

Supplementary Materials: On the Possible Coordination on a ^3MC State Itself? Mechanistic Investigation Using DFT-Based Methods

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Figure S1: MO diagram schematizing the interaction between the metallic fragment in the ^3MC state and the approaching acetonitrile ligand.....p2

Figure S2: MO diagram at selected points along the reaction path.....p3

Cartesian coordinates of the 20 beads along the minimum energy path.....p4

Figure S1 : MO diagram schematizing the interaction between the metallic fragment in the ^3MC state and the approaching acetonitrile ligand

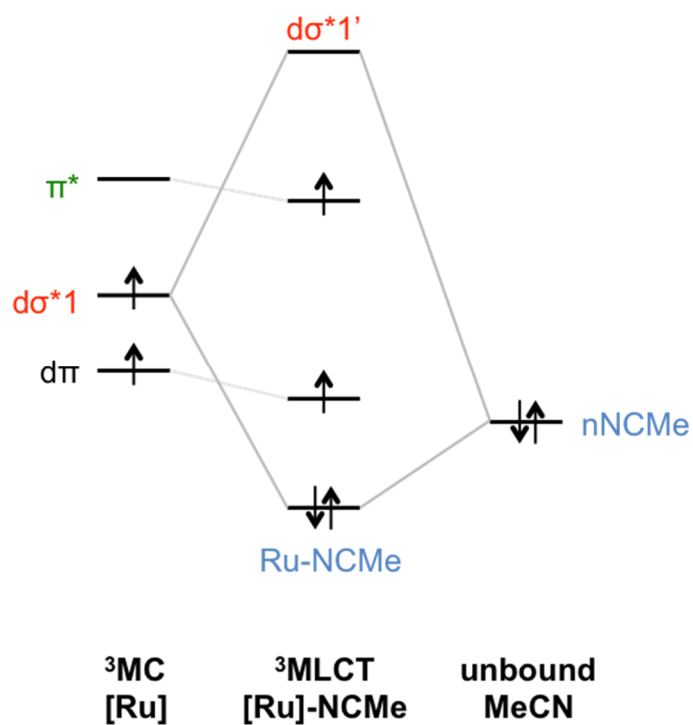
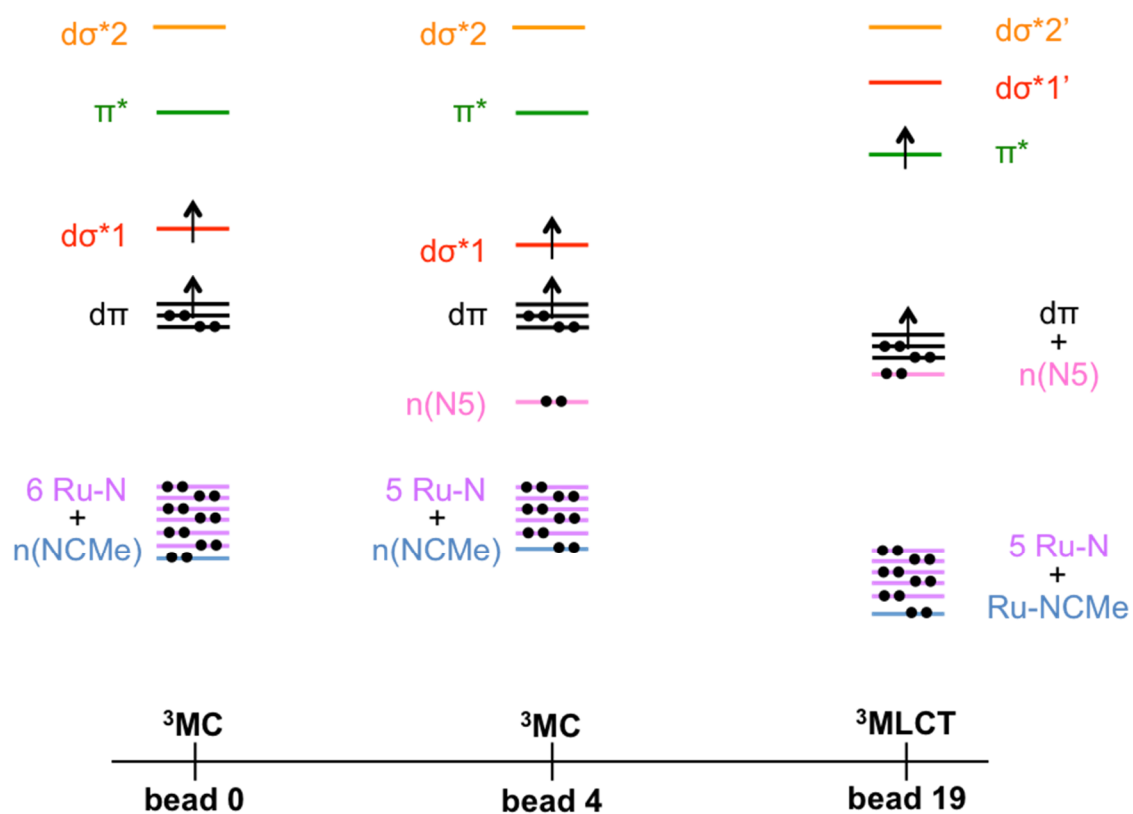


Figure S2 : MO diagram at selected points along the reaction path

- bead 0 = initial $^3\text{MC}_{\text{cis}}$ state + unbound MeCN
- bead 4 = pentacoordinated complex in a ^3MC state + unbound MeCN
- bead 19 = final $^3\text{MLCT}$ state following coordination of MeCN



Cartesian coordinates of the 20 beads along the minimum energy path

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bead0

Ru	0.00195100	0.10139200	0.06887900
N	0.91292700	-1.67210200	-0.69460800
C	2.10754100	-1.73798500	-1.29858300
C	2.59067700	-2.91115100	-1.84783400
C	1.80723300	-4.05548800	-1.76862900
C	0.56586200	-3.98776800	-1.15748600
C	0.12950100	-2.77829700	-0.63088000
C	-1.18262800	-2.59324900	-0.00089800
C	-2.06772500	-3.63636500	0.24389100
C	-3.30174400	-3.36867200	0.81169800
C	-3.62988700	-2.05495800	1.11634500
C	-2.70454600	-1.06035900	0.85826300
N	-1.50137100	-1.31368700	0.32333000
H	2.68268300	-0.82438300	-1.32571900
H	3.56082100	-2.92361200	-2.32275300
H	2.15417300	-4.98976800	-2.18671100
H	-0.06109500	-4.86382900	-1.10321400
H	-1.79515900	-4.64960400	-0.00739300
H	-3.99635500	-4.17291500	1.00890100
H	-4.58342700	-1.79557600	1.55269000
H	-2.91605900	-0.02858900	1.09357400
N	1.52113700	1.48599700	-0.23603600
C	2.70954600	1.43564600	0.38384000
C	3.68412900	2.39819700	0.20051200
C	3.42355500	3.46038800	-0.65472100
C	2.19874800	3.51750100	-1.29962300
C	1.25736200	2.51897300	-1.07626200
C	-0.06980500	2.50306900	-1.71013000
C	-0.44842900	3.38161600	-2.71822700
C	-1.72137300	3.29238800	-3.25824100
C	-2.59326900	2.31954900	-2.78598300
C	-2.15559300	1.46754500	-1.78806800
N	-0.93013000	1.55820500	-1.25409700
H	2.86347000	0.59918100	1.04746600
H	4.62563900	2.30888000	0.72217400
H	4.15986300	4.23514600	-0.81437200
H	1.97282700	4.33806700	-1.96251000
H	0.24340700	4.12291800	-3.08629100
H	-2.02418800	3.97157900	-4.04300600
H	-3.59495600	2.21864300	-3.17748400
H	-2.79586100	0.69275000	-1.39258400
N	-0.74769800	1.32782900	1.97061100
C	-1.54620700	2.38556500	1.80013200
C	-2.12228900	3.07618100	2.85319800

C	-1.84493300	2.65147100	4.14391800
C	-1.00669000	1.56593300	4.32663200
C	-0.46640400	0.91218400	3.21905000
C	0.44289000	-0.24807300	3.36795900
C	0.76497700	-0.77948000	4.61798000
C	1.65906000	-1.83397400	4.69857600
C	2.21634800	-2.33609000	3.53144900
C	1.82798900	-1.77299500	2.32629200
N	0.96491300	-0.75934200	2.24379900
H	-1.73684400	2.68209600	0.77980800
H	-2.77303200	3.91577500	2.65577700
H	-2.26787100	3.16017000	4.99932800
H	-0.77380500	1.23652600	5.32624700
H	0.32981000	-0.37922900	5.51986900
H	1.91777500	-2.25281700	5.66123900
H	2.93272700	-3.14482800	3.54689700
H	2.22977700	-2.14287800	1.39372600
N	-0.18962600	-0.77176100	-4.85056200
C	-0.23358700	-0.97212600	-5.97942900
C	-0.29387500	-1.22770800	-7.40225600
H	0.70639200	-1.15908500	-7.83090700
H	-0.68715200	-2.22866400	-7.58084100
H	-0.94571100	-0.49662700	-7.88163600

