

π -Stacking between Casiopeinas[®] and DNA Bases.
Rodrigo Galindo-Murillo,^a Joseelyne Hernandez-Lima,^a Mayra González-Rendón,^a Fernando Cortés-Guzmán,^{*a,b} Lena Ruíz-Azuara^c and Rafael Moreno-Esparza^c

Complex	ΔE	$\Delta N(\text{adenine})$
A01	-58.63	-0.0938
A02	-58.38	-0.0932
A03	-58.58	-0.0949
A04	-58.79	-0.0952
A05	-57.88	-0.0939
A06	-59.21	-0.0937
A07	-58.25	-0.0941
A10	-57.43	-0.0879
A11	-58.62	-0.0972
A12	-60.19	-0.1012
A13	-61.99	-0.1062
A14	-60.60	-0.1051
A15	-61.20	-0.1032
A16	-60.09	-0.1030
A17	-61.38	-0.1053
A18	-61.11	-0.1025
A20	-62.18	-0.1089
A21	-63.60	-0.1116

Coordenadas de AXA_sp

A01A_sp

Atom	X	Y	Z
Cu	0.51829900	0.04773000	-0.49249200
N	-0.97852700	-0.28447700	0.82215100
C	-1.40233800	-1.50875400	1.18382700
H	-0.84748100	-2.33814500	0.76773600
C	-2.49562800	-1.67008900	2.04441700
H	-2.83609000	-2.66088200	2.30861500
C	-3.14114700	-0.52485200	2.52964500
C	-2.68138300	0.74586300	2.15438200
H	-3.18353900	1.63256100	2.51153900
C	-1.58807500	0.83349500	1.28807600
C	-1.01896500	2.10569200	0.78010500
C	-1.43089800	3.37707900	1.19073400
H	-2.19947700	3.49839600	1.94036000
C	-0.81856200	4.50085100	0.61797700
C	0.18347100	4.32978300	-0.34745300
H	0.66835900	5.17833100	-0.80854300
C	0.55272200	3.02779400	-0.70839200
H	1.32457800	2.80408500	-1.43259500
N	-0.04352100	1.95896000	-0.14941200
C	2.62170700	-3.68133400	-0.61070900

H	3.52056700	-3.70001100	0.01494100
H	2.84566400	-4.23878300	-1.52249600
H	1.79795800	-4.15889900	-0.08167200
C	2.26865700	-2.25261100	-0.92904300
O	1.19325100	-1.77560700	-0.36049200
C	3.11361400	-1.51787700	-1.78387800
H	3.97455700	-2.02919500	-2.19031700
C	2.94688900	-0.16103700	-2.11065000
O	1.95939300	0.58270100	-1.67889000
C	3.96178700	0.52724500	-2.98122700
H	3.49240000	1.35344600	-3.51561700
H	4.41879600	-0.16494000	-3.68886700
H	4.75498400	0.92619400	-2.33931100
O	-0.75915500	-0.31579000	-2.27811800
H	-1.50380800	-1.01573800	-2.16050200
H	-0.19971600	-0.42392000	-3.06590200
N	4.92381600	-1.67964800	1.23842800
C	5.65809000	-0.83846900	0.48770900
H	6.59519600	-1.21543200	0.10664400
N	5.35864600	0.44776200	0.17138300
C	4.19759600	0.99017900	0.61273800
N	3.93731100	2.29686100	0.35448900
H	4.63838800	2.84554200	-0.11876900
H	3.09961500	2.72475300	0.71421200
C	3.31235500	0.16797600	1.34720400
N	2.05264500	0.39600400	1.91433900
C	1.77349500	-0.72678200	2.56758200
H	0.87462000	-0.90298600	3.13087100
N	2.77457800	-1.67357500	2.45124100
H	2.79198300	-2.59750300	2.85550300
C	3.76461700	-1.12403900	1.65459700
N	-2.95277500	-1.46301000	-1.60578700
C	-3.63336600	-2.54620200	-1.18011800
H	-3.22716000	-3.51370100	-1.43297800
N	-4.78057300	-2.54470100	-0.47065700
C	-5.36006000	-1.36132100	-0.12575300
N	-6.50950400	-1.36899600	0.58215700
H	-6.94320000	-2.25395200	0.79922200
H	-6.97758300	-0.50129100	0.79745000
C	-4.72070300	-0.16161100	-0.52053300
N	-5.03029000	1.18559700	-0.32440500
C	-4.05475500	1.84660800	-0.93542400
H	-3.98395500	2.91790000	-0.99747000
N	-3.11731800	0.99886400	-1.51441700
H	-2.25221700	1.21652700	-2.00056200
C	-3.53382000	-0.28794800	-1.25324900
H	-1.11839900	5.49433300	0.92371000
H	-3.99682700	-0.61662500	3.18509800

A02A_sp

Atom	X	Y	Z
Cu	0.54954200	0.07035500	-0.44943800
N	-0.94402300	-0.25210900	0.86412600
C	-1.38976000	-1.46919700	1.22265700
H	-0.82530300	-2.30703100	0.83730800

