

Supporting Information

Mechanism of selective C-H cyanation of 2-phenylpyridine with benzyl nitrile catalyzed by CuBr: a DFT investigation

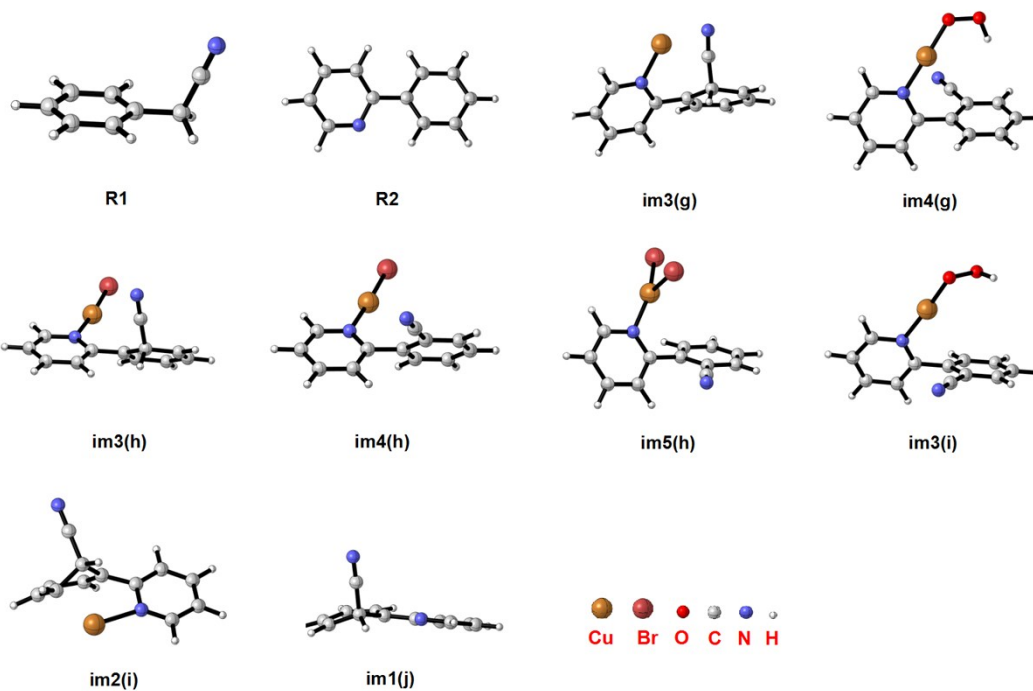
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1. The optimized structures for the reactants and intermediates obtained at the B3LYP/6-31+G(d,p) level of theory in the solvent of DMF.



2. The Cartesian coordinates (Angstrom) for the optimized the reactants, intermediates, transition states, and products obtained at the B3LYP/6-31+G(d,p) level of theory in the solvent of DMF.

R1

C	0.53172600	-1.20884400	0.24319900
C	-0.14032400	0.00100200	0.46003500
C	0.53299000	1.20970100	0.24108400
C	1.86135700	1.20889800	-0.19444700
C	2.52727400	-0.00116400	-0.41353100
C	1.86004100	-1.21018500	-0.19230000
H	0.01852900	-2.15097200	0.41684900
H	0.02076100	2.15265600	0.41304800
H	2.37463100	2.15176700	-0.35860100
H	3.55974100	-0.00203200	-0.75014100
H	2.37237500	-2.15385400	-0.35478000
C	-1.59294900	0.00230100	0.92386300
H	-1.80630500	-0.87705900	1.54072300
H	-1.80584100	0.88468200	1.53657200
C	-2.53978600	-0.00032500	-0.19928000
N	-3.28226700	-0.00192800	-1.09363000

ts1

C	-1.96049800	-0.97651700	-1.09436900
C	-0.61714700	-0.99225900	-0.74077400
C	-0.17606200	-0.31789700	0.42585900
C	-1.12728300	0.38794800	1.20664500
C	-2.46874900	0.39795700	0.84429200
C	-2.89205600	-0.28429300	-0.30534500
H	-2.28894600	-1.50332400	-1.98468500
H	0.09950600	-1.52977900	-1.35411000
H	-0.79876400	0.91381500	2.09819500
H	-3.18854000	0.93350400	1.45507700
H	-3.94060800	-0.27672300	-0.58596300
C	1.22129000	-0.29445500	0.82749600
H	1.67359500	0.95516300	0.18216700
H	1.43510000	0.00998300	1.85289700
C	2.14457000	-1.25358500	0.31309700
N	2.92552000	-2.00724800	-0.11698600
O	0.81580800	2.37009800	-0.87646200
O	1.90739400	1.94824000	-0.33679800

im1

C	-2.02365700	1.20671900	-0.74451900
C	-0.67426500	0.99045600	-0.45328300
C	-0.29257200	-0.10212000	0.33558100
C	-1.27243700	-0.97213500	0.83525000
C	-2.62006800	-0.75655300	0.54104100
C	-2.99742400	0.33383600	-0.24986700
H	-2.31230300	2.05576300	-1.35649000
H	0.07596700	1.67263600	-0.84078000
H	-0.98205400	-1.81698500	1.45381700
H	-3.37270500	-1.43351300	0.93341100
H	-4.04583800	0.50475700	-0.47522900
C	1.16116500	-0.41051500	0.63999100
H	1.23674200	-0.92535700	1.60519500
C	2.02190200	0.79202900	0.71367100
N	2.72017300	1.71682200	0.78035600
O	1.73147500	-0.84561100	-1.59611600
H	2.68548800	-0.75299300	-1.76895500
O	1.75072900	-1.38093600	-0.24396500

ts2(a)

C	2.43077100	-0.97808400	-0.64963200
C	1.03548800	-0.97038800	-0.68032800
C	0.32711800	0.03108200	-0.00014500
C	1.02549500	1.01177300	0.72129000
C	2.42162300	1.00017000	0.74427600
C	3.12848600	0.00583000	0.06081200
H	2.97364300	-1.75116500	-1.18520500
H	0.49492600	-1.73082600	-1.23337600
H	0.48492800	1.78490500	1.25963700
H	2.95441600	1.76650200	1.29899800
H	4.21393400	-0.00315100	0.08117900
C	-1.17838600	0.02671400	-0.00854900
H	-1.56948500	-0.71921400	0.98360700
C	-1.87387800	1.30405000	0.13601000
N	-2.43782900	2.31278800	0.26603600
O	-2.26545200	-1.90643200	0.63571200
H	-3.23821000	-1.83459100	0.73320400
O	-1.83045000	-0.86164300	-0.77061200

ts2(b)

