

Supporting information

C-H reductive elimination during the reaction of cycloplatinated(II) complexes with pyridine-2-thione: kinetic follow up

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The Cartesian coordinates (in Angstroms) for all species discussed in the manuscript.

1a

Pt	-0.55380900	-0.43175700	0.00000000
S	-2.79036200	0.67819600	-0.00004200
N	0.56876200	1.45504500	-0.00002300
C	-3.75628200	0.02293600	1.40571600
H	-4.77500100	0.41618400	1.35962700
H	-3.26834200	0.37362600	2.31748700
H	-3.76693900	-1.06869900	1.39176100
C	-3.75636500	0.02283300	-1.40569700
H	-3.76700400	-1.06880000	-1.39167700
H	-3.26849600	0.37348100	-2.31752300
H	-4.77508600	0.41606900	-1.35955800
C	1.33305700	-1.13524200	0.00002300
C	2.35283600	-0.14009300	-0.00002600
C	3.71155500	-0.50100300	-0.00006500
H	4.48592400	0.26079700	-0.00012500
C	4.08895100	-1.84104000	-0.00003900
H	5.14158100	-2.11014900	-0.00007100
C	3.10126100	-2.82990300	0.00002900
H	3.38473200	-3.88011100	0.00005900
C	1.74901300	-2.47685400	0.00005500
H	1.00708900	-3.26868400	0.00009800
C	1.91822900	1.26723000	-0.00001900
C	0.06908600	2.70204500	-0.00000200
H	-1.01255500	2.78164500	-0.00001200

C	0.87197700	3.83699000	0.00002500
H	0.41907300	4.82236900	0.00004700
C	2.25688400	3.66405300	0.00002900
H	2.92295400	4.52169700	0.00004900
C	2.77874900	2.37517900	0.00000700
H	3.85214300	2.22877800	0.00001500
C	-1.39693600	-2.31581900	0.00004700
H	-1.07814500	-2.88229600	-0.88576200
H	-1.07823300	-2.88220400	0.88594800
H	-2.49426500	-2.30097000	-0.00000800

1b

Pt	0.13899900	-0.30768100	-0.00115500
S	-0.46975300	-2.74681600	-0.00617300
N	2.30165000	-0.67035400	-0.00158100
C	-1.60702400	-3.03996100	-1.40547500
H	-1.99390200	-4.06041100	-1.34641600
H	-1.02378700	-2.92174100	-2.32126700
H	-2.42020700	-2.31207300	-1.39109000
C	-1.59329400	-3.05093900	1.40175900
H	-2.40827300	-2.32496900	1.39856100
H	-1.00209000	-2.93632800	2.31289100
H	-1.97813400	-4.07201600	1.34029800
C	0.82352200	1.58782600	0.00138700
C	2.24147400	1.72083400	0.00244500
C	2.84454900	2.99041900	0.00418500
H	3.92632400	3.08787600	0.00487000
C	2.06598900	4.14471300	0.00484900
H	2.54155400	5.12156900	0.00618100
C	0.67310300	4.03110200	0.00362500
H	0.05572400	4.92667500	0.00395200
C	0.06657400	2.77167600	0.00193300
H	-1.01620600	2.71059600	0.00054000
C	3.03298300	0.47902200	0.00130100
C	2.92611300	-1.85978300	-0.00299200
H	2.28526500	-2.73460700	-0.00545300
C	4.31081700	-1.98373800	-0.00153000
H	4.76761700	-2.96724300	-0.00276800
C	5.07665200	-0.81697000	0.00152600
H	6.16145100	-0.86586000	0.00282300
C	4.43420400	0.41633100	0.00291900
H	5.01888000	1.32840500	0.00535600
C	-1.81458900	0.22180800	0.00133000
C	-2.54015700	0.40089000	1.19687900
C	-2.53259800	0.43811400	-1.19376500
C	-3.89203900	0.76377400	1.19860700
H	-2.04057600	0.26548500	2.15448900
C	-3.88338200	0.80105500	-1.19368500

H	-2.02572900	0.33251700	-2.15126200
C	-4.59337600	0.96866500	0.00342400
H	-4.40831600	0.89494100	2.14878000
H	-4.39282500	0.96222700	-2.14306000
C	-6.06075400	1.33516800	0.00168800
H	-6.30115500	2.02903000	-0.81216100
H	-6.69879600	0.45063900	-0.13332700
H	-6.35684100	1.80591100	0.94557600

