Supporting Information

Ruthenium(II) Isocyanide Complexes Supported by Triazacyclononane/Trithiacyclononane and Aromatic Diimine: Structural, Spectroscopic, and Theoretical Studies

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Table S1. Standard orientation of **1** at the PBE1PBE optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
Ru	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.13260100
N	2.14940700	0.00000000	0.30441300
N	0.30620000	2.13876200	0.26907800
C	1.40268400	-0.16943400	2.66126500
H	1.75963300	0.79442800	3.03265700
H	1.39062700	-0.84103200	3.52664300
C	2.33796400	-0.72344200	1.59749200
H	2.12917400	-1.78082200	1.42885800
H	3.38278900	-0.64596300	1.93350300
C	2.94623400	-0.64370200	-0.77428600
H	3.99648800	-0.74404100	-0.47217800
H	2.89200800	-0.02217400	-1.66964000
H	2.54764300	-1.62383100	-1.02500600
C	2.66515700	1.40565400	0.45072600
H	2.80374300	1.63357000	1.50962600
H	3.65647000	1.49017600	-0.00860100
C	1.70980400	2.37890100	-0.19137600
H	1.70800000	2.25651600	-1.27909300
H	2.01038600	3.41343100	0.02936600
C	-0.53392700	3.07348700	-0.53243000
H	-1.53718100	3.14533300	-0.11976000
H	-0.59428300	2.72003100	-1.56250900
H	-0.09803100	4.08038600	-0.51825800
C	0.16961300	2.46230400	1.73716200
H	1.16122400	2.65179300	2.15653200
H	-0.38947900	3.39660500	1.86110700
C	-0.53564000	1.34771700	2.49865800
H	-1.60322000	1.33384500	2.26414100
H	-0.44213500	1.51592900	3.58189000
C	-0.87393700	-1.03733000	2.74462500
H	-0.47521900	-2.02667300	2.51453500
H	-1.88045100	-0.95762800	2.33154600
H	-0.91904400	-0.91191200	3.83380600
C	-3.02518500	0.86251500	-0.02789800
H	-2.66475100	1.82870200	0.28700500
C	-4.39793600	0.68824900	-0.26044800
H	-5.06901100	1.52729900	-0.12377200
C	-4.86535400	-0.54606700	-0.66229700
H	-5.91862900	-0.71163400	-0.86041200
C	-3.94583000	-1.60707400	-0.79479200

C	-2.57957200	-1.34060800	-0.52909100
C	-1.62590000	-2.40173000	-0.58415900
C	-2.05413500	-3.71151700	-0.91624500
C	-1.09370500	-4.74372700	-0.91224500
H	-1.38400800	-5.75820800	-1.16238600
C	0.20679600	-4.43396300	-0.57269000
H	0.97767700	-5.19412700	-0.54204500
C	0.54069600	-3.10705800	-0.26177000
H	1.56273600	-2.88014500	0.00029700
C	-4.34457600	-2.93275700	-1.16279000
H	-5.39092200	-3.11709600	-1.37986000
C	-3.43402700	-3.94469300	-1.22245900
H	-3.74163200	-4.94986600	-1.48887300
N	-2.11289900	-0.10412700	-0.17185000
N	-0.32977000	-2.09176000	-0.26802800
N	0.08184000	0.12581000	-2.01200000
C	0.08097300	0.15294800	-3.17087300
C	0.08352300	0.18732300	-4.62414300
H	-0.94025300	0.23673000	-5.00752300
H	0.63033800	1.06191700	-4.98985200
H	0.56015100	-0.71098500	-5.02844500