C	2.56447000	-1.25687500	-0.50418900
C	1.18575600	-1.06620900	-0.62461700
C	0.59880000	0.12410300	-0.17220400
C	1.40458900	1.11097600	0.41602300
C	2.78356800	0.91645200	0.52900100
C	3.36930300	-0.26778100	0.07102500
H	3.00961500	-2.17974500	-0.86451400
H	0.56434800	-1.83242200	-1.07545300
H	0.96180600	2.03414000	0.77907100
H	3.39744200	1.69158800	0.97811100
H	4.44081700	-0.41823900	0.16116900
C	-0.89913000	0.31089500	-0.27126600
H	-1.26805200	-0.05892100	0.97855500
C	-1.41548700	1.67539500	-0.31394500
N	-1.85503500	2.75405900	-0.32254100
O	-2.56534600	-1.66537700	-0.25998500
H	-3.40076500	-1.35612800	-0.65073700
O	-1.56417000	-0.51244300	-1.09229800
O	-1.88825900	-0.66633200	1.89492300
H	-1.27604100	-1.18668700	2.44290900
H	-2.34618000	-1.27693200	1.21416600

P2

C	-1.16367100	-2.76498000	-0.01342900
C	-1.92890300	-1.60484700	0.00831700
C	-1.29184400	-0.34746100	0.00270300
C	0.11159000	-0.26513800	-0.02860600
C	0.87196600	-1.43480800	-0.05131600
C	0.23691300	-2.68056100	-0.04354600
H	-1.64970100	-3.73535900	-0.00748200
H	-3.01227600	-1.65194600	0.03243700
H	0.62004400	0.69497400	-0.03612400
H	1.95537400	-1.36953000	-0.07430600
H	0.83038900	-3.58980600	-0.06155100
C	-2.12187500	0.86334200	0.02733200
C	-1.41799700	2.17664500	0.02229400
N	-0.95964800	3.24455800	0.02207300
O	-3.34552700	0.89536500	0.05339000

im2

C	-3.45849800	-0.53165400	1.52878800
C	-2.67229300	0.46729300	0.96956700
C	-2.24401200	0.37509900	-0.38417800
C	-2.63990800	-0.76185500	-1.14282900
C	-3.42554300	-1.75504200	-0.57177200
C	-3.83957900	-1.64710200	0.76510500
H	-3.77870700	-0.44855400	2.56296300
H	-2.38015200	1.32663900	1.56572300
H	-2.32021500	-0.84434300	-2.17766000
H	-3.71949700	-2.61684300	-1.16321700
H	-4.45353500	-2.42494800	1.20859100
C	-1.43788500	1.37603100	-1.00286600
H	-1.12942400	1.25372500	-2.03689400
C	-0.99985900	2.53997000	-0.35509300
N	-0.62472200	3.51852800	0.17183800

im4

O	0.33469600	-2.03331400	0.00000000
H	1.25652300	-1.69284900	0.00000000
O	-0.49176100	-0.98690000	0.00000000
Cu	0.00000000	0.89153700	0.00000000

ts3

C	-2.99278700	-0.28738100	1.60110600
C	-1.91039900	0.38581000	1.04164900
C	-1.73317700	0.41309900	-0.36188800
C	-2.67096200	-0.26019500	-1.18057400
C	-3.74945500	-0.93285100	-0.61231700
C	-3.91553900	-0.94966800	0.77925000
H	-3.12054100	-0.29756800	2.67934300
H	-1.19914800	0.89609500	1.68439400
H	-2.54460600	-0.24544700	-2.25950000
H	-4.46427200	-1.44178300	-1.25182600
H	-4.75857300	-1.47292700	1.22016700
C	-0.60633200	1.08360400	-0.98435900
H	0.33562000	-1.06480900	-0.93306200
H	-0.63104200	1.22695400	-2.05911400
C	0.14788900	2.05547900	-0.26971800
N	0.78135600	2.84888800	0.30607000
O	2.38457900	-1.20359800	-1.00405100
O	0.88476200	-0.28743300	-1.12730600
Cu	3.08079000	-0.50558100	0.54307100

P1

C	-1.65740200	-1.98987500	1.26753400
C	-1.43492100	-0.62143100	1.10189200
C	-1.32434900	-0.07668100	-0.18558300
C	-1.43768300	-0.91298600	-1.30194900
C	-1.66287200	-2.28453200	-1.13621400
C	-1.77348400	-2.82436100	0.14821300
H	-1.74238100	-2.40581900	2.26736600
H	-1.33997000	0.02474900	1.96982200
H	-1.34764100	-0.49581700	-2.30184300
H	-1.74716700	-2.92673300	-2.00804600
H	-1.94728100	-3.88854700	0.27887600
C	-1.07090600	1.42076200	-0.37110600
H	0.85419300	1.59971400	0.00834700
H	-0.89725400	1.60974600	-1.44126300
C	-2.28667200	2.19370300	-0.01482700
N	-3.24509200	2.79309300	0.25336700
O	-0.01145900	1.92507700	0.41393700

ts1(c)

C	-1.37189700	-0.51473000	-1.53755000
C	-1.30766100	-1.23655100	-0.34842700
C	-0.67936700	-0.67969500	0.78440200
C	-0.13202400	0.61681100	0.70586500
C	-0.19766700	1.32861400	-0.48995900
C	-0.81740400	0.76882300	-1.61411500
H	-1.85236000	-0.95404500	-2.40599200
H	-1.73839600	-2.23193000	-0.29931300
H	0.34442100	1.05144000	1.57677700
H	0.23399300	2.32308500	-0.54538400
H	-0.86815300	1.32856000	-2.54285200
C	-0.64805200	-1.41242900	2.06508000
H	0.15274800	-1.35231300	3.84842500
H	-1.88120100	-1.02633500	2.68255900
C	-0.79784600	-2.85223100	2.03698200
N	-0.96904600	-4.00414100	2.07352500
O	0.27490600	-0.93629800	2.97936900
O	-2.22546800	-0.47533600	4.56944700
O	-2.73144700	-0.64002900	3.39717500

ts1(d)