2a

Pt	0.12275400	-0.39427600	-0.43535400
N	1.21775800	1.46257000	-0.02729700
C	1.93255900	-1.13821500	0.03489100
C	2.92127900	-0.16807000	0.37427900
C	4.22474600	-0.55910000	0.72732700
H	4.97346200	0.18457500	0.98578500
C	4.57959700	-1.90510200	0.75135200
H	5.58955600	-2.19743100	1.02547200
C	3.62405700	-2.86984900	0.41831600
H	3.89061300	-3.92456100	0.43187800
C	2.32674400	-2.48700500	0.06760000
H	1.60816500	-3.26029100	-0.18589100
C	2.51271900	1.24675600	0.33633700
C	0.74315300	2.71713700	-0.09681400
H	-0.29679500	2.81111500	-0.39142200
C	1.52045100	3.83387800	0.18925500
H	1.09137900	4.82740800	0.11747500
C	2.84935500	3.63271400	0.56658800
H	3.49293600	4.47545700	0.80116200
C	3.34452200	2.33529900	0.63977600
H	4.37438100	2.16731800	0.93146700
C	-0.70989500	-2.25335800	-0.77353600
H	-1.77737400	-2.19403800	-1.02006500
H	-0.20264400	-2.75598100	-1.60949900
H	-0.60426600	-2.89857900	0.10980700
S	-2.01084200	0.75139000	-1.11116700
C	-3.28262500	0.26100300	-0.06226200
C	-3.14878900	-0.50913000	1.12000300
C	-5.66510700	0.35416500	0.36364100
H	-4.67952700	1.19966700	-1.22018500
C	-4.25379000	-0.82617900	1.88435500
H	-2.15272900	-0.83373000	1.39539600
C	-5.54417800	-0.39022100	1.50913300
H	-6.60333100	0.73907100	-0.01589300
H	-4.12755300	-1.41593800	2.78726800
H	-6.42062500	-0.62839800	2.09853900
N	-4.56143600	0.64989500	-0.37362600

2b

Pt	0.38309100	0.04698600	-0.31775200
N	2.11947300	-1.28777300	-0.28621800
C	1.81403700	1.32494500	0.30340000
C	3.11878800	0.76397100	0.42453500
C	4.20800000	1.55245400	0.83390300
H	5.20024700	1.11928700	0.92271900
C	4.03442800	2.90145200	1.13131600
H	4.88261000	3.50323600	1.44601800
C	2.76127400	3.46752600	1.01989700
H	2.61409700	4.52064000	1.24979700
C	1.67426300	2.68911800	0.61209600
H	0.69620500	3.15210200	0.53690300
C	3.26658300	-0.66558100	0.10368500
C	2.13832700	-2.59377000	-0.59859400
H	1.18582800	-3.01758600	-0.89835100
C	3.29528400	-3.36316700	-0.54566900
H	3.26083900	-4.41490300	-0.80813100
C	4.48144300	-2.74309000	-0.14937800
H	5.40899100	-3.30517100	-0.09344000
C	4.46507300	-1.39109400	0.17610300
H	5.37994300	-0.90026100	0.48600100
S	-1.20062100	-1.67871800	-1.25136600
C	-2.28005500	-2.19751800	-0.01731700
C	-2.22010000	-1.85466500	1.35650500
C	-4.23159700	-3.54111100	0.48595200
C	-3.14859500	-2.35205700	2.24910000
H	-1.42399000	-1.19374000	1.67549700
C	-4.18010100	-3.21480400	1.81704000
H	-4.97821800	-4.19137400	0.04782100
H	-3.08219300	-2.07713500	3.29743300
H	-4.91508700	-3.61426400	2.50441900
N	-3.30682500	-3.03592200	-0.37325000
H	-3.37071400	-3.29017800	-1.35498600
C	-1.11292200	1.41071300	-0.29722500
C	-1.67109800	1.90865700	-1.49377000
C	-1.67203300	1.91364300	0.89533200
C	-2.71290600	2.84083000	-1.49828600
H	-1.28442000	1.56177400	-2.45016200
C	-2.72199400	2.83924900	0.89365500
H	-1.27487600	1.58835000	1.85501000
C	-3.26573900	3.32249700	-0.30314700
H	-3.10353000	3.20085400	-2.44964100
H	-3.12045900	3.19652000	1.84270900
C	-4.41651600	4.30416500	-0.30830200
H	-5.38393400	3.79520500	-0.42315300
H	-4.46137600	4.87384700	0.62660400
H	-4.33275100	5.01902100	-1.13526100