Table S2. Standard orientation of **2** at the PBE1PBE optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
Ru	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.18857400
N	2.14871700	0.00000000	0.33424300
N	0.30976200	2.14425300	0.30049500
C	1.40391100	-0.16763600	2.70099000
H	1.76663200	0.79524400	3.06987800
H	1.40400300	-0.83968400	3.56659800
C	2.32977000	-0.72546100	1.62925900
H	2.11114600	-1.78093900	1.45884100
H	3.37660700	-0.65763300	1.96097400
C	2.96414800	-0.64104600	-0.73434400
H	4.00828900	-0.74372400	-0.41244000
H	2.92600500	-0.01694500	-1.62868900
H	2.56990700	-1.61929800	-0.99768900
C	2.66605200	1.40502700	0.48676800
H	2.80339400	1.62775200	1.54682500
H	3.65841400	1.48886300	0.02997100
C	1.71641100	2.38525000	-0.15220300
H	1.72068400	2.27597800	-1.24108100
H	2.01778200	3.41641800	0.08346000
C	-0.52089400	3.10135800	-0.48658100
H	-1.51751700	3.19081600	-0.06047100
H	-0.59712200	2.76158200	-1.52018800
H	-0.06633200	4.09976200	-0.46359900
C	0.17538000	2.45808600	1.77243100
H	1.16857500	2.63838600	2.19174900
H	-0.37600700	3.39626200	1.90093600
C	-0.53735300	1.34884200	2.53363000
H	-1.60270200	1.33539000	2.28585200
H	-0.45766800	1.53125800	3.61616300
C	-0.87184100	-1.03190100	2.80691500
H	-0.47674200	-2.02397300	2.58070100
H	-1.88083800	-0.95297300	2.39859400
H	-0.91502900	-0.90406700	3.89621900
C	-3.02096800	0.86923800	-0.04776200
H	-2.64413300	1.85771200	0.15609900
C	-4.40268500	0.68271100	-0.20713400
H	-5.06535600	1.53484700	-0.11936500
C	-4.88896800	-0.57958300	-0.47707300
H	-5.95016500	-0.75667000	-0.61331500
C	-3.97666700	-1.65136100	-0.56505400

C	-2.59988300	-1.37002600	-0.38274100
C	-1.64728300	-2.43188200	-0.42446600
C	-2.08744600	-3.75906700	-0.65659800
C	-1.12102900	-4.78556800	-0.66536500
H	-1.42001500	-5.81304200	-0.84128500
C	0.19826000	-4.45222000	-0.44056200
H	0.97637300	-5.20549400	-0.43101900
C	0.54247100	-3.10971400	-0.22157600
H	1.57901200	-2.86410800	-0.05009700
C	-4.39150900	-2.99889800	-0.81671800
H	-5.44755800	-3.19639700	-0.96386900
C	-3.48221100	-4.01268100	-0.86162500
H	-3.80041900	-5.03280400	-1.04598100
N	-2.11882200	-0.11223500	-0.13927200
N	-0.33571300	-2.10174000	-0.21254900
C	0.10156600	0.13981800	-1.92340400
N	0.15982300	0.23401900	-3.09018400
C	0.21754000	0.32089300	-4.54209400
C	1.69374000	0.27557000	-4.96019100
H	2.16350300	-0.66064800	-4.64367000
H	1.76050600	0.33817600	-6.04987400
H	2.24894200	1.11912800	-4.53797500
C	-0.55325500	-0.87667400	-5.11483400
H	-1.60146400	-0.85370200	-4.80258300
H	-0.52012500	-0.83430200	-6.20708100
H	-0.10382300	-1.82121500	-4.79432200
C	-0.43282600	1.64607000	-4.96276100
H	0.10708500	2.50048500	-4.54272700
H	-0.40429000	1.73012100	-6.05264200
H	-1.47873000	1.68863600	-4.64433300

Table S3. Standard orientation of **2'** at the PBE1PBE optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
Ru	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.18918700
N	2.15408300	0.00000000	0.34360200
N	0.31580900	2.14574300	0.29927900
C	1.40211600	-0.16653000	2.70713100
H	1.76190800	0.79720400	3.07674000
H	1.39900700	-0.83774400	3.57338000
C	2.33314800	-0.72331000	1.64006000
H	2.12003900	-1.78012800	1.47317900
H	3.37866600	-0.65114700	1.97497000
C	2.97592400	-0.63860200	-0.72197900
H	4.01921200	-0.73697200	-0.39604600
H	2.93891300	-0.01460100	-1.61647700
H	2.58765900	-1.61888000	-0.98696000
C	2.67064300	1.40465800	0.50107400
H	2.80014200	1.62680800	1.56216500
H	3.66637600	1.48862900	0.05164700
C	1.72629200	2.38502300	-0.14328600
H	1.73796600	2.27616900	-1.23215500
H	2.02676300	3.41593800	0.09428500
C	-0.50199300	3.10528800	-0.50038300
H	-1.50918200	3.19216800	-0.10019300
H	-0.55479700	2.76902000	-1.53662800
H	-0.04902300	4.10392800	-0.46415100
C	0.17011100	2.46125000	1.77029400
H	1.15958400	2.65290300	2.19380000
H	-0.39080100	3.39459800	1.89293000
C	-0.53582600	1.34899900	2.53611800
H	-1.60322300	1.33361700	2.29946400
H	-0.44796400	1.53236800	3.61789200
C	-0.87331200	-1.03313800	2.80404000
H	-0.47650500	-2.02466900	2.57827100
H	-1.88091700	-0.95509500	2.39190700
H	-0.92066000	-0.90648400	3.89329300
C	-2.98541300	0.89728700	0.01917300
H	-2.56708700	1.85148100	0.29109400
C	-4.35979300	0.77096200	-0.14476000
H	-5.00055800	1.63176200	0.00173800
C	-4.87890600	-0.47139200	-0.49931300
H	-5.94269700	-0.61384700	-0.64695500
C	-3.99394100	-1.53294300	-0.64642000