C	-1.42090600	-0.51452100	-1.60192600
C	-1.34197500	-1.21331500	-0.39933800
C	-0.73897500	-0.61320100	0.72098400
C	-0.23854500	0.69819200	0.63324600
C	-0.31920900	1.38753700	-0.57450300
C	-0.90994900	0.78529400	-1.69270900
H	-1.87933200	-0.98310800	-2.46663700
H	-1.74117800	-2.22072100	-0.33460300
H	0.21640400	1.15988400	1.50169800
H	0.07797900	2.39503500	-0.64497100
H	-0.97239000	1.32775500	-2.63092800
C	-0.68293000	-1.33592700	2.02602700
H	-0.05631000	-1.02849900	3.85064300
H	-1.77839400	-1.10674000	2.56314500
C	-0.69611400	-2.80862500	1.95889100
N	-0.70923400	-3.96964400	1.94004500
O	0.22068100	-0.83941100	2.91960800
O	-1.60141300	-0.43787900	4.58445400
O	-2.42008600	-0.94310800	3.72576600

im1(e or f)

C	-1.28336500	2.26560100	-1.31256400
C	-1.63567100	0.94132200	-1.04891000
C	-1.71864400	0.49127800	0.27834700
C	-1.45700100	1.37366800	1.33535400
C	-1.10786700	2.69975200	1.06643700
C	-1.02035000	3.14529100	-0.25578900
H	-1.21837300	2.61137500	-2.33950400
H	-1.84485700	0.26273600	-1.87108100
H	-1.52331300	1.02649600	2.36246100
H	-0.90571000	3.38058700	1.88739600
H	-0.75010000	4.17622400	-0.46386400
C	-2.05468900	-0.95139400	0.58366000
H	-1.04641200	-2.69561200	0.50716200
H	-2.22322800	-1.08008800	1.65700800
C	-3.26739900	-1.41586500	-0.12487800
N	-4.22831800	-1.78875200	-0.65857100
O	-0.93490900	-1.78913300	0.17552600
Br	3.11882400	-0.45047000	-0.03503400
Cu	0.93329000	-1.11053600	0.09764300

ts1(e)

C	-1.35633000	-0.52915900	-1.58025500
C	-1.27285500	-1.26771200	-0.40511700
C	-0.68694900	-0.69749000	0.74872500
C	-0.20678100	0.63098400	0.70200900
C	-0.29510300	1.35910500	-0.47967400
C	-0.86883800	0.78483100	-1.62324700
H	-1.79868700	-0.97538600	-2.46499600
H	-1.65061200	-2.28495700	-0.37846700
H	0.23075200	1.07679500	1.58777700
H	0.08192100	2.37633300	-0.51276200
H	-0.93610400	1.35832500	-2.54261500
C	-0.65017300	-1.44672800	2.00856200
H	-0.17827900	-0.83358700	3.83740600
H	-1.85859400	-1.06008400	2.68450100
C	-0.78341700	-2.88655600	1.98013200
N	-0.93555100	-4.04091000	1.99747500
O	0.27347200	-0.99917500	2.97462200
Cu	2.25029600	-1.19198000	2.96515400
Br	4.52568600	-1.38107000	2.99292100
O	-1.83226400	-0.41952600	4.56413800
O	-2.56960200	-0.66872400	3.53415000

ts1(f)

C	-3.96960800	-1.77572400	0.80358700
C	-3.17134400	-0.65990000	1.03844600
C	-2.15870400	-0.31890700	0.11940100
C	-1.97565200	-1.08373400	-1.04805500
C	-2.78158200	-2.19548800	-1.27454800
C	-3.77820100	-2.54408400	-0.35194000
H	-4.74071300	-2.04554100	1.51760400
H	-3.32639800	-0.06313700	1.93193100
H	-1.20279900	-0.81494800	-1.75883700
H	-2.63264200	-2.79397800	-2.16737600
H	-4.40358400	-3.41254100	-0.53388100
C	-1.33237800	0.90297700	0.34579700
H	-0.29524100	1.73435900	-1.13871000
H	-2.02955500	1.80542000	-0.09566600
C	-1.10161500	1.29507600	1.74185300
N	-0.92295700	1.62686400	2.83975400
O	-0.17740000	1.02794600	-0.41318100
Cu	1.60264600	0.20154700	-0.15381200
Br	3.63968000	-0.80698400	0.07783600
O	-1.03912500	3.02646700	-1.58365100
O	-2.17840000	2.80565900	-1.02120600

R2

C	-0.76440800	0.01818200	-0.00191900
C	-2.71760000	-1.18444600	-0.29520000
C	-3.52338100	-0.07719300	-0.02220600
C	-2.89202800	1.12955600	0.28345800
C	-1.49943800	1.17896000	0.29869400
C	0.72489300	0.01477700	-0.00439200
C	1.42951700	-1.17222200	0.26585900
C	2.82518900	-1.18870000	0.27539300
C	3.54619400	-0.01967300	0.00725700
C	2.85720200	1.16488400	-0.27112900
C	1.46030900	1.18253200	-0.27663700
H	-3.16851800	-2.14556700	-0.53299500
H	-4.60447400	-0.16427100	-0.04447100
H	-3.47257100	2.01718700	0.51593500
H	-0.99274900	2.10109400	0.55977600
H	0.87217900	-2.07875100	0.47542000
H	3.35022400	-2.11396800	0.49479200
H	4.63210800	-0.03261900	0.01221100
H	3.40563100	2.07590400	-0.49223900
H	0.94660900	2.10795900	-0.51696600
N	-1.37816300	-1.14956000	-0.28950400

im1(g)