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bead1

Ru	0.01043900	0.15689300	0.16924400
N	0.92004500	-1.61304400	-0.56949100
C	2.11967900	-1.68518900	-1.16305700
C	2.61537600	-2.86478000	-1.68485800
C	1.83926500	-4.01340600	-1.59257500
C	0.59293800	-3.94047200	-0.99194600
C	0.14618700	-2.72607900	-0.48753900
C	-1.16943900	-2.53935100	0.13385700
C	-2.05472400	-3.58088200	0.38451500
C	-3.29220400	-3.30838500	0.94250900
C	-3.62289400	-1.99127200	1.23036700
C	-2.69720500	-0.99859400	0.96871000
N	-1.49016800	-1.25647600	0.44359400
H	2.69351700	-0.77105700	-1.20022300
H	3.59145500	-2.87913400	-2.14579700
H	2.19758100	-4.95339400	-1.98806300
H	-0.02895900	-4.81936700	-0.92211700
H	-1.77713700	-4.59662400	0.14932100
H	-3.98437000	-4.11186600	1.15083500
H	-4.57724800	-1.72771700	1.66210900
H	-2.91242100	0.03505800	1.19335100
N	1.52301700	1.54985200	-0.14308000
C	2.71175600	1.49980600	0.47499600
C	3.68509900	2.46357100	0.29255600

C	3.42234900	3.52232400	-0.56558700
C	2.19619300	3.57976200	-1.20702500
C	1.25404000	2.58282300	-0.98123600
C	-0.07841200	2.57016500	-1.60401200
C	-0.47079700	3.45604700	-2.60090900
C	-1.75096400	3.36651400	-3.12531300
C	-2.61285000	2.38578500	-2.65222200
C	-2.16286000	1.53086300	-1.66268800
N	-0.93332400	1.62401800	-1.14189300
H	2.86787000	0.66143700	1.13598800
H	4.62688700	2.37375400	0.81360200
H	4.15870900	4.29592900	-0.73202100
H	1.96998600	4.40040800	-1.86965900
H	0.21482200	4.20238300	-2.97104800
H	-2.06865100	4.05270000	-3.89792600
H	-3.61638300	2.28139300	-3.03725500
H	-2.79700200	0.75247300	-1.26308800
N	-0.72543000	1.35504500	2.06712200
C	-1.50832800	2.42733400	1.90068000
C	-2.07680500	3.11862800	2.95643900
C	-1.81074600	2.68405400	4.24639200
C	-0.98151000	1.59021100	4.42522600
C	-0.44765400	0.93356900	3.31580400
C	0.45164200	-0.23620700	3.46777800
C	0.71738700	-0.80917400	4.71295500
C	1.60953300	-1.86594200	4.79862100
C	2.21268100	-2.33690700	3.64142200
C	1.87752300	-1.73335700	2.43943100
N	1.02089700	-0.71553100	2.35275600
H	-1.69124100	2.73687300	0.88290600
H	-2.70730600	3.97426500	2.76277900
H	-2.23668700	3.18978800	5.10163600
H	-0.74978300	1.25396700	5.42305500
H	0.23691100	-0.44287800	5.60590900
H	1.83119300	-2.31387600	5.75778900
H	2.92256500	-3.15145700	3.66289400
H	2.31735500	-2.07714600	1.51403100
N	-0.17631100	-0.71390300	-4.58531900
C	-0.21935400	-0.91774900	-5.71817500
C	-0.27113200	-1.17782500	-7.14516100
H	0.73231700	-1.12940000	-7.56793000
H	-0.68669000	-2.17045000	-7.32468300
H	-0.90022500	-0.43880100	-7.63928600
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bead2			
Ru	0.01191300	0.16931600	0.14400700
N	0.92562500	-1.60209900	-0.56717800
C	2.13007600	-1.67826000	-1.15026700
C	2.63396300	-2.86334500	-1.65104200

C	1.86154400	-4.01363500	-1.54825400
C	0.61167400	-3.93719800	-0.95591100
C	0.15707800	-2.71779500	-0.47172500
C	-1.16127600	-2.52841300	0.14161400
C	-2.04436000	-3.56929100	0.40225000
C	-3.28519800	-3.29309600	0.95079600
C	-3.62135600	-1.97305200	1.21882800
C	-2.69717800	-0.98109200	0.94909500
N	-1.48633300	-1.24265000	0.43406100
H	2.70069700	-0.76263400	-1.19655300
H	3.61276100	-2.87980800	-2.10601700
H	2.22533300	-4.95751700	-1.92900600
H	-0.00773700	-4.81700400	-0.87698500
H	-1.76164300	-4.58718400	0.18307100
H	-3.97555700	-4.09592600	1.16729000
H	-4.57836700	-1.70699300	1.64302700
H	-2.91721800	0.05497500	1.15779700
N	1.51775400	1.56619000	-0.18143600
C	2.70823300	1.51833400	0.43287900
C	3.67802800	2.48534000	0.24978500
C	3.40963200	3.54417100	-0.60644300
C	2.18069900	3.59997300	-1.24301500
C	1.24133000	2.60096200	-1.01474000
C	-0.09699500	2.59006500	-1.62594500
C	-0.50236000	3.48525300	-2.60934300
C	-1.78870100	3.39854500	-3.11945300
C	-2.64351800	2.41198300	-2.64606200
C	-2.18030500	1.54847300	-1.67005500
N	-0.94515100	1.63861400	-1.16371300
H	2.86628700	0.67933100	1.09240900
H	4.62069800	2.39814600	0.76962300
H	4.14381300	4.31947000	-0.77458200
H	1.94998000	4.42165700	-1.90278900
H	0.17685900	4.23771700	-2.97878900
H	-2.11679000	4.09201700	-3.88114100
H	-3.65147000	2.30950100	-3.01993200
H	-2.80849600	0.76565700	-1.26981700
N	-0.70000600	1.34462600	2.03862000
C	-1.46647000	2.43048700	1.87827200
C	-2.03376900	3.11792200	2.93660600
C	-1.77998000	2.66894900	4.22398900
C	-0.96126700	1.56631500	4.39731500
C	-0.43315100	0.90924800	3.28555200
C	0.44880000	-0.27377600	3.43707700
C	0.64636700	-0.89445000	4.67212100
C	1.53750200	-1.95171600	4.76641600
C	2.19918300	-2.38049400	3.62476900
C	1.92107000	-1.73749200	2.42806600
N	1.07020800	-0.71493700	2.33416300

H	-1.63776400	2.75370300	0.86306200
H	-2.65280600	3.98271600	2.74645800
H	-2.20719400	3.17052900	5.08097200
H	-0.73016300	1.22331400	5.39300000
H	0.11084200	-0.56641100	5.54853500
H	1.71185900	-2.43258700	5.71949300
H	2.90866800	-3.19535400	3.65445000
H	2.40424700	-2.05415300	1.51407900
N	-0.17462800	-0.70934800	-4.47667300
C	-0.21205400	-0.92021400	-5.60842900
C	-0.25679300	-1.18848300	-7.03438400
H	0.75136100	-1.17017500	-7.44812700
H	-0.69690500	-2.17069400	-7.21219600
H	-0.86112600	-0.43622300	-7.53954500

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bead3

Ru	0.01400700	0.18130500	0.12014100
N	0.93210900	-1.59173000	-0.56162600
C	2.14120200	-1.67064500	-1.13436500
C	2.65268300	-2.85993300	-1.61667100
C	1.88431200	-4.01200800	-1.50450800
C	0.63127100	-3.93349500	-0.91937500
C	0.16860500	-2.70992900	-0.45417700
C	-1.15291100	-2.51798400	0.15057300
C	-2.03435600	-3.55792000	0.42035300
C	-3.27876100	-3.27804300	0.95877500
C	-3.62001000	-1.95548700	1.20759600
C	-2.69693000	-0.96450300	0.93052700
N	-1.48226900	-1.22950300	0.42571200
H	2.70896400	-0.75372300	-1.18769900
H	3.63381000	-2.87752900	-2.06636800
H	2.25362800	-4.95877300	-1.87238900
H	0.01506200	-4.81470500	-0.83195000
H	-1.74703400	-4.57785700	0.21723200
H	-3.96788300	-4.07991500	1.18251800
H	-4.57992300	-1.68695400	1.62362100
H	-2.92173700	0.07355100	1.12425500
N	1.51369300	1.58176100	-0.21791900
C	2.70574000	1.53712500	0.39315800
C	3.67163800	2.50756700	0.20863800
C	3.39733900	3.56580700	-0.64635000
C	2.16578400	3.61911000	-1.27837100
C	1.22977600	2.61750100	-1.04739600
C	-0.11407000	2.60702900	-1.64755400
C	-0.53234800	3.51056000	-2.61792100
C	-1.82462300	3.42599300	-3.11368300
C	-2.67232900	2.43393700	-2.63936000
C	-2.19606500	1.56268900	-1.67655500
N	-0.95536900	1.65031100	-1.18484600

H	2.86603900	0.69869000	1.05275200
H	4.61514000	2.42380600	0.72748100
H	4.12887400	4.34326500	-0.81597700
H	1.93027600	4.44177100	-1.93524400
H	0.14040500	4.26886100	-2.98718300
H	-2.16305900	4.12595100	-3.86482900
H	-3.68450600	2.33301800	-3.00205300
H	-2.81859300	0.77613000	-1.27490100
N	-0.67613100	1.33796700	2.00986000
C	-1.42734100	2.43644400	1.85835100
C	-1.99152700	3.11822400	2.92159100
C	-1.74571900	2.65501000	4.20537300
C	-0.93542200	1.54492300	4.37022400
C	-0.41709600	0.88840700	3.25390900
C	0.44603200	-0.30834900	3.40234400
C	0.56936400	-0.97975600	4.62002600
C	1.45846700	-2.03792900	4.72490700
C	2.18388000	-2.42223900	3.60619900
C	1.96745300	-1.73742500	2.41947700
N	1.12409300	-0.70882500	2.31761700
H	-1.58965500	2.77450300	0.84666400
H	-2.60082900	3.99119600	2.73765000
H	-2.17279700	3.15114600	5.06549900
H	-0.70063600	1.19441100	5.36252600
H	-0.02563800	-0.69173800	5.47197900
H	1.58100000	-2.55357400	5.66784500
H	2.89204000	-3.23803000	3.64520900
H	2.49637500	-2.02576900	1.52091800
N	-0.17642900	-0.70312800	-4.37087300
C	-0.20786200	-0.92164800	-5.50141000
C	-0.24463100	-1.19995300	-6.92587600
H	0.76764700	-1.21162200	-7.32964400
H	-0.70838700	-2.17147200	-7.10156500
H	-0.82383200	-0.43587700	-7.44286400