2a'

Pt	-0.07151500	-0.37702800	-0.56363200
N	-1.13447900	1.46857800	-0.05174100
C	-1.83813400	-1.13529900	0.04871300
C	-2.80087700	-0.16898000	0.46311300
C	-4.07060400	-0.56527900	0.91775200
H	-4.80002000	0.17494600	1.23443400
C	-4.41546300	-1.91321800	0.97138600
H	-5.39914800	-2.20983800	1.32482800
C	-3.48468600	-2.87417900	0.56634300
H	-3.74419700	-3.93002200	0.60260900
C	-2.22060900	-2.48545700	0.11395500
H	-1.52077300	-3.25570300	-0.19506600
C	-2.40204000	1.24799000	0.39492900
C	-0.66834700	2.72404000	-0.15270800
H	0.35072100	2.81864000	-0.51268300
C	-1.42995700	3.83820700	0.18184900
H	-1.01001800	4.83322100	0.08256000
C	-2.73183300	3.63272800	0.64172400
H	-3.36261400	4.47365800	0.91433400
C	-3.21720200	2.33369200	0.74808200
H	-4.22667200	2.16288400	1.10262000
C	0.72067900	-2.23109100	-1.02431300
H	1.75734800	-2.17048100	-1.37856300
H	0.69749400	-2.90762200	-0.15877800
H	0.12486400	-2.69932400	-1.82052300
S	2.05673200	0.75937400	-1.28975100
C	3.21222400	0.31070200	-0.09491000
C	4.57738500	0.68763300	-0.12962800
C	3.65694900	-0.86038600	1.96864400
C	5.44010100	0.29096700	0.87266000
H	4.92283700	1.29129300	-0.96049400
C	4.98140300	-0.50026400	1.94933000
H	3.20322500	-1.46406000	2.74490000
H	6.48315500	0.58949300	0.83090600
H	5.64479400	-0.82043200	2.74295700
N	2.82872800	-0.45352900	0.97273000
H	1.83575300	-0.72460900	0.97680400

2b'

Pt	0.35626400	0.04726600	-0.37411400
N	2.23654900	-1.06893100	-0.34632300
C	1.61290200	1.46680800	0.32979000
C	2.96693200	1.04981400	0.48553700
C	3.94514800	1.93906300	0.96286600
H	4.97525400	1.61528900	1.08165400
C	3.61163300	3.25100800	1.28928400
H	4.37484900	3.93125000	1.65712100

C	2.29061500	3.67895900	1.13436200
H	2.01965600	4.70313100	1.38150300
C	1.31275600	2.79853800	0.66169400
H	0.29506300	3.15732000	0.55439400
C	3.28934800	-0.33866700	0.11522400
C	2.41926700	-2.34533900	-0.72271300
H	1.53382800	-2.86129600	-1.07805900
C	3.65675500	-2.97630000	-0.66307000
H	3.75548700	-4.00885400	-0.97961300
C	4.74720300	-2.24571500	-0.18848300
H	5.73179100	-2.69912200	-0.12275800
C	4.56118900	-0.92376000	0.20138000
H	5.40088200	-0.34714200	0.57026900
S	-1.00392500	-1.85676600	-1.32008300
C	-1.99396600	-2.40698400	-0.02478600
C	-2.94992400	-3.44543000	-0.14665100
C	-2.61840600	-2.19542600	2.29770300
C	-3.70679800	-3.83281200	0.94100600
H	-3.07042300	-3.92224200	-1.11217700
C	-3.54640400	-3.20142100	2.19448700
H	-2.41725100	-1.64483400	3.20827300
H	-4.43491400	-4.63048200	0.82989300
H	-4.13317700	-3.49209400	3.05681100
N	-1.88384000	-1.83704700	1.21309700
H	-1.19648500	-1.07814900	1.28263300
C	-1.29609800	1.22258300	-0.36020500
C	-1.95435100	1.55685200	-1.56330700
C	-1.86953800	1.74563400	0.81684600
C	-3.09621000	2.36176200	-1.58834700
H	-1.56585500	1.18171200	-2.50780700
C	-3.02293600	2.53885300	0.79585400
H	-1.40020600	1.54903800	1.77920400
C	-3.66069300	2.86474300	-0.40696800
H	-3.55945500	2.60141500	-2.54488300
H	-3.42806500	2.91655700	1.73390100
C	-4.91731600	3.70596500	-0.43331600
H	-5.81840100	3.08505000	-0.53435300
H	-5.02743600	4.28919700	0.48746400
H	-4.91652100	4.40521100	-1.27780300