C	0.57552300	-0.97295800	0.19927300
C	2.57498200	0.24893600	0.02759200
C	3.32631700	-0.93146900	0.05586300
C	2.66620100	-2.15695800	0.15439800
C	1.27253100	-2.18478800	0.21959000
C	-0.88173800	-0.82064000	0.20056800
C	-1.43333400	0.34545500	0.86057500
C	-2.79394800	0.66847200	0.70732900
C	-3.61044500	-0.16715500	-0.04559400
C	-3.08168500	-1.34536900	-0.63050600
C	-1.73418000	-1.67402000	-0.50989700
H	3.04319600	1.22431200	-0.03217600
H	4.40782900	-0.87143800	0.02397700
H	3.23015100	-3.08293900	0.17773900
H	0.73132300	-3.12185900	0.27958200
H	-0.88648200	0.77492200	1.70409000
H	-3.20504100	1.52685700	1.22690100
H	-4.66632300	0.05451300	-0.15486600
H	-3.73681000	-1.98885800	-1.20834200
H	-1.33924200	-2.54673900	-1.01732100
N	1.23975100	0.21162300	0.10962400
Cu	0.00242200	1.70688800	-0.18541200

im2(g)

C	1.32797000	0.71122400	0.09759200
C	2.46943000	-1.33773100	0.00739500
C	3.69988900	-0.68561400	-0.01875500
C	3.72630300	0.71034300	0.00776100
C	2.52678200	1.42220900	0.06200200
C	-0.02264200	1.30344800	0.13732100
C	-1.00785300	0.66375100	0.95761300
C	-2.35364000	1.08895100	0.91605200
C	-2.71102000	2.15247800	0.10105400
C	-1.73058400	2.80573700	-0.67342700
C	-0.39727200	2.38473800	-0.66247000
H	2.39296200	-2.41874800	-0.01393600
H	4.61262900	-1.26840100	-0.05425200
H	4.67232200	1.24097800	-0.01044700
H	2.51718600	2.50552400	0.08833200
H	-0.68577100	0.03123900	1.78620500
H	-3.08597100	0.60282700	1.55088900
H	-3.73866200	2.49808000	0.07085900
H	-2.01854700	3.63827400	-1.30733000
H	0.33140000	2.87156200	-1.30161100
N	1.31750700	-0.64654400	0.06828400
Cu	-0.46895800	-1.38927900	-0.07430600
C	-3.15206800	-2.77801300	-0.44343500
N	-2.12458300	-2.21936600	-0.29486400

ts1(g)

C	-0.83704300	-0.93142300	0.06039300
C	-2.83528300	0.28231600	0.09996500
C	-3.60210300	-0.87631300	0.17555500
C	-2.94784600	-2.10704900	0.18318900
C	-1.55515900	-2.13275900	0.12600700
C	0.65203500	-0.97911400	0.02009700
C	1.28603800	-1.82342400	-0.88304200
C	2.68362700	-1.99806200	-0.86063000
C	3.47687000	-1.36116700	0.11206100
C	2.88363000	-0.51412300	1.02565600
C	1.47350000	-0.23774900	0.95392900
H	-3.30428600	1.25964400	0.07688800
H	-4.68250000	-0.80437200	0.22246700
H	-3.50844800	-3.03419300	0.24204700
H	-1.01892600	-3.07375800	0.15975700
H	0.69808600	-2.37011100	-1.61301300
H	3.14624000	-2.65221100	-1.59241600
H	4.54473400	-1.54718000	0.14947200
H	3.46649400	-0.01576400	1.79245600
H	0.99699600	0.18205000	1.83395000
N	-1.48802400	0.26266900	0.03906600
Cu	-0.46725600	1.91735200	-0.24022400
C	1.57139000	1.76050700	0.15527100
N	1.44717600	2.87488100	-0.22703700

im3(g)

C	-0.76168600	-0.93605100	0.04436000
C	-2.85116500	0.12990700	0.13407500
C	-3.53298700	-1.07722600	0.22778900
C	-2.78924200	-2.25816400	0.22530000
C	-1.40220400	-2.18469300	0.14136100
C	0.71651000	-0.88579400	-0.03178000
C	1.39965700	-1.82722900	-0.77932800
C	2.80306800	-1.95077200	-0.76719300
C	3.58534100	-1.14463200	0.10587900
C	3.01140700	-0.18031300	0.87646600
C	1.52422500	0.12021900	0.80188900
H	-3.38888100	1.07158200	0.12866600
H	-4.61414700	-1.08210700	0.30307300
H	-3.27910600	-3.22314500	0.30659800
H	-0.80466400	-3.08704900	0.18400400
H	0.82936500	-2.51234000	-1.39925800
H	3.28069600	-2.69231200	-1.39747300
H	4.65628900	-1.31182300	0.17162900
H	3.59423900	0.43807300	1.55075800
H	1.10916100	0.16023400	1.82205400
N	-1.50676300	0.20789000	0.03628300
Cu	-0.65026000	1.95095700	-0.30426500
C	1.37693600	1.50888800	0.28267200
N	1.36011400	2.61737900	-0.11284600

ts2(g)

C	0.74750500	1.21048200	-0.09388800
C	2.84231800	0.14845400	0.16850100
C	3.53502400	1.35046500	0.16257400
C	2.80329900	2.53074700	-0.03788900
C	1.43067000	2.45880600	-0.16851100
C	-0.70210500	1.18397800	-0.10401300
C	-1.42589900	2.34231500	0.27357800
C	-2.80336300	2.40271500	0.32000700
C	-3.60533100	1.26256400	-0.05284200
C	-3.01302200	0.09925000	-0.42476400
C	-1.54788900	-0.04178900	-0.41348700
H	3.38183300	-0.78761800	0.26875000
H	4.61314100	1.35324000	0.26992900
H	3.30511300	3.49083000	-0.09819700
H	0.86820200	3.36577000	-0.34277500
H	-0.87594200	3.21683700	0.59753100
H	-3.28954100	3.31287000	0.65245100
H	-4.68753800	1.33997100	-0.04317800
H	-3.59783600	-0.76451100	-0.72220400
H	-1.42544800	-0.87252000	0.88344100
N	1.50283000	0.05847400	0.01973600
Cu	0.82690000	-1.81642300	-0.17797700
C	-1.04268500	-1.04287700	-1.27706300
N	-0.57400300	-1.97694400	-1.83368800
O	-1.26419400	-1.55806600	1.77087200
O	-0.24643300	-2.31443000	1.51413200

im4(g)

