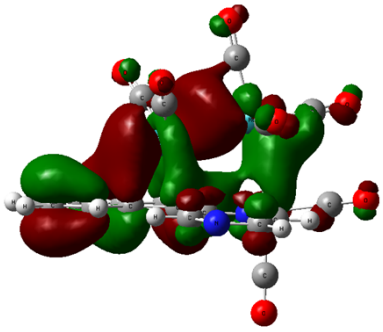

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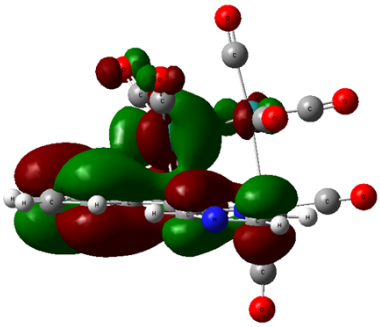

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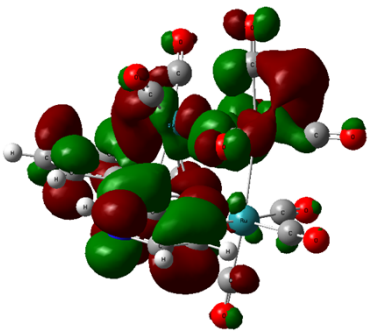

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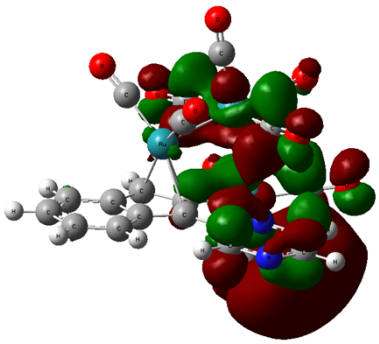

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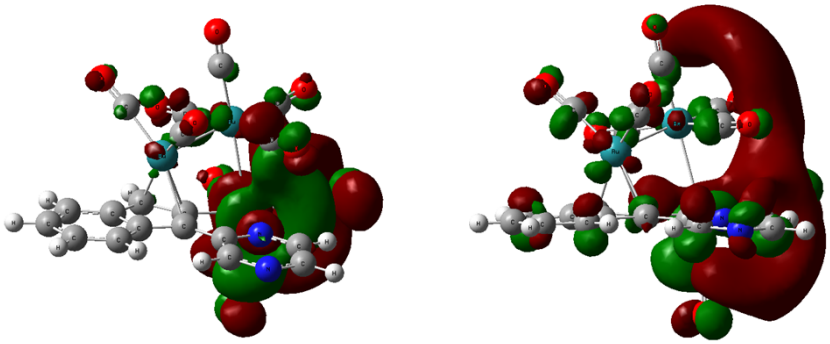

LUMO+3(+0.0761eV) LUMO+4(+0.0836eV)

Fig. *S*1 Frontier molecular orbitals of complex **1**

Table S1 Cartesian coordinates of the optimized complex **1**

Ru	0.00000000	0.00000000	0.00000000
Ru	0.00000000	0.00000000	3.81491800
Ru	2.23561300	0.00000000	1.80084200
C	-2.14541300	-1.02369000	0.07537800
C	-2.76786700	-1.72740600	-0.99132500
H	-2.62045800	-2.80483100	-1.08951000
C	-3.57890600	-1.03470000	-1.86720799
H	-4.08140200	-1.56683700	-2.67758899
C	-3.76872400	0.36674900	-1.73542299
H	-4.41126400	0.88627000	-2.44921400
C	-3.15323800	1.08754600	-0.72996199
H	-3.31433900	2.16311100	-0.66016099
C	-2.33411300	0.40432600	0.21245301
C	-1.59212700	0.79999400	1.41152200
C	-1.01916800	-0.38326500	2.03485600
C	-1.29097000	-1.47605999	1.15974801
H	-1.01663500	-2.51492099	1.33331400
C	-1.48201600	2.05324401	2.12996801
C	-2.08175500	3.28320401	1.77902101
H	-2.68745500	3.35255601	0.87448400
C	-1.21145600	4.30545201	3.61030801
H	-1.09258500	5.20939501	4.21240301
C	-0.60786400	3.11675501	3.99935501