H	-4.37693600	-2.51189000	-0.90039700
C	-2.62206900	-1.33677900	-0.45505100
C	-1.64697400	-2.43003600	-0.52522200
C	-2.01444200	-3.74630200	-0.82457300
H	-3.04262600	-3.98731100	-1.05766900
C	-1.06083000	-4.75683300	-0.82118700
H	-1.33611100	-5.77898000	-1.05169800
C	0.25161800	-4.41572800	-0.50684200
H	1.03880300	-5.15898100	-0.47628700
C	0.54875100	-3.08593500	-0.23234600
H	1.56557700	-2.81671800	0.00297200
N	-2.10976900	-0.11428300	-0.14222700
N	-0.35849200	-2.08875600	-0.24196000
C	0.10959600	0.14618600	-1.92297800
N	0.17430000	0.24292900	-3.08909800
C	0.24606100	0.33759400	-4.54023400
C	1.72488400	0.26855000	-4.94564400
H	2.17563800	-0.67719100	-4.62985700
H	1.80214500	0.33530400	-6.03437800
H	2.29092300	1.10037100	-4.51461300
C	-0.37733400	1.67649000	-4.95807300
H	0.17433200	2.51872000	-4.52882700
H	-0.33843700	1.76627000	-6.04716600
H	-1.42487500	1.73591100	-4.64787600
C	-0.54069400	-0.84276400	-5.12682700
H	-0.49626700	-0.79504600	-6.21844200
H	-0.11154700	-1.79717200	-4.80764600
H	-1.59144500	-0.80213700	-4.82497300

Table S4. Standard orientation of **4** at the PBE1PBE optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
Ru	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	2.39665200
S	2.33393500	0.00000000	0.09447300
S	0.08704100	2.33264300	0.09455300
C	1.69942300	-0.58341100	2.75724700
H	1.90907900	-0.41145900	3.81887200
H	1.65602300	-1.66781600	2.61066900
C	2.77277000	0.05579300	1.89046800
H	3.72108300	-0.47760800	2.01198000
H	2.94671600	1.09831700	2.17249400
C	2.76932700	1.70392000	-0.43170700
H	3.82271300	1.88546900	-0.19217000
H	2.68168300	1.68421200	-1.52294700
C	1.88376600	2.77805700	0.17865700
H	2.00821400	3.72084600	-0.36290300
H	2.14008500	2.96443800	1.22570700
C	-0.45034100	2.70363400	1.81069800
H	-0.20484400	3.74860600	2.03130500
H	-1.54264700	2.63115700	1.78060500
C	0.12876900	1.77945200	2.86958600
H	-0.41677000	1.90676700	3.81016600
H	1.17941500	2.00810900	3.06942300
C	-3.00809800	0.80847500	-0.15048900
H	-2.63540400	1.81352300	-0.31370700
C	-4.38963100	0.56467200	-0.09194500
H	-5.07874100	1.39415600	-0.19222100
C	-4.84745100	-0.72691800	0.08951500
H	-5.90973500	-0.93864300	0.14441500
C	-3.91258600	-1.78014100	0.18483500
C	-2.54053300	-1.44545800	0.11196600
C	-1.55155200	-2.47606000	0.14022600
C	-1.94455200	-3.83028500	0.24493200
C	-0.92827900	-4.80943300	0.21255500
H	-1.18561200	-5.85994000	0.29342800
C	0.38639500	-4.41022300	0.06126800
H	1.18946300	-5.13526300	0.01248300
C	0.68987800	-3.04233600	-0.03446600
H	1.71429600	-2.71458400	-0.16997300
C	-4.28455000	-3.15749800	0.32886900
H	-5.33793700	-3.40420500	0.40263100
C	-3.33980800	-4.14163100	0.35815700