C	-0.77232900	-1.03155900	-0.04649500
C	-2.76371900	-0.29131400	0.93192900
C	-3.53171300	-0.96667100	-0.00973800
C	-2.88225200	-1.70885900	-0.99604500
C	-1.48727800	-1.74030000	-1.01342700
C	0.71879700	-1.03842000	-0.02709100
C	1.40458200	-2.22369800	0.26129700
C	2.80149400	-2.25061600	0.29931400
C	3.53694400	-1.09039700	0.04132900
C	2.87681600	0.09797300	-0.26610000
C	1.47110700	0.13044300	-0.30263900
H	-3.22696100	0.28734000	1.72272700
H	-4.61286300	-0.91071700	0.04014400
H	-3.45013000	-2.25145100	-1.74467900
H	-0.94963700	-2.29572600	-1.77310800
H	0.83852700	-3.12583200	0.47005800
H	3.31298900	-3.17869800	0.53382600
H	4.62126900	-1.11087500	0.07083100
H	3.43705000	0.99979300	-0.48759800
H	2.22136200	0.62981500	3.29557100
N	-1.41290500	-0.32428400	0.92054200
Cu	-0.40726600	0.50722000	2.36051600
C	0.82012200	1.35460300	-0.67611400
N	0.31370000	2.35428800	-0.99313900
O	1.85517800	1.20532000	4.00341100
O	0.53983600	1.32440800	3.79549500

im5(g)

C	-0.77945500	-0.90789600	-0.04713800
C	-2.75568800	-0.75787700	1.18352600
C	-3.53386800	-1.00908800	0.05786500
C	-2.89407000	-1.21258000	-1.16462900
C	-1.50093400	-1.16473600	-1.21607700
C	0.71034900	-0.89958000	-0.03500400
C	1.39877500	-1.82570100	0.76067100
C	2.79639700	-1.85708100	0.78011300
C	3.53159900	-0.95750300	0.00329800
C	2.86914800	-0.02621500	-0.79441400
C	1.46340600	0.00676000	-0.81867200
H	-3.20054200	-0.59618500	2.15940000
H	-4.61368800	-1.04318100	0.14631100
H	-3.46688600	-1.41537600	-2.06373300
H	-0.97290900	-1.34245500	-2.14588700
H	0.83427100	-2.54501100	1.34606800
H	3.30714400	-2.59087200	1.39553700
H	4.61618200	-0.98009800	0.01623300
H	3.42897700	0.68259400	-1.39480800
H	2.39955500	-0.18292800	3.63133300
N	-1.40973400	-0.70068000	1.13521500
Cu	-0.40731900	-0.08890000	2.78874600
C	0.81755600	1.00181400	-1.62711600
N	0.32309000	1.82396700	-2.28686800
O	2.02492600	0.51566900	4.19918400
O	0.94195200	1.02818900	3.47756100
Br	-1.67734500	-0.79051400	4.72932200

P3

C	0.87118000	-0.33489900	0.03959400
C	2.76611300	0.74798100	0.78158400
C	3.61125600	-0.13637800	0.10737000
C	3.03087000	-1.16344300	-0.63809200
C	1.64090300	-1.26655600	-0.67542500
C	-0.61539400	-0.41907900	0.04755700
C	-1.43797700	0.72715000	-0.08191300
C	-2.83972700	0.61091600	-0.04576800
C	-3.43714600	-0.63650000	0.11930100
C	-2.63580200	-1.77490300	0.23832300
C	-1.24463700	-1.66262200	0.20042700
H	3.17956600	1.56184300	1.37280800
H	4.68792800	-0.01716300	0.16561700
H	3.64726700	-1.86860800	-1.18700900
H	1.15955400	-2.04182800	-1.26147200
H	-3.44913200	1.50155200	-0.15526400
H	-4.51859900	-0.71738600	0.15096800
H	-3.09136200	-2.75123200	0.37045900
H	-0.63398600	-2.55193900	0.31696800
N	1.42938300	0.65952000	0.75572800
N	-0.55149000	3.12722600	-0.53625300
C	-0.89738700	2.03792200	-0.31119300

im1(h)

C	-2.00403600	0.24568500	0.07611000
C	-2.11896800	-2.09640700	0.04048900
C	-3.50942700	-2.05843400	-0.03238200
C	-4.15089000	-0.81809500	-0.06072000
C	-3.39180400	0.35226400	-0.00957200
C	-1.05498100	1.37599300	0.12807300
C	0.08458400	1.24983600	0.98505800
C	1.10888700	2.22292100	0.95367200
C	0.99160700	3.31734500	0.10780300
C	-0.15064700	3.45768400	-0.70171600
C	-1.16565400	2.49399000	-0.69958300
H	-1.57101900	-3.03165900	0.05904500
H	-4.06962700	-2.98547300	-0.06418800
H	-5.23283000	-0.76162200	-0.11735700
H	-3.86222800	1.32856500	-0.02139800
H	0.04343800	0.56485100	1.83414100
H	1.95750800	2.12346700	1.62144200
H	1.76700200	4.07540600	0.08314400
H	-0.23922800	4.31851300	-1.35686600
H	-2.01453200	2.59833400	-1.36688600
N	-1.39336500	-0.96644300	0.09450400
Cu	0.56268900	-0.80459300	0.03721200
Br	2.82326900	-1.05136400	-0.20079100

im2(h)