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bead4

Ru	0.01478800	0.19308500	0.09557400
N	0.93723000	-1.58153100	-0.55776200
C	2.15132100	-1.66398200	-1.11896400
C	2.67140600	-2.85829900	-1.57896600
C	1.90674100	-4.01179400	-1.45686100
C	0.64970800	-3.93016500	-0.88106300
C	0.17879200	-2.70194800	-0.43730100
C	-1.14615200	-2.50712700	0.15760400
C	-2.02600700	-3.54608800	0.43613400
C	-3.27394300	-3.26287500	0.96425100
C	-3.62002800	-1.93810600	1.19428900
C	-2.69810500	-0.94807600	0.90984300
N	-1.47974400	-1.21620800	0.41512600

H	2.71636700	-0.74602100	-1.18058200
H	3.65579600	-2.87798600	-2.02129800
H	2.28193900	-4.96191500	-1.80963100
H	0.03630200	-4.81239000	-0.78481100
H	-1.73413700	-4.56772800	0.24862200
H	-3.96199500	-4.06379000	1.19455300
H	-4.58272500	-1.66732300	1.60232500
H	-2.92741700	0.09174100	1.08877900
N	1.50843700	1.59682800	-0.25492800
C	2.70220700	1.55494300	0.35246300
C	3.66465700	2.52830400	0.16604500
C	3.38486400	3.58598700	-0.68779800
C	2.15051700	3.63731200	-1.31475600
C	1.21748800	2.63357600	-1.08057600
C	-0.13165800	2.62390100	-1.66939900
C	-0.56240900	3.53610800	-2.62626000
C	-1.86039200	3.45403500	-3.10778400
C	-2.70113900	2.45658000	-2.63273400
C	-2.21208000	1.57700700	-1.68388400
N	-0.96600900	1.66159700	-1.20673900
H	2.86419300	0.71695500	1.01211400
H	4.60912100	2.44762800	0.68357100
H	4.11420200	4.36505800	-0.85951400
H	1.91053300	4.46071000	-1.96913900
H	0.10429100	4.29982500	-2.99526600
H	-2.20869200	4.16036700	-3.84838900
H	-3.71749600	2.35748900	-2.98408600
H	-2.82958700	0.78732100	-1.28077900
N	-0.65181700	1.33041300	1.97974300
C	-1.38874600	2.44047000	1.83730200
C	-1.94973000	3.11676200	2.90532100
C	-1.71385100	2.63810000	4.18518100
C	-0.91439700	1.51884700	4.34136000
C	-0.40194700	0.86576200	3.22068600
C	0.44639100	-0.34179600	3.36574300
C	0.50061100	-1.05866800	4.56213400
C	1.38340000	-2.12112400	4.67654400
C	2.16934100	-2.46461500	3.58566600
C	2.01563100	-1.73775500	2.41382100
N	1.17977100	-0.70340800	2.30397700
H	-1.54268800	2.79240400	0.82922800
H	-2.54840800	3.99832500	2.72764800
H	-2.14000300	3.12955900	5.04840800
H	-0.67974000	1.15829700	5.33025000
H	-0.14532800	-0.80342500	5.38729500
H	1.45403700	-2.67152100	5.60507500
H	2.87404100	-3.28307200	3.63333400
H	2.59186500	-1.99636900	1.53468100
N	-0.17384900	-0.69347400	-4.25470600

C	-0.20096700	-0.91993300	-5.38404600
C	-0.23204700	-1.20761900	-6.80733100
H	0.78290300	-1.24894700	-7.20247500
H	-0.71922100	-2.16775700	-6.98155200
H	-0.78644100	-0.43246100	-7.33531100
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bead5			
Ru	0.01453200	0.20511100	0.06977400
N	0.94186200	-1.57095800	-0.55515300
C	2.16262600	-1.65742700	-1.10086600
C	2.69117900	-2.85647800	-1.53835800
C	1.92966800	-4.01104000	-1.40759300
C	0.66805900	-3.92628200	-0.84250600
C	0.18839900	-2.69340800	-0.42176100
C	-1.14038600	-2.49583600	0.16241700
C	-2.01837700	-3.53392900	0.45029900
C	-3.26989000	-3.24769800	0.96809200
C	-3.62060700	-1.92102400	1.17986400
C	-2.69982500	-0.93196900	0.88809500
N	-1.47822700	-1.20276300	0.40246700
H	2.72458500	-0.73837300	-1.17064800
H	3.67884500	-2.87814300	-1.97315100
H	2.31056500	-4.96419500	-1.74560300
H	0.05744800	-4.80946700	-0.73767700
H	-1.72225300	-4.55709600	0.27823200
H	-3.95710900	-4.04759400	1.20439000
H	-4.58598800	-1.64819100	1.58010300
H	-2.93329800	0.10928900	1.05318200
N	1.50273000	1.61109300	-0.29164400
C	2.69806000	1.57192500	0.31197000
C	3.65718400	2.54809800	0.12341500
C	3.37198000	3.60523700	-0.72917100
C	2.13485900	3.65457300	-1.35100200
C	1.20504000	2.64850300	-1.11374400
C	-0.14908100	2.63910300	-1.69156600
C	-0.59238500	3.56035500	-2.63415000
C	-1.89584900	3.48081700	-3.10135000
C	-2.73012600	2.47875600	-2.62473500
C	-2.22863900	1.59096200	-1.69009800
N	-0.97615800	1.67039200	-1.22997800
H	2.86181500	0.73446600	0.97190900
H	4.60265400	2.47068900	0.63961100
H	4.09908500	4.38599100	-0.90303600
H	1.89041300	4.47873200	-2.00287100
H	0.06840100	4.32939200	-3.00274700
H	-2.25362100	4.19289000	-3.83190600
H	-3.75050500	2.38150000	-2.96478400
H	-2.84119000	0.79844300	-1.28522700
N	-0.62677300	1.32437500	1.94944700

C	-1.35038000	2.44510700	1.81700800
C	-1.90766500	3.11549700	2.89033700
C	-1.68183000	2.62056700	4.16570700
C	-0.89393300	1.49171000	4.31218000
C	-0.38588100	0.84415000	3.18672200
C	0.44923700	-0.37298000	3.32753500
C	0.43449600	-1.13403300	4.49752400
C	1.30809500	-2.20286700	4.62082300
C	2.15369100	-2.50736600	3.56322000
C	2.06496200	-1.73774600	2.41180800
N	1.23819100	-0.69650200	2.29411300
H	-1.49730800	2.81056000	0.81284900
H	-2.49567400	4.00561600	2.71984100
H	-2.10642700	3.10714600	5.03245300
H	-0.66088900	1.11947200	5.29728900
H	-0.25894900	-0.90833000	5.29246700
H	1.32535100	-2.78852200	5.53011800
H	2.85333700	-3.32975000	3.61947100
H	2.68926500	-1.96535900	1.55636200
N	-0.17009200	-0.68310000	-4.13539000
C	-0.19400300	-0.91726500	-5.26338400
C	-0.22009800	-1.21520200	-6.68558400
H	0.79656700	-1.28649700	-7.07217000
H	-0.73058400	-2.16325900	-6.85842600
H	-0.74918200	-0.42986600	-7.22481400

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Ru	0.01304900	0.21735000	0.04191600
N	0.94788500	-1.56143200	-0.54764400
C	2.17499300	-1.65181400	-1.07821500
C	2.71143800	-2.85507700	-1.49395000
C	1.95266000	-4.01043200	-1.35517200
C	0.68622200	-3.92236700	-0.80177700
C	0.19819300	-2.68510800	-0.40410000
C	-1.13527600	-2.48445200	0.16672700
C	-2.01164300	-3.52143500	0.46377300
C	-3.26662200	-3.23236400	0.97129200
C	-3.62171100	-1.90400300	1.16511300
C	-2.70211600	-0.91613900	0.86547300
N	-1.47763800	-1.18938400	0.38819100
H	2.73460500	-0.73217400	-1.15612800
H	3.70233400	-2.87865400	-1.92121900
H	2.33912000	-4.96644900	-1.67837400
H	0.07785200	-4.80613100	-0.68923500
H	-1.71114600	-4.54594200	0.30778400
H	-3.95301100	-4.03115400	1.21372100
H	-4.58960500	-1.62910800	1.55778500
H	-2.93971800	0.12638100	1.01650600
N	1.49597600	1.62469900	-0.32955300