I

Pt	0.03489300	-0.03415400	-0.58004100
N	2.23765300	0.10892500	-0.72560200
C	0.59429000	-1.77136300	0.34036500
C	1.99504700	-1.96679500	0.43580200
C	2.49808300	-3.10350300	1.09299200
H	3.56914700	-3.25858700	1.17996200
C	1.63345000	-4.04439300	1.64497400

H	2.03468500	-4.91852700	2.14956500
C	0.25307700	-3.85631900	1.54270300
H	-0.42904800	-4.58820900	1.96802700
C	-0.25998800	-2.72939700	0.89235500
H	-1.33400500	-2.59899700	0.82365600
C	2.87630400	-0.94946500	-0.16332100
C	2.93266600	1.09917200	-1.30499700
H	2.34040400	1.90592200	-1.72380700
C	4.32173600	1.09420900	-1.35973300
H	4.84912600	1.91230200	-1.83748300
C	5.00127400	0.01643900	-0.78879400
H	6.08595300	-0.02716900	-0.81139800
C	4.27722100	-1.00810100	-0.18855100
H	4.79591400	-1.84936200	0.25482200
C	-1.97977300	-0.34169200	-0.43818200
C	-2.75996400	-0.67735000	-1.55843700
C	-2.64334700	-0.21216300	0.78999300
C	-4.13900700	-0.86943700	-1.45095100
H	-2.29323800	-0.78893100	-2.53290700
C	-4.02596000	-0.40671700	0.89383700
H	-2.08602800	0.03750500	1.68769200
C	-4.80206100	-0.73644700	-0.22246000
H	-4.70857600	-1.13055600	-2.34141300
H	-4.50502500	-0.29807200	1.86528000
C	-6.29800500	-0.92998200	-0.11707000
H	-6.62131400	-0.97855800	0.92793200
H	-6.84445100	-0.10482100	-0.59293300
H	-6.62043100	-1.85320900	-0.61341600
S	-0.40679900	2.37364600	-1.35672900
C	-0.16055900	2.65118800	0.36147800
C	-0.18671800	3.88779900	1.02875500
C	0.04539400	3.91393900	2.39834100
H	-0.38354100	4.79719500	0.47112900
C	0.31052000	1.53341200	2.37155200
C	0.30204900	2.72119500	3.09062900
H	0.02955400	4.86050800	2.93128600
H	0.50036300	0.57367800	2.84282000
H	0.48889900	2.71466700	4.15856300
N	0.07977700	1.50670300	1.04923600
H	-0.01768000	-0.91589800	-1.86963600

I'

Pt	0.03489300	-0.03415400	-0.58004100
N	2.23765300	0.10892500	-0.72560200
C	0.59429000	-1.77136300	0.34036500
C	1.99504700	-1.96679500	0.43580200
C	2.49808300	-3.10350300	1.09299200
H	3.56914700	-3.25858700	1.17996200

C	1.63345000	-4.04439300	1.64497400
H	2.03468500	-4.91852700	2.14956500
C	0.25307700	-3.85631900	1.54270300
H	-0.42904800	-4.58820900	1.96802700
C	-0.25998800	-2.72939700	0.89235500
H	-1.33400500	-2.59899700	0.82365600
C	2.87630400	-0.94946500	-0.16332100
C	2.93266600	1.09917200	-1.30499700
H	2.34040400	1.90592200	-1.72380700
C	4.32173600	1.09420900	-1.35973300
H	4.84912600	1.91230200	-1.83748300
C	5.00127400	0.01643900	-0.78879400
H	6.08595300	-0.02716900	-0.81139800
C	4.27722100	-1.00810100	-0.18855100
H	4.79591400	-1.84936200	0.25482200
C	-1.97977300	-0.34169200	-0.43818200
C	-2.75996400	-0.67735000	-1.55843700
C	-2.64334700	-0.21216300	0.78999300
C	-4.13900700	-0.86943700	-1.45095100
H	-2.29323800	-0.78893100	-2.53290700
C	-4.02596000	-0.40671700	0.89383700
H	-2.08602800	0.03750500	1.68769200
C	-4.80206100	-0.73644700	-0.22246000
H	-4.70857600	-1.13055600	-2.34141300
H	-4.50502500	-0.29807200	1.86528000
C	-6.29800500	-0.92998200	-0.11707000
H	-6.62131400	-0.97855800	0.92793200
H	-6.84445100	-0.10482100	-0.59293300
H	-6.62043100	-1.85320900	-0.61341600
S	-0.40679900	2.37364600	-1.35672900
C	-0.16055900	2.65118800	0.36147800
C	-0.18671800	3.88779900	1.02875500
C	0.04539400	3.91393900	2.39834100
H	-0.38354100	4.79719500	0.47112900
C	0.31052000	1.53341200	2.37155200
C	0.30204900	2.72119500	3.09062900
H	0.02955400	4.86050800	2.93128600
H	0.50036300	0.57367800	2.84282000
H	0.48889900	2.71466700	4.15856300
N	0.07977700	1.50670300	1.04923600
H	-0.01768000	-0.91589800	-1.86963600