C	-1.11948100	1.30568200	-0.30403200
C	0.90913300	2.39255300	0.17746200
C	0.36921800	3.64126300	-0.10331600
C	-0.97040500	3.71410300	-0.49136200
C	-1.71393300	2.54196800	-0.59654700
C	-1.87204900	0.03366900	-0.42673500
C	-1.29959700	-1.07878200	-1.06870300
C	-2.01698600	-2.27216700	-1.18506700
C	-3.31095200	-2.36689500	-0.66469500
C	-3.88974600	-1.26027000	-0.03310700
C	-3.17800200	-0.06517000	0.08304200
H	1.94123100	2.28072900	0.49039300
H	0.98831200	4.52632100	-0.01502000
H	-1.42720300	4.67135700	-0.72099200
H	-2.74597200	2.56623400	-0.92640600
H	-0.31237800	-1.00299500	-1.51571300
H	-1.56755900	-3.12083200	-1.69162100
H	-3.86735500	-3.29504300	-0.75413300
H	-4.89309800	-1.32919900	0.37608700
H	-3.62639000	0.78308400	0.59112500
N	0.17738500	1.26479900	0.08636400
Cu	1.02166800	-0.43323700	0.75110300
Br	2.68536200	-0.90533200	-0.80887800
N	0.15382700	-0.71195300	2.42906400
C	-0.31964000	-0.91159000	3.49046200

ts1(h)

C	-1.75950700	0.88254300	-0.24079900
C	-0.41744300	2.78245000	-0.14727500
C	-1.52432500	3.62743600	-0.16718600
C	-2.79725300	3.05907800	-0.20755300
C	-2.91565100	1.66917800	-0.24496600
C	-1.83456900	-0.59975300	-0.33234400
C	-1.29680200	-1.26949100	-1.42467700
C	-1.38054800	-2.66929100	-1.51713000
C	-2.02386400	-3.41899200	-0.51133100
C	-2.54194500	-2.78405200	0.59910300
C	-2.37961700	-1.36303400	0.76488700
H	0.58997300	3.18237700	-0.09830700
H	-1.38254600	4.70192700	-0.14297000
H	-3.68433900	3.68410800	-0.21781300
H	-3.88910600	1.19443100	-0.29827200
H	-0.83940400	-0.70391600	-2.23051300
H	-0.96502900	-3.17250600	-2.38421400
H	-2.12162600	-4.49427300	-0.61980500
H	-3.03937400	-3.34486900	1.38319400
H	-3.03930900	-0.85745900	1.46348400
N	-0.52504600	1.43929300	-0.17484800
Cu	1.11847100	0.31683400	0.26881600
Br	3.36452600	-0.19700400	-0.24079200
N	0.26933200	-0.66826900	1.92774100
C	-0.79138100	-1.18261100	2.00854700

im3(h)

C	-1.49353300	0.92475000	-0.37743900
C	-0.19283600	2.86810500	-0.26345600
C	-1.31364800	3.69134600	-0.25327900
C	-2.57419300	3.09227800	-0.28388600
C	-2.66215400	1.70493900	-0.34500300
C	-1.54884500	-0.54025900	-0.50757600
C	-0.65544300	-1.23161300	-1.30355300
C	-0.70129300	-2.63000600	-1.46638100
C	-1.70514200	-3.39400200	-0.80738000
C	-2.63869000	-2.80075600	-0.01312600
C	-2.65988000	-1.30051700	0.21702700
H	0.80573200	3.28874600	-0.21695500
H	-1.19351200	4.76759400	-0.20972500
H	-3.47627700	3.69548800	-0.27220100
H	-3.63423800	1.22975800	-0.40230700
H	0.08621900	-0.67021200	-1.86541700
H	0.01785800	-3.11865300	-2.11407300
H	-1.73615300	-4.46986800	-0.95279800
H	-3.41456000	-3.37679500	0.47990800
H	-3.64510100	-0.92515900	-0.11245300
N	-0.26867800	1.52137900	-0.30886200
Cu	1.39518300	0.52156500	-0.03122600
Br	3.41485200	-0.49318100	0.38318000
N	-2.56753800	-0.82939400	2.81804200
C	-2.61074100	-1.02755600	1.67381300

ts2(h)

C	0.61419100	-0.59021200	-0.08104700
C	2.68230900	0.28487800	0.61983500
C	3.38167600	-0.83411100	0.15886000
C	2.66133400	-1.84975800	-0.48153000
C	1.28765000	-1.72555400	-0.61317000
C	-0.81084300	-0.47240600	-0.06764900
C	-1.48111700	0.24395900	0.98418100
C	-2.84048800	0.36135900	1.04861900
C	-3.67269000	-0.19520500	-0.00513600
C	-3.11450700	-0.91370500	-1.03097600
C	-1.69813600	-1.20004000	-1.07299200
H	3.21129900	1.10629400	1.09176300
H	4.45576400	-0.88993300	0.29029800
H	3.16598600	-2.73121800	-0.86298900
H	0.72468200	-2.51903600	-1.08607100
H	-0.87933700	0.62037000	1.80559600
H	-3.30919200	0.85383600	1.89294000
H	-4.74538800	-0.03492400	0.01840000
H	-3.73752200	-1.30354600	-1.82920600
H	-1.81614500	-2.60435300	-0.41382900
N	1.35408400	0.42487400	0.50113300
Cu	0.61525700	2.22221200	0.72451000
Br	-0.07112600	4.40404900	0.92988800
N	-0.77516800	-1.77705000	-3.43212300
C	-1.17819600	-1.49452400	-2.37221900
O	-2.03007100	-3.53873000	0.15724900
O	-3.26392800	-3.47707700	0.52526600

im4(h)

C	-0.48617300	1.53383100	-0.25468800
C	1.40557300	2.87806600	-0.47768200
C	0.64635900	4.04257500	-0.42545300
C	-0.73613200	3.93318500	-0.27750800
C	-1.30668900	2.66362300	-0.19228200
C	-1.05772300	0.15834700	-0.21233400
C	-0.85286000	-0.71037100	-1.29260300
C	-1.39232400	-1.99920300	-1.29035200
C	-2.14945900	-2.44410000	-0.20030200
C	-2.36436000	-1.59783300	0.88827600
C	-1.82425800	-0.29906500	0.88596300
H	2.48365600	2.91848600	-0.58550900
H	1.13561500	5.00703800	-0.49859800
H	-1.36250200	4.81824000	-0.23623800
H	-2.37971800	2.54339500	-0.09673900
H	-0.28560800	-0.36527300	-2.15092900
H	-1.22331000	-2.65349800	-2.13951400
H	-2.55683800	-3.45020300	-0.18841600
H	-2.93888900	-1.93590400	1.74358000
H	-4.18604600	-1.62416700	-1.34132500
N	0.85900300	1.64605600	-0.39256400
Cu	2.05183000	0.09453100	-0.35918200
Br	3.54827000	-1.64697900	-0.34443800
N	-2.21880000	1.16987500	2.99425800
C	-2.03697700	0.52777900	2.04035400
O	-5.79659900	-1.39661300	-0.43742200
O	-5.10119000	-1.33806700	-1.56957400

im5(h)