C	2.69305000	1.58776100	0.27034500
C	3.64900500	2.56665200	0.07983700
C	3.35878500	3.62361800	-0.77132500
C	2.11883400	3.67159200	-1.38773800
C	1.19180300	2.66354300	-1.14735800
C	-0.16752000	2.65551700	-1.71247400
C	-0.62283300	3.58518000	-2.64119300
C	-1.93158400	3.50837600	-3.09402100
C	-2.75917300	2.50157700	-2.61586700
C	-2.24589000	1.60625000	-1.69479500
N	-0.98772900	1.68145600	-1.24995400
H	2.85840600	0.75061700	0.93037600
H	4.59545700	2.49217700	0.59461500
H	4.08398500	4.40571300	-0.94737600
H	1.87013200	4.49651800	-2.03711900
H	0.03245700	4.35890100	-3.00984200
H	-2.29861900	4.22604500	-3.81450900
H	-3.78325900	2.40570800	-2.94506900
H	-2.85356100	0.81048700	-1.28934400
N	-0.60041800	1.31906000	1.91975300
C	-1.31098800	2.44978900	1.79723100
C	-1.86518700	3.11401000	2.87558600
C	-1.65130700	2.60177200	4.14609100
C	-0.87625800	1.46267100	4.28294900
C	-0.36958600	0.82270300	3.15300100
C	0.45416400	-0.40267300	3.28914400
C	0.37235300	-1.20699400	4.42706000
C	1.23497300	-2.28376000	4.55741000
C	2.13746200	-2.55060300	3.53718100
C	2.11451600	-1.73715000	2.41267200
N	1.29761100	-0.68845000	2.28810400
H	-1.45056800	2.82827000	0.79702200
H	-2.44194400	4.01276400	2.71219400
H	-2.07464400	3.08332500	5.01621800
H	-0.64846800	1.07646600	5.26406300
H	-0.36427300	-1.00759700	5.18987600
H	1.19951700	-2.90433000	5.44275000
H	2.83134700	-3.37751000	3.60072200
H	2.78655300	-1.93402500	1.58553300
N	-0.16578800	-0.67332400	-4.01742700
C	-0.18618700	-0.91509000	-5.14388400
C	-0.20771300	-1.22269800	-6.56406900
H	0.81001500	-1.32381600	-6.94113000
H	-0.74150200	-2.15796800	-6.73490900
H	-0.71126900	-0.42733900	-7.11324800
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Ru	0.01026100	0.22939100	0.01175500
N	0.95445000	-1.55280800	-0.53844400

C	2.18806600	-1.64686300	-1.05307200
C	2.73218500	-2.85392400	-1.44716100
C	1.97571000	-4.00981500	-1.30088200
C	0.70409600	-3.91848500	-0.76013300
C	0.20783200	-2.67716100	-0.38571400
C	-1.13085200	-2.47330400	0.17037500
C	-2.00573800	-3.50906100	0.47631000
C	-3.26411300	-3.21723400	0.97362800
C	-3.62334700	-1.88748300	1.14990500
C	-2.70507900	-0.90085300	0.84194100
N	-1.47814600	-1.17644700	0.37217100
H	2.74563500	-0.72684000	-1.13814800
H	3.72636900	-2.87931400	-1.86663600
H	2.36756600	-4.96843700	-1.60943400
H	0.09753000	-4.80260700	-0.64095300
H	-1.70103700	-4.53466400	0.33642700
H	-3.94977900	-4.01487200	1.22201400
H	-4.59355000	-1.61061000	1.53541700
H	-2.94641000	0.14269700	0.97972600
N	1.48869500	1.63764300	-0.36759200
C	2.68750800	1.60255100	0.22872400
C	3.64044800	2.58408900	0.03647600
C	3.34571900	3.64092500	-0.81336100
C	2.10297200	3.68803600	-1.42425600
C	1.17835700	2.67850100	-1.18046800
C	-0.18597500	2.67227700	-1.73256200
C	-0.65307600	3.60986200	-2.64751200
C	-1.96683900	3.53551600	-3.08611200
C	-2.78783200	2.52407700	-2.60640800
C	-2.26302900	1.62136600	-1.69909600
N	-0.99934700	1.69253700	-1.26930800
H	2.85485200	0.76590900	0.88910100
H	4.58787400	2.51225800	0.54981500
H	4.06927900	4.42408700	-0.99162000
H	1.85016100	4.51370800	-2.07118000
H	-0.00309900	4.38791600	-3.01650000
H	-2.34285800	4.25845700	-3.79668200
H	-3.81550800	2.42962900	-2.92473700
H	-2.86585700	0.82241900	-1.29321600
N	-0.57418200	1.31450900	1.89143500
C	-1.27169100	2.45457200	1.77851700
C	-1.82289100	3.11275300	2.86171400
C	-1.62177500	2.58297800	4.12697800
C	-0.86038000	1.43340300	4.25437100
C	-0.35394500	0.80194100	3.12017600
C	0.45924400	-0.43121500	3.25073000
C	0.31335600	-1.27783500	4.35093700
C	1.16463400	-2.36312800	4.48627300
C	2.12045000	-2.59366400	3.50650600

C	2.16209300	-1.73562400	2.41591600
N	1.35502300	-0.67962800	2.28558900
H	-1.40376000	2.84538500	0.78216800
H	-2.38787900	4.02014900	2.70540200
H	-2.04364800	3.05958700	5.00044900
H	-0.63962400	1.03264900	5.23140400
H	-0.46169300	-1.10158100	5.08100500
H	1.07900200	-3.01714800	5.34374000
H	2.80897200	-3.42474500	3.57613800
H	2.88169500	-1.90151600	1.62223200
N	-0.16078800	-0.66276800	-3.89935500
C	-0.17815700	-0.91243900	-5.02396800
C	-0.19543100	-1.23036500	-6.44168100
H	0.82267000	-1.36126400	-6.80852400
H	-0.75223400	-2.15231700	-6.61009500
H	-0.67315400	-0.42575900	-7.00065500

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Ru	0.00650800	0.24061900	-0.02052600
N	0.96113300	-1.54526900	-0.52834200
C	2.20103100	-1.64250700	-1.02678700
C	2.75286700	-2.85297200	-1.39888900
C	1.99841500	-4.00922000	-1.24552600
C	0.72146300	-3.91491600	-0.71801900
C	0.21720900	-2.66997700	-0.36672100
C	-1.12706600	-2.46283300	0.17358300
C	-2.00079800	-3.49708200	0.48812500
C	-3.26251700	-3.20259500	0.97517300
C	-3.62558600	-1.87166500	1.13445800
C	-2.70863700	-0.88649800	0.81776300
N	-1.47949600	-1.16439000	0.35479900
H	2.75665100	-0.72215700	-1.11867200
H	3.75058600	-2.88006100	-1.80982800
H	2.39558200	-4.97019200	-1.53949400
H	0.11633000	-4.79923100	-0.59323500
H	-1.69216700	-4.52355800	0.36405900
H	-3.94766100	-3.99894600	1.22917300
H	-4.59788600	-1.59273800	1.51313800
H	-2.95345000	0.15793400	0.94257800
N	1.48109900	1.64947000	-0.40591600
C	2.68135900	1.61628800	0.18748400
C	3.63162300	2.60016000	-0.00631000
C	3.33286300	3.65688400	-0.85493000
C	2.08742600	3.70348700	-1.46048600
C	1.16506200	2.69247300	-1.21391900
C	-0.20414500	2.68818300	-1.75293400
C	-0.68272000	3.63383100	-2.65365200
C	-2.00143300	3.56234000	-3.07779900
C	-2.81604800	2.54641700	-2.59671600

C	-2.28006800	1.63636700	-1.70337400
N	-1.01103100	1.70322700	-1.28877400
H	2.85056000	0.78035300	0.84851400
H	4.57997600	2.53058600	0.50561600
H	4.05504000	4.44086700	-1.03533200
H	1.83077600	4.53000600	-2.10488100
H	-0.03778100	4.41613100	-3.02256100
H	-2.38607800	4.29054900	-3.77834700
H	-3.84720100	2.45350600	-2.90418900
H	-2.87835400	0.83453100	-1.29698600
N	-0.54867300	1.31023500	1.86405600
C	-1.23288900	2.45916500	1.76042900
C	-1.78110000	3.11145000	2.84834500
C	-1.59340300	2.56408300	4.10803800
C	-0.84617100	1.40395700	4.22614300
C	-0.33935600	0.78148400	3.08789600
C	0.46447700	-0.45882300	3.21238600
C	0.25827500	-1.34540800	4.27071300
C	1.09820200	-2.43946000	4.40872800
C	2.10424000	-2.63551400	3.47255700
C	2.20818400	-1.73356300	2.42217500
N	1.41034800	-0.67080600	2.28718600
H	-1.35714100	2.86168500	0.76782200
H	-2.33378900	4.02749600	2.69911900
H	-2.01363900	3.03590800	4.98475200
H	-0.63375300	0.98823700	5.19887900
H	-0.55204100	-1.19023300	4.96689100
H	0.96556600	-3.12519700	5.23497300
H	2.78783900	-3.47034900	3.54757900
H	2.97272300	-1.86952200	1.66541300
N	-0.15626700	-0.64882900	-3.78028800
C	-0.16978100	-0.90803300	-4.90275400
C	-0.18288600	-1.23731800	-6.31774800
H	0.83464300	-1.39786100	-6.67432400
H	-0.76224100	-2.14552600	-6.48360000
H	-0.63480600	-0.42466100	-6.88667900

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Ru	0.00154500	0.25093200	-0.05484100
N	0.96752100	-1.53857000	-0.51793800
C	2.21388000	-1.63866900	-0.99917500
C	2.77330000	-2.85207300	-1.34939800
C	2.02045400	-4.00850200	-1.18970900
C	0.73798900	-3.91148400	-0.67620000
C	0.22573100	-2.66332300	-0.34828000
C	-1.12442400	-2.45301900	0.17554400
C	-1.99700400	-3.48558000	0.49886900
C	-3.26191300	-3.18852700	0.97582600
C	-3.62854000	-1.85664800	1.11847700