3

Pt	0.24496000	-1.22393400	0.94679800
Pt	0.24611300	1.22370900	-0.94685100
S	1.38471400	0.31025600	2.34858400
S	1.38394100	-0.31189300	-2.34850200

N	2.17268000	-1.64885500	-0.09749200
C	-1.51761100	1.05026800	-1.89314500
N	-0.82070300	2.74410300	0.01926300
C	-1.51832800	-1.04918800	1.89356300
C	-2.90440800	3.91345400	0.14976600
H	-3.92336300	4.04633500	-0.19386800
C	4.56178300	2.52455200	1.24411900
H	5.48798900	2.86302900	1.69945900
C	4.23974300	-2.87911200	0.07336600
H	4.89629000	-3.49508600	0.67761100
N	2.17413700	1.64680700	0.09751900
C	3.04549400	-2.41436400	0.59817900
H	2.74197800	-2.65540000	1.61107800
C	-2.10744200	-2.90918500	0.41537600
C	-2.51138900	-1.97777500	1.47121100
N	-0.82356700	-2.74288500	-0.01962600
C	-2.10447700	2.91152700	-0.41558700
C	-2.50962000	1.98001600	-1.47087300
C	2.48425700	1.27833400	1.36538000
C	-1.88087500	-0.13329800	2.89511100
H	-1.15769500	0.60037600	3.23696800
C	-0.32594600	3.53946200	0.98564300
H	0.69743100	3.34885900	1.27984800
C	4.55924400	-2.52897100	-1.24449400
H	5.48503500	-2.86838800	-1.69997600
C	3.68514500	-1.72495800	-1.95822500
H	3.91445400	-1.41582500	-2.97205500
C	3.04748800	2.41167900	-0.59820100
H	2.74397200	2.65319400	-1.61099800
C	-3.15947500	-0.13829800	3.46092400
H	-3.40629500	0.58343700	4.23622900
C	3.68711100	1.72120000	1.95789900
H	3.91638000	1.41166800	2.97161300
C	2.48284100	-1.28087200	-1.36549600
C	-3.79546700	-1.97706000	2.04100300
H	-4.54612600	-2.68963200	1.71103200
C	-0.32976000	-3.53842900	-0.98633800
H	0.69376400	-3.34882300	-1.28058300
C	-1.88137200	0.13433000	-2.89419700
H	-1.15902300	-0.60017000	-3.23604200
C	-4.12166500	-1.06034000	3.03649500
H	-5.11544500	-1.06304700	3.47511900
C	-1.07664500	4.54720400	1.57603900
H	-0.63487300	5.16395000	2.35049700
C	-2.39770600	-4.73187200	-1.14808600
H	-3.01753600	-5.50856100	-1.58519800
C	4.24228400	2.87525800	-0.07358400
H	4.89920600	3.49080500	-0.67785500

C	-2.90851000	-3.91002600	-0.15027300
H	-3.92753700	-4.04198100	0.19352000
C	-4.12133300	1.06342800	-3.03518200
H	-5.11526900	1.06688300	-3.47344300
C	-3.79391800	1.98024700	-2.04018600
H	-4.54382100	2.69360700	-1.71020600
C	-2.39257900	4.73517200	1.14716000
H	-3.01153600	5.51268100	1.58405900
C	-3.16016200	0.14031000	-3.45957300
H	-3.40792000	-0.58150100	-4.23450800
C	-1.08161900	-4.54515600	-1.57702000
H	-0.64057400	-5.16206700	-2.35176500