C	-0.51431600	1.54437400	-0.25536800
C	1.37356900	2.87137700	-0.64092000
C	0.64996500	4.04399800	-0.46508600
C	-0.70697800	3.94790100	-0.16441600
C	-1.29304900	2.68696800	-0.06085200
C	-1.09134100	0.17430400	-0.21300800
C	-0.91347800	-0.67971100	-1.30980300
C	-1.43977400	-1.97404400	-1.31002300
C	-2.15997900	-2.43870400	-0.20910300
C	-2.35488200	-1.60728800	0.89175400
C	-1.82304300	-0.30580200	0.89846000
H	2.43353100	2.89719300	-0.86457800
H	1.14604900	5.00258700	-0.56081700
H	-1.30476600	4.84082200	-0.02007200
H	-2.35049600	2.58475600	0.14592200
H	-0.39611600	-0.31273000	-2.18975400
H	-1.29154800	-2.61249000	-2.17396600
H	-2.57082400	-3.44266400	-0.20558400
H	-2.90755000	-1.95951900	1.75473300
N	0.80704300	1.65134800	-0.53951400
Cu	2.00335300	0.06812900	-0.70032800
Br	2.58895900	-0.29519100	1.61697900
N	-2.18691200	1.11495600	3.04346500
C	-2.01772800	0.49750500	2.07140600
Br	3.24112800	-1.46050500	-1.93695500

im1(i)

C	0.82595700	0.65960900	0.11057900
C	2.70360200	-0.72620900	-0.07829200
C	3.57119400	0.35383700	0.04978000
C	3.02974100	1.63146400	0.20826200
C	1.64447000	1.78642200	0.24147400
C	-0.65671300	0.72890500	0.13434100
C	-1.39397100	-0.20581900	0.89449800
C	-2.79349700	-0.19625800	0.86380700
C	-3.46914100	0.74399900	0.08100900
C	-2.74349500	1.68644000	-0.65602800
C	-1.34643500	1.68162100	-0.63085100
H	3.07318200	-1.73627000	-0.21547400
H	4.64246800	0.19141800	0.01958600
H	3.67745300	2.49588300	0.31321700
H	1.19592900	2.76240100	0.38741700
H	-0.88275100	-0.86382000	1.59721200
H	-3.34824800	-0.90775600	1.46746400
H	-4.55439300	0.75082200	0.05457500
H	-3.26531100	2.42003800	-1.26294800
H	-0.79191500	2.39812800	-1.22902200
N	1.36497300	-0.57581900	-0.05541100
Cu	0.00680000	-1.99616500	-0.29844700

ts1(i)

C	-1.12392000	0.60490600	0.27446500
C	-2.93767600	-0.67591700	-0.46507000
C	-3.83717900	0.34748600	-0.16719800
C	-3.34263400	1.53411400	0.37834100
C	-1.96964800	1.66882900	0.59782300
C	0.34591400	0.55654500	0.46114900
C	1.18068900	0.28643100	-0.72155200
C	2.16862300	-0.74579100	-0.48304500
C	2.79598800	-0.73498000	0.79296700
C	2.26711300	0.00830300	1.84252700
C	0.96247800	0.55407200	1.69830500
H	-3.27443500	-1.62107000	-0.87932300
H	-4.89654100	0.20877300	-0.35252700
H	-4.01636000	2.34995400	0.62172100
H	-1.55293700	2.58551800	1.00037400
H	0.67407700	0.28502800	-1.68172500
H	2.69029300	-1.18210300	-1.33068300
H	3.68719000	-1.33711800	0.95129400
H	2.75042500	0.01379500	2.81441200
H	0.39955700	0.83691200	2.58503400
N	-1.61889600	-0.56063200	-0.23943200
Cu	0.11897600	-1.76099200	-0.35692700
N	2.78003500	2.92537900	-1.45752000
C	2.15032800	1.99197600	-1.12521800

im2(i)

C	-1.13719300	0.65373900	0.20898900
C	-2.88579000	-0.78533400	-0.39117900
C	-3.84084900	0.20712200	-0.17650700
C	-3.41007400	1.46297700	0.25734000
C	-2.04539200	1.69228100	0.44257000
C	0.33108400	0.74445000	0.37688000
C	1.23692200	0.47386000	-0.84361400
C	2.02812800	-0.78746400	-0.48519500
C	2.72103200	-0.63949200	0.77095100
C	2.28233200	0.24188900	1.74489100
C	0.96024400	0.79223200	1.59308700
H	-3.17191000	-1.78107900	-0.71559800
H	-4.89171300	-0.00726000	-0.33677400
H	-4.12635800	2.25910000	0.43665000
H	-1.67780300	2.66477100	0.75104800
H	0.63244100	0.32993100	-1.74525900
H	2.57401000	-1.25447100	-1.30450800
H	3.57875200	-1.27834400	0.97509000
H	2.78928700	0.31143800	2.70221400
H	0.39192900	1.04659900	2.48669700
N	-1.57286500	-0.58208000	-0.18705300
Cu	0.18251400	-1.73476600	-0.20996100
N	2.79200600	2.54914600	-1.42506800
C	2.10530300	1.65175100	-1.14419000

ts2(i)