C	-2.71299900	-0.87312700	0.79254800
N	-1.48215400	-1.15330000	0.33552600
H	2.76765200	-0.71803200	-1.09715800
H	3.77477400	-2.88077100	-1.75104000
H	2.42285000	-4.97162800	-1.46903900
H	0.13396600	-4.79585600	-0.54670500
H	-1.68461500	-4.51270400	0.39057600
H	-3.94655800	-3.98349200	1.23552200
H	-4.60262000	-1.57563600	1.49102900
H	-2.96083500	0.17201800	0.90522900
N	1.47295300	1.66025800	-0.44454500
C	2.67439500	1.62878800	0.14658800
C	3.62237300	2.61463400	-0.04845200
C	3.32015400	3.67133600	-0.89595800
C	2.07218500	3.71791400	-1.49634700
C	1.15169900	2.70574600	-1.24735800
C	-0.22225700	2.70393600	-1.77327400
C	-0.71195100	3.65766300	-2.65937700
C	-2.03534800	3.58910400	-3.06926100
C	-2.84393000	2.56890300	-2.58703000
C	-2.29739600	1.65159600	-1.70769300
N	-1.02311400	1.71402700	-1.30833200
H	2.84524900	0.79361300	0.80844800
H	4.57156000	2.54691900	0.46219300
H	4.04126800	4.45586200	-1.07835900
H	1.81198200	4.54542700	-2.13808400
H	-0.07165900	4.44375700	-3.02835000
H	-2.42831200	4.32267300	-3.75953200
H	-3.87841500	2.47757800	-2.88370500
H	-2.89098200	0.84673000	-1.30100100
N	-0.52371800	1.30602100	1.83691000
C	-1.19473800	2.46337100	1.74240300
C	-1.73988400	3.10978000	2.83490200
C	-1.56596700	2.54463300	4.08865500
C	-0.83347100	1.37397300	4.19726100
C	-0.32531700	0.76101500	3.05515700
C	0.47034700	-0.48586900	3.17342700
C	0.20759100	-1.40876800	4.18740700
C	1.03639800	-2.51143100	4.32665000
C	2.09057000	-2.67531000	3.43817400
C	2.25388400	-1.73247300	2.43210000
N	1.46469000	-0.66355500	2.29314200
H	-1.31091900	2.87715600	0.75350900
H	-2.27987600	4.03445400	2.69301700
H	-1.98447200	3.01169700	4.96862200
H	-0.63060600	0.94274600	5.16539000
H	-0.63541600	-1.27288200	4.84819300
H	0.85971900	-3.22704000	5.11874400
H	2.76876800	-3.51420600	3.51811300

H	3.05972200	-1.84052700	1.71455400
N	-0.15202300	-0.63337500	-3.66001800
C	-0.16115100	-0.90184400	-4.78008500
C	-0.17028800	-1.24287300	-6.19209900
H	0.84583200	-1.43280900	-6.53813000
H	-0.77163400	-2.13702700	-6.35515100
H	-0.59649700	-0.42333200	-6.77108100

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Ru	-0.00535100	0.25946300	-0.09343100
N	0.97303100	-1.53392100	-0.50554900
C	2.22543900	-1.63728400	-0.96950100
C	2.79169700	-2.85365400	-1.29747400
C	2.03957200	-4.00971600	-1.13162200
C	0.75177100	-3.90926600	-0.63233600
C	0.23275100	-2.65801500	-0.32759400
C	-1.12297400	-2.44438300	0.17971000
C	-1.99301600	-3.47513200	0.51552200
C	-3.26073700	-3.17574300	0.98318600
C	-3.63174700	-1.84311200	1.10657000
C	-2.71917700	-0.86139900	0.76698900
N	-1.48693100	-1.14367600	0.31489200
H	2.77747700	-0.71657700	-1.07451000
H	3.79684700	-2.88435600	-1.68971200
H	2.44589800	-4.97500100	-1.39728100
H	0.14768200	-4.79294800	-0.49890600
H	-1.67602500	-4.50253100	0.42473100
H	-3.94375300	-3.96924600	1.25153000
H	-4.60728000	-1.56001300	1.47371000
H	-2.97124200	0.18431000	0.86409400
N	1.46424100	1.66852900	-0.48612500
C	2.66662600	1.63738500	0.10331200
C	3.61306800	2.62483000	-0.09107600
C	3.30893500	3.68243100	-0.93690900
C	2.05873400	3.73055800	-1.53251700
C	1.13896600	2.71799500	-1.28216000
C	-0.23961200	2.72060000	-1.79456500
C	-0.73932200	3.68325300	-2.66523700
C	-2.06728200	3.61919600	-3.06083900
C	-2.87057300	2.59467900	-2.57882500
C	-2.31436100	1.66908600	-1.71440900
N	-1.03547000	1.72649900	-1.32916200
H	2.83878300	0.80174100	0.76449700
H	4.56279000	2.55757900	0.41866500
H	4.03006000	4.46662200	-1.12096600
H	1.79609900	4.55946400	-2.17148400
H	-0.10287000	4.47293500	-3.03314000
H	-2.46777100	4.35914800	-3.73990400
H	-3.90826000	2.50575400	-2.86501900

H	-2.90365200	0.86065300	-1.30914400
N	-0.49982300	1.30010700	1.80831000
C	-1.15743000	2.46538600	1.72188400
C	-1.70227600	3.10536400	2.81776900
C	-1.54570400	2.52152200	4.06513400
C	-0.82916400	1.33992100	4.16526500
C	-0.31527700	0.73789300	3.02049100
C	0.47550300	-0.51375600	3.13289600
C	0.16330700	-1.46976000	4.10141200
C	0.98544300	-2.57741700	4.24257800
C	2.08434300	-2.70979500	3.40409700
C	2.29979600	-1.73034100	2.44389000
N	1.51685800	-0.65718600	2.30219900
H	-1.26239600	2.89065300	0.73669300
H	-2.22897600	4.03859100	2.68251900
H	-1.96380600	2.98402800	4.94754500
H	-0.64060200	0.89216500	5.12889700
H	-0.71026900	-1.35428000	4.72568800
H	0.77129500	-3.32008400	4.99988400
H	2.75864000	-3.55152200	3.48775600
H	3.14243400	-1.81138000	1.76614500
N	-0.14557900	-0.61463700	-3.53726600
C	-0.15146400	-0.89045500	-4.65532300
C	-0.15719800	-1.24022000	-6.06516500
H	0.85693700	-1.45642300	-6.40158500
H	-0.77823200	-2.12082500	-6.22740300
H	-0.55942300	-0.41428700	-6.65232400

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Ru	-0.01217000	0.26685200	-0.13224900
N	0.97901400	-1.52964400	-0.49299000
C	2.23762000	-1.63488400	-0.93870500
C	2.81107500	-2.85319000	-1.24583400
C	2.05985400	-4.00920100	-1.07548000
C	0.76622400	-3.90669600	-0.59171300
C	0.23968300	-2.65313500	-0.30970900
C	-1.12223900	-2.43664600	0.17970900
C	-1.99071400	-3.46512900	0.52645700
C	-3.26127600	-3.16319800	0.98468400
C	-3.63557800	-1.83000100	1.09118900
C	-2.72485500	-0.85056800	0.74022600
N	-1.49165700	-1.13530000	0.29214600
H	2.78814100	-0.71394000	-1.04823100
H	3.82025300	-2.88501200	-1.62758900
H	2.47128100	-4.97614100	-1.32664600
H	0.16292600	-4.79040600	-0.45503300
H	-1.67011200	-4.49271800	0.45207300
H	-3.94359000	-3.95494200	1.25999600
H	-4.61236000	-1.54456800	1.45323700

H	-2.97965000	0.19555800	0.82523300
N	1.45540800	1.67686700	-0.52634600
C	2.65832000	1.64730700	0.06254400
C	3.60320000	2.63623700	-0.13188100
C	3.29701300	3.69396300	-0.97693500
C	2.04454600	3.74316000	-1.56771100
C	1.12571700	2.73006700	-1.31576100
C	-0.25758900	2.73687100	-1.81440100
C	-0.76729100	3.70717600	-2.67070700
C	-2.09960200	3.64659800	-3.05196700
C	-2.89755000	2.61800100	-2.56957600
C	-2.33188100	1.68575500	-1.71877400
N	-1.04871400	1.73951000	-1.34731500
H	2.83197200	0.81246400	0.72468600
H	4.55344400	2.57007800	0.37712700
H	4.01784200	4.47806200	-1.16268100
H	1.77922900	4.57341300	-2.20384200
H	-0.13479300	4.49995200	-3.03879000
H	-2.50763900	4.39185000	-3.72063400
H	-3.93816200	2.53058500	-2.84555900
H	-2.91666000	0.87391800	-1.31425800
N	-0.47624100	1.29586100	1.78105000
C	-1.12056200	2.46872100	1.70346200
C	-1.66293900	3.10276700	2.80355000
C	-1.52145100	2.50105500	4.04420900
C	-0.82024800	1.30917200	4.13479400
C	-0.30312600	0.71742600	2.98666100
C	0.48153500	-0.53989500	3.09212700
C	0.12195000	-1.52602300	4.01278800
C	0.93490300	-2.64047600	4.15494000
C	2.07530800	-2.74529800	3.36939400
C	2.34093900	-1.73245600	2.45754700
N	1.56585600	-0.65403100	2.31314700
H	-1.21632800	2.90457000	0.72198200
H	-2.17619500	4.04446900	2.67592200
H	-1.93793200	2.95897100	4.92966200
H	-0.64380300	0.84571700	5.09342300
H	-0.77947600	-1.42778700	4.59969400
H	0.68306300	-3.40907500	4.87382600
H	2.74482700	-3.59042600	3.45746100
H	3.21829700	-1.78907300	1.82290300
N	-0.13939700	-0.59585300	-3.41536100
C	-0.14213400	-0.88047500	-4.53102100
C	-0.14463400	-1.24183100	-5.93725800
H	0.86679100	-1.48611100	-6.26232200
H	-0.78614800	-2.10802900	-6.09666000
H	-0.52153800	-0.41081200	-6.53390500