H	-0.00828800	3.05945501	4.90791800
C	-1.57097800	-0.26734800	4.89652300
C	1.19338400	0.67908600	5.22763900
C	0.58127500	-1.78846300	4.05615300
C	3.52938800	-0.16195600	3.22271400
C	2.03407400	-1.92883300	1.51436700
C	3.43897200	0.19307100	0.30213800
C	2.00242200	1.92190000	2.01215500
C	0.86904600	-1.10952100	-1.24165600
C	0.63543000	1.54083700	-0.88098000
N	-0.73692800	1.98892801	3.27378600
N	-1.95698800	4.39407801	2.49663001
O	0.98069200	2.50421400	-1.42042200
O	1.35248799	-1.81599100	-2.01948800
O	4.18849499	0.33414300	-0.55661700
O	4.34083700	-0.26975400	4.03140200
O	1.95783900	-3.05862501	1.32103900
O	1.91787700	3.06536901	2.11022700
O	1.88249000	1.10818800	6.04044600
O	-2.48987500	-0.48957100	5.54947800
O	0.86312400	-2.88782101	4.25036700

Table S2 Cartesian coordinates of the optimized complex **4**

Ru	-0.74863600	-0.73001000	0.37796600
Ru	1.90638800	-1.05900800	-0.50764700
Ru	-3.40280700	0.51676900	0.05079700
Br	4.76154200	1.06744900	0.65630100
N	2.08824900	1.17853600	-0.23475300
O	-1.53776700	-3.42430500	1.51186000
O	-0.05736600	0.31452900	3.14231800
O	1.11169000	-3.93717800	-1.05192700
O	3.27116200	-1.92408800	2.15562200
O	4.20852400	-1.21043700	-2.54937300
O	-3.39245500	1.79949500	2.79462500
O	-4.94499400	-1.78528200	1.27621400
C	-0.11335700	0.96233500	-1.09451600
C	0.25154000	-0.39140700	-1.50774900
C	-0.96278600	-1.02247600	-1.93022800
H	-1.05292800	-2.02992900	-2.33119600
C	-2.03421100	-0.05362200	-1.93444500
C	-1.51305100	1.20452900	-1.40650700
C	-2.42420500	2.26807800	-1.16143200
H	-2.08723800	3.19281700	-0.69542100
C	-3.79880200	2.15526700	-1.53214700
H	-4.46343800	3.00832800	-1.39822400
C	-4.29532500	0.93898500	-2.05221800
H	-5.34804400	0.84538100	-2.31836200
C	-3.42472400	-0.17841800	-2.19589800
H	-3.82568600	-1.13473700	-2.53379800
C	0.93233700	1.83756700	-0.60189600
C	0.83856800	3.23458400	-0.51881600
H	-0.07063600	3.73261500	-0.84808900
C	1.91593200	3.97232000	-0.04402100
H	1.85524800	5.06004200	0.02802000
C	3.08614200	3.31146400	0.32505500
H	3.96020400	3.84369600	0.69367700
C	3.11691100	1.92213200	0.19561800

C	-1.24681400	-2.38291500	1.09875900
C	-0.34820700	-0.09675700	2.10061700
C	1.40970300	-2.84971000	-0.82075700
C	2.83321400	-1.57425900	1.15449100
C	3.38484900	-1.11275200	-1.75252100
C	-3.38580900	1.29944000	1.75112800
C	-4.34309000	-0.91298600	0.81286800

Table S3 Topological properties at the BCP of Ru-C bond

Ru-C bond	ρ_b	$\nabla^2\rho_b$	V_b	G_b	$-G_b / V_b$	H_b
Ru1-C2	0.085	0.264	-0.104	0.085	0.817	-0.019
Ru3-C6	0.057	0.226	-0.064	0.060	0.938	-0.004
Ru3-C7	0.062	0.243	-0.072	0.066	0.917	-0.006
Ru3-C8	0.060	0.241	-0.070	0.065	0.928	-0.005
Ru3-C9	0.056	0.219	-0.062	0.059	0.952	-0.003