C	1.10094900	0.92952400	-0.06725700
C	2.90171500	-0.59070300	0.07647100
C	3.84588900	0.42355200	0.09140800
C	3.39084300	1.74839500	0.00722300
C	2.02904700	1.99732400	-0.06425200
C	-0.33961700	1.19194000	-0.10669900
C	-1.35214300	0.35319300	0.61322300
C	-2.70723500	0.94402400	0.72513700
C	-3.08873500	2.01667100	-0.02826400
C	-2.14373700	2.68508600	-0.86369600
C	-0.80889300	2.28624900	-0.85116000
H	3.19964400	-1.63254500	0.12611300
H	4.90020700	0.18413800	0.16700600
H	4.09400500	2.57540100	0.02367800
H	1.66303200	3.01683100	-0.07438700
H	-1.85629000	-0.79364600	-0.19000400
H	-3.41670500	0.44172800	1.37621400
H	-4.11363800	2.37301300	0.02296800
H	-2.45322200	3.52326500	-1.47896900
H	-0.09815000	2.84120600	-1.45682200
N	1.57254300	-0.35734900	-0.01083100
Cu	0.32210100	-1.75976900	-0.42993500
N	-0.62201500	-0.89260900	2.78754300
C	-0.92149900	-0.31308400	1.81692000
O	-1.33834600	-2.60855400	-0.93743300
O	-2.33078000	-1.73886900	-0.75994200

im3(i)

C	-1.19593700	-0.85561600	-0.25814100
C	-2.67393400	0.94054500	-0.09682500
C	-3.77952300	0.10633700	-0.22649700
C	-3.56993300	-1.26279600	-0.38997300
C	-2.26183600	-1.74690100	-0.40579200
C	0.21357700	-1.34395200	-0.26621100
C	1.02469900	-1.28776600	0.89296700
C	2.34938000	-1.75809300	0.86113000
C	2.87175700	-2.28528300	-0.31867300
C	2.07299300	-2.35683400	-1.46316600
C	0.75461000	-1.89319600	-1.43384600
H	-2.79247700	2.01188200	0.01831900
H	-4.77703700	0.52997400	-0.20438800
H	-4.40765900	-1.94402800	-0.49830600
H	-2.05896700	-2.80586900	-0.51739900
H	3.19738600	2.43025000	-0.33603200
H	2.95348400	-1.71265800	1.76079900
H	3.89531500	-2.64454100	-0.34069900
H	2.47488900	-2.77057300	-2.38263700
H	0.14188300	-1.94442000	-2.32826900
N	-1.40463600	0.47779400	-0.11573100
Cu	0.05977900	1.75162700	-0.08873300
N	0.09222400	-0.43318200	3.16450100
C	0.49902200	-0.80083100	2.13713300
O	1.39966800	3.04978700	-0.05047800
O	2.47498400	2.57606700	-0.96604200

ts1(j)

C	-1.00549300	-0.25684500	-0.09849300
C	-2.83684600	1.12524500	-0.51415000
C	-3.76246600	0.18216300	-0.07419800
C	-3.25884500	-1.05023400	0.37235800
C	-1.89157600	-1.27340300	0.35813800
C	0.44059600	-0.42417100	-0.13262400
C	1.26425600	0.64937200	-0.70865700
C	2.61276000	0.22923400	-1.10481400
C	3.20639100	-0.86095900	-0.51382700
C	2.47508900	-1.70443300	0.36606400
C	1.10219600	-1.50083900	0.49064800
H	-3.17812100	2.09520500	-0.87487500
H	-4.82584000	0.39745000	-0.08518600
H	-3.93277800	-1.82928700	0.71902900
H	-1.50406900	-2.23293500	0.68123800
H	0.73818300	1.26863200	-1.42643100
H	3.17337700	0.86443100	-1.78609400
H	4.23949500	-1.10637300	-0.75485100
H	2.95418000	-2.55085600	0.84869100
H	0.52643300	-2.22250000	1.06499500
N	-1.50901800	0.93496800	-0.52927800
N	1.90325200	2.36567200	1.59426800
C	1.49552300	1.92016100	0.58597900

im1(j)

C	-0.97908900	-0.26437000	-0.06449100
C	-2.81858500	1.11781100	-0.49384600
C	-3.75274400	0.15246700	-0.12730900
C	-3.24816300	-1.09649200	0.28661000
C	-1.88330700	-1.31054200	0.31143100
C	0.44970400	-0.41547100	-0.04803600
C	1.30643000	0.75544300	-0.53223300
C	2.66778400	0.28153500	-1.02341600
C	3.22493700	-0.85261300	-0.51233000
C	2.49405900	-1.73421500	0.35271900
C	1.12345900	-1.53139900	0.48659700
H	-3.15688700	2.09911300	-0.82815300
H	-4.81709400	0.35942000	-0.16661000
H	-3.92643500	-1.89619200	0.57451600
H	-1.50059100	-2.28255600	0.60275300
H	0.77211700	1.30086700	-1.31897200
H	3.20120100	0.91496600	-1.72690300
H	4.23230600	-1.13174000	-0.82056100
H	2.96795500	-2.61847500	0.76705600
H	0.54218300	-2.29769100	0.99621500
N	-1.48845700	0.94678600	-0.46374600
N	1.66721600	2.52691500	1.42834500
C	1.48783700	1.77057600	0.55904800

ts2(j)

C	1.27832900	0.41721900	-0.01895800
C	2.80842500	-1.32746000	-0.15032600
C	3.90259900	-0.46835100	-0.25272400
C	3.64730300	0.91037000	-0.21997600
C	2.33970100	1.35693700	-0.09748200
C	-0.12101200	0.82014200	0.09204500
C	-1.16733700	-0.17513200	0.49797200
C	-2.53426100	0.37172100	0.68006100
C	-2.86797700	1.63555100	0.28254200
C	-1.87420700	2.51626200	-0.23913500
C	-0.54524300	2.09608400	-0.30184500
H	2.95798200	-2.40619000	-0.16149300
H	4.90983800	-0.86116100	-0.34290000
H	4.46315800	1.62558800	-0.27572700
H	2.13956800	2.42060500	-0.03805900
H	-1.29862700	-0.99961900	-0.57965700
H	-3.28492700	-0.29095800	1.09948100
H	-3.89601900	1.97569800	0.37622300
H	-2.14385200	3.51466000	-0.56792300
H	0.19024700	2.79192700	-0.69451700
N	1.53891300	-0.91680700	-0.03726300
N	-0.67043900	-1.93449900	2.36365400
C	-0.83261800	-1.12936500	1.53162800
O	-1.49501300	-1.72385100	-1.61469800
O	-2.78690900	-2.01202900	-1.62418700