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Ru	-0.01911600	0.27265200	-0.17306300
N	0.98540600	-1.52694000	-0.47872300
C	2.24978900	-1.63364900	-0.90640100
C	2.83022300	-2.85342200	-1.19330400
C	2.07965500	-4.00928800	-1.01918200
C	0.78019400	-3.90505700	-0.55136600
C	0.24645200	-2.64959700	-0.29145400
C	-1.12176100	-2.43031700	0.17942500
C	-1.98873200	-3.45615800	0.53790700
C	-3.26193500	-3.15166400	0.98704100
C	-3.63929400	-1.81805100	1.07624100
C	-2.73052100	-0.84132200	0.71283000
N	-1.49663000	-1.12862600	0.26801000
H	2.79882000	-0.71248100	-1.02039000
H	3.84339600	-2.88602400	-1.56436400
H	2.49604500	-4.97761700	-1.25616200
H	0.17752100	-4.78892800	-0.41288300
H	-1.66536600	-4.48389600	0.47949500
H	-3.94363900	-3.94141000	1.26962700
H	-4.61708700	-1.53008400	1.43363500
H	-2.98808700	0.20505700	0.78534900
N	1.44654100	1.68441800	-0.56736400
C	2.64977200	1.65643100	0.02181800
C	3.59335500	2.64666100	-0.17206300
C	3.28576300	3.70458100	-1.01654400
C	2.03118600	3.75532000	-1.60275500
C	1.11272600	2.74202200	-1.34963800
C	-0.27538400	2.75383500	-1.83407700
C	-0.79460100	3.73144900	-2.67629300
C	-2.13115200	3.67445100	-3.04316900
C	-2.92391500	2.64185000	-2.56069100
C	-2.34926700	1.70344100	-1.72301000
N	-1.06231000	1.75406200	-1.36457800
H	2.82478200	0.82257000	0.68515000
H	4.54386300	2.58130400	0.33665400
H	4.00663600	4.48832000	-1.20376000
H	1.76365100	4.58713400	-2.23591900
H	-0.16590500	4.52704400	-3.04481500
H	-2.54650400	4.42496200	-3.70133100
H	-3.96727500	2.55572700	-2.82673100
H	-2.92953500	0.88798900	-1.31974200
N	-0.45327600	1.29144800	1.75442500
C	-1.08402700	2.47156300	1.68534400
C	-1.62429400	3.10001400	2.78925100
C	-1.49858800	2.48090800	4.02305700
C	-0.81310700	1.27887800	4.10444800
C	-0.29242000	0.69718300	2.95331800
C	0.48646500	-0.56544800	3.05124200
C	0.08451800	-1.58000200	3.92169200

C	0.88988900	-2.69999700	4.06501800
C	2.06721900	-2.77906500	3.33293600
C	2.37697600	-1.73552300	2.47075800
N	1.60848300	-0.65291900	2.32345200
H	-1.17019500	2.91731100	0.70740500
H	-2.12383400	4.04998600	2.66916900
H	-1.91375900	2.93439100	4.91128600
H	-0.64971100	0.80018300	5.05804300
H	-0.84209300	-1.49815500	4.47106000
H	0.60428200	-3.49216900	4.74461600
H	2.73304800	-3.62666100	3.42554000
H	3.28621200	-1.76907200	1.88121900
N	-0.13437800	-0.57497900	-3.29283600
C	-0.13293400	-0.86884400	-4.40552800
C	-0.13190100	-1.24189700	-5.80803900
H	0.87621100	-1.51365100	-6.12133200
H	-0.79310800	-2.09350400	-5.96474600
H	-0.48344000	-0.40672600	-6.41420900

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Ru	-0.02580400	0.27695800	-0.21522400
N	0.99226600	-1.52638700	-0.46195800
C	2.26171100	-1.63412200	-0.87272100
C	2.84905400	-2.85479600	-1.14023000
C	2.09905800	-4.01052100	-0.96292800
C	0.79384400	-3.90505000	-0.51126900
C	0.25333600	-2.64814000	-0.27194200
C	-1.12142000	-2.42614400	0.17908300
C	-1.98725500	-3.44891100	0.54963400
C	-3.26283500	-3.14159200	0.99019800
C	-3.64278800	-1.80767600	1.06180100
C	-2.73610300	-0.83427000	0.68439000
N	-1.50164500	-1.12430800	0.24241500
H	2.80896900	-0.71269000	-0.99202100
H	3.86610800	-2.88774300	-1.50064100
H	2.52039900	-4.97993200	-1.18618500
H	0.19165000	-4.78916700	-0.37200500
H	-1.66091800	-4.47657200	0.50895800
H	-3.94395900	-3.92889200	1.28112800
H	-4.62121000	-1.51680800	1.41533800
H	-2.99634400	0.21222500	0.74426400
N	1.43776100	1.69134000	-0.60972000
C	2.64104600	1.66504100	-0.01954600
C	3.58367400	2.65647300	-0.21191500
C	3.27540000	3.71461200	-1.05600600
C	2.01878600	3.76728600	-1.63787300
C	1.10009000	2.75414800	-1.38392300
C	-0.29299400	2.77219800	-1.85349500
C	-0.82136200	3.75669600	-2.68219400

C	-2.16203100	3.70328800	-3.03460600
C	-2.94979200	2.66672700	-2.55229000
C	-2.36643300	1.72270700	-1.72728700
N	-1.07617800	1.77082000	-1.38100500
H	2.81748100	0.83236900	0.64517000
H	4.53422700	2.59156700	0.29693500
H	3.99665400	4.49778700	-1.24439000
H	1.74957100	4.60111300	-2.26770100
H	-0.19647100	4.55486900	-3.05164700
H	-2.58458500	4.45896500	-3.68216800
H	-3.99571200	2.58154500	-2.80870900
H	-2.94207900	0.90331000	-1.32580300
N	-0.43063300	1.28717200	1.72926100
C	-1.04784100	2.47409000	1.66810300
C	-1.58637400	3.09726400	2.77556700
C	-1.47714500	2.46145200	4.00245900
C	-0.80779100	1.24939800	4.07508700
C	-0.28307200	0.67763100	2.92139000
C	0.49031900	-0.58999000	3.01127000
C	0.05029100	-1.63196100	3.82857000
C	0.84929900	-2.75665300	3.97250600
C	2.05946600	-2.81134800	3.29434300
C	2.40847000	-1.73857700	2.48425600
N	1.64555800	-0.65246400	2.33465500
H	-1.12319100	2.92943600	0.69363300
H	-2.07210000	4.05524300	2.66300100
H	-1.89141600	2.91069100	4.89315700
H	-0.65852200	0.75574100	5.02350400
H	-0.89955700	-1.56611600	4.33926000
H	0.53377600	-3.57038300	4.61224000
H	2.72306100	-3.66017900	3.39230000
H	3.34663600	-1.75027800	1.94135800
N	-0.13015000	-0.55274500	-3.17097800
C	-0.12403500	-0.85598600	-4.28054200
C	-0.11902500	-1.24076800	-5.67898800
H	0.88531600	-1.53919500	-5.97984300
H	-0.79922400	-2.07760600	-5.83309600
H	-0.44528200	-0.40218900	-6.29438700
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Ru	-0.03250400	0.28004800	-0.25838800
N	1.00015500	-1.52857300	-0.44170000
C	2.27416500	-1.63691500	-0.83678000
C	2.86855000	-2.85803400	-1.08567300
C	2.11876800	-4.01345800	-0.90567000
C	0.80769100	-3.90733200	-0.47031700
C	0.26057900	-2.64936500	-0.25026800
C	-1.12085600	-2.42450900	0.18144900
C	-1.98659000	-3.44356300	0.56367500

C	-3.26467200	-3.13297400	0.99547600
C	-3.64700400	-1.79885600	1.04886000
C	-2.74167200	-0.82969500	0.65725300
N	-1.50632000	-1.12285600	0.21918500
H	2.81885000	-0.71485600	-0.96240400
H	3.88965200	-2.89094700	-1.43514600
H	2.54514700	-4.98370900	-1.11532800
H	0.20604400	-4.79196100	-0.33122700
H	-1.65821000	-4.47115200	0.53927800
H	-3.94561000	-3.91747100	1.29482600
H	-4.62637500	-1.50424600	1.39735400
H	-3.00457000	0.21683500	0.70285000
N	1.42901000	1.69981300	-0.65237700
C	2.63261900	1.67457100	-0.06172100
C	3.57511100	2.66639000	-0.25284600
C	3.26619100	3.72493300	-1.09631400
C	2.00712200	3.78045800	-1.67314500
C	1.08742200	2.76808100	-1.41827600
C	-0.31098900	2.79297000	-1.87355100
C	-0.84870200	3.78397600	-2.68912500
C	-2.19357200	3.73399900	-3.02680000
C	-2.97669600	2.69365300	-2.54491900
C	-2.38436100	1.74422600	-1.73277500
N	-1.09099600	1.79027100	-1.39816500
H	2.81078700	0.84310000	0.60432200
H	4.52638000	2.60106500	0.25513700
H	3.98857200	4.50678300	-1.28642800
H	1.73660300	4.61598700	-2.30022900
H	-0.22813000	4.58506300	-3.05967900
H	-2.62335700	4.49485600	-3.66353000
H	-4.02539900	2.60987000	-2.79115700
H	-2.95505700	0.92044700	-1.33345600
N	-0.40661700	1.28403400	1.70739400
C	-1.01081600	2.47707600	1.65337800
C	-1.54902900	3.09530800	2.76370400
C	-1.45721200	2.44273300	3.98337600
C	-0.80536200	1.22010100	4.04768400
C	-0.27472500	0.65859100	2.89212700
C	0.49360200	-0.61406200	2.97246100
C	0.01818100	-1.68339600	3.73175200
C	0.81223500	-2.81176300	3.87666100
C	2.05259700	-2.84272600	3.25468900
C	2.43705200	-1.74190200	2.49969300
N	1.67945400	-0.65211900	2.34953600
H	-1.07467100	2.94052600	0.68180200
H	-2.02081300	4.06127800	2.65880200
H	-1.86970200	2.88816400	4.87671200
H	-0.67242700	0.71158600	4.99086900
H	-0.95429400	-1.63382500	4.19989200