H	-3.63208400	-5.18132700	0.45589800
N	-2.09802600	-0.16145700	-0.02998600
N	-0.24638900	-2.09077300	0.02100000
C	0.01918500	-0.00850200	-1.96177800
N	0.01836600	-0.02860700	-3.12751900
C	-0.00828300	-0.07772300	-4.58470700
C	-0.38213500	1.32131900	-5.09271300
H	-1.36707800	1.62399200	-4.72545300
H	-0.41478600	1.30520700	-6.18551600
H	0.35932000	2.06469100	-4.78512800
C	-1.06222600	-1.11608300	-4.99341900
H	-0.80440500	-2.10898800	-4.61344000
H	-1.10470000	-1.16780800	-6.08484000
H	-2.05351000	-0.83577100	-4.62525400
C	1.39019400	-0.48873700	-5.06439300
H	2.14368000	0.24318700	-4.75834600
H	1.39031800	-0.53944900	-6.15664000
H	1.66657700	-1.47329800	-4.67602200

Table S5. Standard orientation of **5** at the PBE1PBE optimized geometry

Atom	Coordinates in Å		
	X	Y	Z
Ru	0.00000000	0.00000000	0.00000000
Ru	0.00000000	0.00000000	3.21716800
Cl	1.89237300	0.00000000	1.60585400
Cl	-0.91868900	1.65501300	1.60542000
Cl	-0.97161000	-1.63758300	1.61584800
N	0.84428100	-1.39097700	-1.33157900
N	-1.62497100	-0.04570000	-1.33261900
N	0.77042400	1.41927500	-1.34174900
N	0.73409000	-1.45307600	4.56038700
N	-1.61228700	-0.04969200	4.55878000
C	1.34022000	-2.62862100	-0.67861600
H	0.49365500	-3.16804500	-0.25193200
H	2.01524700	-2.35387900	0.13336000
H	1.86286300	-3.26429600	-1.40786700
C	-2.94322800	0.15051500	-0.67858700
H	-2.98486600	1.15679100	-0.25987900
H	-3.03984300	-0.56379700	0.14016000
H	-3.75678300	0.00945900	-1.40456900
C	1.60458400	2.46548300	-0.69823500
H	1.88318800	3.23709100	-1.43009500
H	2.49998900	1.99985100	-0.28459000
H	1.04196900	2.90895900	0.12424900
N	0.83334500	1.37791000	4.54346200
C	-2.88711700	0.45551500	3.99009300
H	-3.07747100	-0.05321900	3.04455500
H	-2.79193900	1.52267400	3.78613000
H	-3.71566700	0.28044100	4.69141400
C	1.67778000	-2.40309300	3.91110900
H	1.95096700	-3.20900300	4.60738300
H	2.57269100	-1.86267600	3.59981600
H	1.20143600	-2.81452500	3.02023500
C	-0.27895300	1.85655700	5.42087300
H	0.12056600	2.33118500	6.33027200
H	-0.79938000	2.62689000	4.84314400
C	-0.44402400	-2.22693300	5.08400300
H	-0.49840000	-3.15628800	4.51163400
H	-0.26104400	-2.50502300	6.13027200
C	1.90268700	0.63205700	5.27082100
H	2.73810200	0.55280600	4.56839900
H	2.24802800	1.20350200	6.14682400
C	1.46464000	2.57270600	3.92209000

H	0.71490300	3.10592100	3.33718300
H	2.25469400	2.24410100	3.24612000
H	1.88007300	3.23299300	4.69689600
C	1.45739700	-0.75906800	5.68723000
H	0.81023700	-0.72043200	6.56357200
H	2.33376200	-1.35187800	5.97910000
C	-1.26344100	0.75387500	5.77672800
H	-2.17345700	1.19706900	6.20281300
H	-0.86345300	0.08349000	6.53781200
C	-1.78547400	-1.48723100	4.90920400
H	-2.41118900	-1.58413800	5.80972300
H	-2.32747600	-1.93349500	4.07251800
C	-1.43412400	1.00257900	-2.39306300
H	-2.39599700	1.47299600	-2.62922500
H	-1.09066300	0.52323200	-3.31467800
C	-0.44519900	2.05914000	-1.92525900
H	-0.88759100	2.66262000	-1.12707800
H	-0.17398300	2.72914300	-2.75670500
C	1.57705300	0.71993900	-2.40091800
H	2.46197300	1.31685500	-2.65182300
H	0.98139600	0.65011300	-3.31590800
C	2.00258200	-0.65966500	-1.92352600
H	2.74906800	-0.57117000	-1.12842400
H	2.44626400	-1.23393500	-2.75257200
C	-0.16627500	-1.75207800	-2.38509200
H	-0.09611800	-2.82135600	-2.61747000
H	0.07560000	-1.21923200	-3.30933500
C	-1.57356400	-1.41884300	-1.91428400
H	-1.87461600	-2.10102100	-1.11368100
H	-2.29146900	-1.52027100	-2.74379400