H	0.46966600	-3.64589100	4.47487600
H	2.71418100	-3.69263600	3.35785100
H	3.40103200	-1.73340400	2.00414100
N	-0.12349000	-0.52907200	-3.05502000
C	-0.11343200	-0.84209200	-4.16088300
C	-0.10579600	-1.23968100	-5.55361400
H	0.89444000	-1.56477600	-5.83993000
H	-0.80529000	-2.06122700	-5.70312900
H	-0.40654100	-0.39774800	-6.17709300

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Ru	-0.03203000	0.27847700	-0.28602400
N	1.00995700	-1.53133300	-0.42478000
C	2.28824800	-1.63457000	-0.80422700
C	2.88846000	-2.85511500	-1.03150300
C	2.13684100	-4.00872200	-0.84776000
C	0.81990200	-3.90439100	-0.43000800
C	0.26693000	-2.64825400	-0.22930000
C	-1.12151500	-2.42068300	0.18528600
C	-1.98570800	-3.43458800	0.57695900
C	-3.26531800	-3.11973800	1.00087400
C	-3.65351300	-1.78664500	1.03588800
C	-2.75029500	-0.82092800	0.63395300
N	-1.51294200	-1.12075400	0.20520700
H	2.82743700	-0.70945600	-0.93652800
H	3.91347500	-2.88669800	-1.36802500
H	2.56697100	-4.97939100	-1.04153000
H	0.21643900	-4.78675800	-0.28949300
H	-1.65077700	-4.45968200	0.56866400
H	-3.94295200	-3.90215400	1.31006200
H	-4.63377000	-1.48961900	1.37944300
H	-3.01439400	0.22657000	0.66445300
N	1.42355600	1.70882800	-0.68593600
C	2.62738600	1.68248800	-0.09546500
C	3.56853700	2.67286400	-0.28959100
C	3.25548700	3.72915700	-1.13428900
C	1.99459800	3.78685600	-1.70721300
C	1.07463700	2.77768300	-1.44870400
C	-0.33020400	2.80983100	-1.89302600
C	-0.87504000	3.80684700	-2.69409800
C	-2.22450300	3.75985300	-3.01503800
C	-3.00621400	2.71666900	-2.53644300
C	-2.40652300	1.76151900	-1.73854400
N	-1.11157900	1.81081500	-1.41812900
H	2.80414700	0.85117900	0.57229300
H	4.51979600	2.60640400	0.21751800
H	3.97662600	4.51048100	-1.32653500
H	1.72036000	4.62157400	-2.33310700
H	-0.25552400	4.60916500	-3.06250800

H	-2.65990800	4.52702400	-3.63869300
H	-4.05718700	2.63332200	-2.77196100
H	-2.96913800	0.93098200	-1.34013300
N	-0.38359700	1.28527600	1.68785900
C	-0.97550500	2.48165000	1.63181700
C	-1.51258500	3.09268600	2.74362800
C	-1.43595400	2.42113300	3.95447900
C	-0.80235500	1.18815400	4.01324600
C	-0.26608900	0.63801700	2.85842100
C	0.49644800	-0.64074300	2.92675600
C	-0.01218600	-1.73401300	3.62737800
C	0.77803700	-2.86474600	3.77630700
C	2.04719000	-2.87388200	3.21541700
C	2.46482500	-1.74871400	2.51560100
N	1.71174300	-0.65627300	2.36280300
H	-1.02691900	2.94822400	0.66013000
H	-1.96684500	4.06673800	2.64289100
H	-1.84588800	2.86205600	4.84949800
H	-0.68114800	0.66156800	4.94734700
H	-1.00544100	-1.69863900	4.05107900
H	0.41119400	-3.71695400	4.33332400
H	2.70588100	-3.72518600	3.32505400
H	3.45257600	-1.72135100	2.07009000
N	-0.11982400	-0.50355900	-2.94240200
C	-0.10415000	-0.82710900	-4.04284700
C	-0.09303000	-1.23630600	-5.42605600
H	0.90362100	-1.58585100	-5.69363100
H	-0.81183000	-2.04187000	-5.56699400
H	-0.36892400	-0.38941700	-6.05320100

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Ru	-0.04669100	0.29409400	-0.30490800
N	1.01196800	-1.51041100	-0.40918500
C	2.29432500	-1.62076300	-0.77146300
C	2.89979500	-2.84330600	-0.97769100
C	2.14931200	-3.99781200	-0.79209000
C	0.82806700	-3.88812700	-0.39185100
C	0.27201200	-2.62767300	-0.21170900
C	-1.11751500	-2.39946100	0.18579400
C	-1.97801000	-3.41442200	0.58913200
C	-3.25947400	-3.10273500	1.00767100
C	-3.65198900	-1.77032900	1.02325700
C	-2.75282300	-0.80538300	0.60916800
N	-1.51245100	-1.10063700	0.18620100
H	2.83690600	-0.69967100	-0.91121700
H	3.92878800	-2.87795400	-1.30218300
H	2.58348900	-4.97034300	-0.97095200
H	0.22542700	-4.77147800	-0.25045200
H	-1.63908300	-4.43859300	0.59777000

H	-3.93384600	-3.88400700	1.32858000
H	-4.63366800	-1.47365700	1.36279700
H	-3.02497300	0.23949800	0.62582600
N	1.40453600	1.70609500	-0.70994900
C	2.61107100	1.68083000	-0.12555600
C	3.55327600	2.67014800	-0.32500600
C	3.24099900	3.72720700	-1.16961800
C	1.97846500	3.78400500	-1.73750900
C	1.05804400	2.77473700	-1.47292700
C	-0.34683100	2.81014600	-1.90398000
C	-0.89757000	3.81812700	-2.69005200
C	-2.24938800	3.77905400	-2.99863000
C	-3.02577600	2.73143300	-2.52051300
C	-2.41954200	1.76681500	-1.73804300
N	-1.12097300	1.80518100	-1.42823300
H	2.79339300	0.85265100	0.54347500
H	4.50594700	2.60492700	0.17975400
H	3.96242700	4.50855300	-1.36382600
H	1.70376100	4.61982400	-2.36223000
H	-0.28125800	4.62363100	-3.05791900
H	-2.69030800	4.55319600	-3.61078300
H	-4.07897800	2.65233200	-2.74783300
H	-2.98313800	0.93486600	-1.34589000
N	-0.36459000	1.26482300	1.63493100
C	-0.93959200	2.47187100	1.59502000
C	-1.47223400	3.07908900	2.71204900
C	-1.41452500	2.39617500	3.91723400
C	-0.79854700	1.15412700	3.96315300
C	-0.26144400	0.61025100	2.80529400
C	0.49767700	-0.66910900	2.87574300
C	-0.03817700	-1.77982800	3.52612800
C	0.74877400	-2.91211500	3.67993500
C	2.04242500	-2.90179000	3.17845500
C	2.48865500	-1.75635600	2.53090900
N	1.73879100	-0.66307000	2.37167700
H	-0.98009100	2.95551500	0.63208500
H	-1.90989600	4.06177800	2.62128500
H	-1.82159300	2.83443500	4.81566000
H	-0.69099800	0.61538800	4.89239600
H	-1.04904900	-1.75671400	3.90704900
H	0.36054700	-3.78094300	4.19524000
H	2.69779700	-3.75481500	3.29311400
H	3.49581500	-1.71264500	2.13326100
N	-0.11385500	-0.47173300	-2.81289100
C	-0.09490200	-0.80457100	-3.91026900
C	-0.08083000	-1.22561800	-5.29004700
H	0.91017800	-1.59920700	-5.54664300
H	-0.81538700	-2.01695500	-5.43093400
H	-0.33267200	-0.37857100	-5.92706400

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Ru	-0.05571900	0.30100400	-0.33021400
N	1.01954200	-1.50723900	-0.38407900
C	2.30473800	-1.61657100	-0.73256200
C	2.91485600	-2.83857500	-0.92256600
C	2.16348100	-3.99269100	-0.73629300
C	0.83752600	-3.88276500	-0.35283500
C	0.27759500	-2.62189000	-0.18811800
C	-1.11722000	-2.39218300	0.18948500
C	-1.97423700	-3.40428600	0.60752600
C	-3.25664100	-3.09197000	1.02180800
C	-3.65568500	-1.76113200	1.01540400
C	-2.76152700	-0.79942400	0.58414800
N	-1.51873300	-1.09544900	0.16750200
H	2.84504500	-0.69537200	-0.88092500
H	3.94685700	-2.87311400	-1.23694300
H	2.60154600	-4.96557700	-0.90201900
H	0.23397300	-4.76576100	-0.21454100
H	-1.62941900	-4.42605900	0.63515400
H	-3.92613000	-3.87073400	1.35833000
H	-4.63778300	-1.46299200	1.35254000
H	-3.03915700	0.24403300	0.58363900
N	1.39220700	1.71190500	-0.74097400
C	2.60009400	1.68438600	-0.15852700
C	3.54366100	2.67104000	-0.36049000
C	3.23194500	3.72801200	-1.20655800
C	1.96841500	3.78851200	-1.77130100
C	1.04438000	2.78268300	-1.50181300
C	-0.36456900	2.82615500	-1.91759100
C	-0.92246000	3.84127700	-2.68981900
C	-2.27726000	3.80461300	-2.98412600
C	-3.05062100	2.75255700	-2.50843000
C	-2.43768300	1.78181100	-1.74051200
N	-1.13721000	1.82013700	-1.44280100
H	2.78330300	0.85789100	0.51257000
H	4.49644500	2.60382300	0.14401300
H	3.95434100	4.50796700	-1.40269600
H	1.69623000	4.62535700	-2.39626300
H	-0.30927000	4.64829800	-3.05990100
H	-2.72285300	4.58397700	-3.58575600
H	-4.10522000	2.67226800	-2.72819700
H	-2.99651900	0.94256700	-1.35578900
N	-0.34753600	1.25033000	1.59047100
C	-0.90486400	2.46583400	1.55773800
C	-1.43255100	3.06852200	2.67813100
C	-1.39452200	2.37165300	3.87585100
C	-0.79815800	1.12005100	3.91208600
C	-0.25833600	0.58290400	2.75416600

C	0.49884300	-0.69752800	2.82418300
C	-0.06146500	-1.82516700	3.42170700
C	0.72279600	-2.95877900	3.57966400
C	2.03845500	-2.92927600	3.14003800
C	2.51048500	-1.76457800	2.54734600
N	1.76337900	-0.67074400	2.38210500
H	-0.93309600	2.96057200	0.60020100
H	-1.85197400	4.05920400	2.59508200
H	-1.79971800	2.80642700	4.77644400
H	-0.70421600	0.56837600	4.83470000
H	-1.08826600	-1.81446800	3.75824400
H	0.31480400	-3.84423400	4.04948000
H	2.69045700	-3.78415400	3.25840500
H	3.53499200	-1.70483000	2.19928100
N	-0.10585000	-0.43911000	-2.68280000
C	-0.08575200	-0.78016200	-3.77564400
C	-0.06897000	-1.20889600	-5.14857300
H	0.91743800	-1.60307900	-5.39049500
H	-0.81863800	-1.98593100	-5.28693100
H	-0.29800500	-0.35943500	-5.79035600

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Ru	-0.09288100	0.30766300	-0.48993800
N	1.02212900	-1.47762200	-0.31101100
C	2.30244100	-1.59216000	-0.69310300
C	2.90737100	-2.81615600	-0.89894300
C	2.16171400	-3.97262700	-0.71300600
C	0.83457800	-3.86098000	-0.33662100
C	0.27635400	-2.60077900	-0.15839800
C	-1.12579500	-2.38157800	0.18717800
C	-1.97350300	-3.39592700	0.61698200
C	-3.25810900	-3.08528800	1.02406400
C	-3.66155600	-1.75601900	1.01470300
C	-2.78075500	-0.79498900	0.55625700
N	-1.55043000	-1.09633400	0.11548700
H	2.84756100	-0.67784200	-0.85418200
H	3.93909800	-2.85189400	-1.21475600
H	2.60157500	-4.94597100	-0.87608000
H	0.22919600	-4.74450200	-0.21083700
H	-1.62237500	-4.41507500	0.65480900
H	-3.92412900	-3.86473600	1.36514600
H	-4.64102700	-1.45845500	1.35774200
H	-3.05900200	0.24754000	0.55501600
N	1.39228700	1.69099700	-0.78447300
C	2.59535200	1.67372600	-0.17465600
C	3.53349800	2.65606000	-0.36175100
C	3.22147200	3.73152900	-1.22712800
C	1.97857900	3.80384000	-1.79235000
C	1.01837700	2.79817100	-1.52877400

C	-0.34293500	2.84707400	-1.89554600
C	-0.94045600	3.85742000	-2.68307500
C	-2.27604600	3.81446800	-2.96847200
C	-3.05915100	2.73370100	-2.48304500
C	-2.45335100	1.77499700	-1.71965600
N	-1.14434400	1.82010500	-1.38514100
H	2.77736500	0.85175400	0.50341200
H	4.48481800	2.59425000	0.14578300
H	3.95145800	4.50672900	-1.41819200
H	1.70914900	4.64177500	-2.41790400
H	-0.32361700	4.65747700	-3.06506100
H	-2.72950200	4.58766700	-3.57298300
H	-4.11090100	2.65063100	-2.71282800
H	-3.01200200	0.92880400	-1.35261900
N	-0.37017400	1.18171100	1.46601600
C	-0.88960000	2.42947000	1.47953400
C	-1.38625100	3.03703000	2.61615200
C	-1.36524200	2.34257400	3.81339200
C	-0.77747600	1.08944200	3.82727700
C	-0.26347900	0.53750900	2.65835400
C	0.49816800	-0.72883700	2.77430600
C	-0.06924100	-1.84868300	3.37697500
C	0.71621800	-2.97898900	3.54702200
C	2.03893900	-2.94305200	3.12936400
C	2.52319500	-1.77319500	2.55664800
N	1.77377600	-0.68601600	2.37177300
H	-0.92522900	2.95175400	0.54240300
H	-1.79482500	4.03411700	2.54637200
H	-1.76942500	2.77510500	4.71915200
H	-0.67641200	0.54081100	4.75289900
H	-1.09976200	-1.83575400	3.70260400
H	0.30080800	-3.86841000	4.00166800
H	2.68847100	-3.79891900	3.24809600
H	3.55373200	-1.70590900	2.22958100
N	-0.07305500	-0.38149500	-2.50878400
C	-0.07554400	-0.73046700	-3.60368400
C	-0.06799800	-1.17028700	-4.98972200
H	0.91132900	-1.57769500	-5.24925900
H	-0.81767200	-1.94603200	-5.14938300
H	-0.28575600	-0.33322900	-5.65480800

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Ru	-0.09808200	0.23254200	-0.47158500
N	1.02694200	-1.55180800	-0.27552200
C	2.31246300	-1.66657800	-0.63873800
C	2.92477100	-2.88979800	-0.82374100
C	2.18315700	-4.04806700	-0.63621800
C	0.84918900	-3.93641300	-0.28445000
C	0.28297900	-2.67670800	-0.12824400

C	-1.12529200	-2.46119900	0.19679400
C	-1.97170100	-3.47439900	0.63208000
C	-3.26012500	-3.16216900	1.02777000
C	-3.67200600	-1.83581700	0.99489400
C	-2.79275200	-0.87682000	0.53004200
N	-1.55490600	-1.17797900	0.11125100
H	2.85989100	-0.75256900	-0.79188400
H	3.96518900	-2.92386200	-1.11080600
H	2.63092900	-5.02173300	-0.77591600
H	0.24455400	-4.82032000	-0.15720500
H	-1.61700100	-4.49222300	0.68802300
H	-3.92473500	-3.93924000	1.37711400
H	-4.65691700	-1.53996300	1.32360300
H	-3.07512700	0.16424700	0.50721700
N	1.38011100	1.61587100	-0.78720000
C	2.58370200	1.59775400	-0.18105100
C	3.52133400	2.57930500	-0.36948600
C	3.20566800	3.65765700	-1.23095700
C	1.96455400	3.72643100	-1.80130400
C	1.00394800	2.72031600	-1.53498900
C	-0.35948500	2.76994200	-1.89299300
C	-0.96217000	3.79131400	-2.66474000
C	-2.30023300	3.75682700	-2.93681900
C	-3.08015200	2.67138200	-2.45849600
C	-2.46833800	1.69966500	-1.71431800
N	-1.15879400	1.74070600	-1.38343600
H	2.76003800	0.77468300	0.49685000
H	4.47232900	2.51791800	0.13830800
H	3.93331100	4.43665400	-1.41349100
H	1.69564400	4.56455700	-2.42736900
H	-0.34836400	4.59896900	-3.03629100
H	-2.75816000	4.54152600	-3.52287100
H	-4.13549500	2.59687300	-2.67534600
H	-3.02492700	0.84620700	-1.36223900
N	-0.35344500	1.08951500	1.46408600
C	-0.85510900	2.34332600	1.48242600
C	-1.35892500	2.94167900	2.61952400
C	-1.36374200	2.22515300	3.80514300
C	-0.79966200	0.95980000	3.81025600
C	-0.27069300	0.42343600	2.64315100
C	0.48390000	-0.84957500	2.74530900
C	-0.11541200	-1.99291100	3.26470000
C	0.66286900	-3.12796100	3.43708700
C	2.00721600	-3.07382200	3.09857800
C	2.52076500	-1.88225500	2.59995000
N	1.78062500	-0.78846500	2.41613100
H	-0.87383200	2.87047100	0.54720100
H	-1.74898100	3.94710600	2.55702200
H	-1.77139500	2.64885300	4.71216200

H	-0.72490800	0.39015500	4.72459300
H	-1.16564100	-1.99222600	3.51985600
H	0.22649000	-4.03677200	3.82870000
H	2.65281900	-3.93143800	3.22497500
H	3.56916400	-1.80487000	2.33821500
N	-0.06718800	-0.44903500	-2.41010600
C	-0.05243200	-0.80326300	-3.49868600
C	-0.02835500	-1.24858000	-4.86962600
H	0.94847900	-1.67965700	-5.09126600
H	-0.79839000	-2.00534700	-5.01980500
H	-0.20465200	-0.40061400	-5.53147100

end of Supplementary Information