C	-2.52334600	-1.61891700	2.02794000
H	-2.87779200	-2.60918600	2.27999000
C	-3.20864900	-0.47786300	2.47834200
C	-2.70559400	0.78513300	2.11068500
H	-3.22414100	1.67783300	2.43212800
C	-1.57485300	0.86755200	1.29935400
C	-0.99339200	2.13724500	0.79604000
C	-1.40705800	3.41033800	1.19508400
H	-2.18371300	3.52999200	1.93836500
C	-0.79804700	4.54892400	0.63667100
C	0.21252100	4.35175400	-0.32288300
H	0.70137800	5.19803500	-0.78711600
C	0.58655700	3.05264600	-0.67681300
H	1.36147000	2.83194100	-1.39874500
N	-0.00958800	1.98061200	-0.12237700
C	2.62014900	-3.67779700	-0.60244700
H	3.52369100	-3.70297900	0.01624800
H	2.83341700	-4.23568900	-1.51648000
H	1.79742800	-4.15031500	-0.06725600
C	2.27383600	-2.24615000	-0.91617400
O	1.21112800	-1.76049200	-0.33232400
C	3.11256100	-1.51849600	-1.78315900
H	3.96413700	-2.03622300	-2.20116400
C	2.94988200	-0.16105300	-2.10952500
O	1.97401700	0.59002300	-1.66512900
C	3.95778500	0.51836600	-2.99556400
H	3.48923100	1.35269100	-3.51786200
H	4.39293700	-0.17666900	-3.71424200
H	4.76792700	0.90402400	-2.36674900
O	-0.77687300	-0.28580500	-2.21161900
H	-1.49878000	-1.00509400	-2.08903400
H	-0.23306000	-0.36925300	-3.01332000
N	4.96998000	-1.69431100	1.21905300
C	5.70481300	-0.86193800	0.45903800
H	6.63594800	-1.24791100	0.07236200
N	5.41292900	0.42513100	0.13877600
C	4.25924600	0.97808000	0.58645200
N	4.00382100	2.28424200	0.32150400
H	4.70140300	2.82561900	-0.16493100
H	3.16472600	2.71505500	0.67457500
C	3.37482800	0.16662100	1.33344700
N	2.12112600	0.40729700	1.90797100
C	1.83633700	-0.71085800	2.56644400
H	0.93767700	-0.87843600	3.13246300
N	2.82931300	-1.66618600	2.44770600
H	2.84009300	-2.58973300	2.85286700
C	3.81861000	-1.12776000	1.64247000
N	-2.94840100	-1.49445300	-1.53486500
C	-3.62160100	-2.59675400	-1.14887300
H	-3.18654100	-3.55237000	-1.39872800
N	-4.79613800	-2.62785000	-0.48610600
C	-5.41299500	-1.46145900	-0.14926000
N	-6.60352200	-1.50508200	0.48748400
H	-7.03275600	-2.40265700	0.65689800
H	-7.10258000	-0.65158900	0.68898700
C	-4.77417900	-0.24381800	-0.48495600

N	-5.11183900	1.09443300	-0.27406400
C	-4.12558600	1.78188600	-0.83856800
H	-4.06679500	2.85508900	-0.87327000
N	-3.15834400	0.96096300	-1.40466700
H	-2.27958300	1.19973100	-1.85676200
C	-3.56063500	-0.33691000	-1.17925100
C	-1.19643200	5.93521800	1.06996600
H	-2.20817400	5.95370400	1.47701700
H	-0.51764800	6.29508900	1.84888800
H	-1.14534400	6.63956700	0.23816700
C	-4.45158300	-0.58517900	3.31922000
H	-4.23199300	-0.34069800	4.36274900
H	-5.21315200	0.11429700	2.96617800
H	-4.86722000	-1.59242400	3.28610100

A03A_sp			
Atom	X	Y	Z
Cu	0.53182700	0.07812100	-0.51254000
N	-0.98721100	-0.25629000	0.79760200
C	-1.46716700	-1.42973200	1.21340300
H	-0.97660300	-2.31004700	0.82127400
C	-2.55569700	-1.49554500	2.11656100
C	-3.12536600	-0.31878100	2.58981700
C	-2.61112500	0.93339100	2.16310800
C	-1.53972400	0.90293400	1.25158100
C	-0.98472100	2.12705400	0.74578600
C	-1.48879400	3.36743000	1.17900200
C	-0.88811700	4.53030400	0.62907300
C	0.13881600	4.40200800	-0.29895100
C	0.57739300	3.11084800	-0.68354300
H	1.37030700	2.94596600	-1.40097300
N	0.02123300	2.01514400	-0.16507500
C	2.54876800	-3.69320700	-0.65769800
H	3.44863000	-3.73914400	-0.03504000
H	2.75710000	-4.24675600	-1.57561200
H	1.71505700	-4.15626400	-0.13150500
C	2.22820100	-2.25360400	-0.96170500
O	1.15610400	-1.76233500	-0.39868500
C	3.09754000	-1.52694000	-1.79901200
H	3.95187800	-2.05219600	-2.20174400
C	2.96235600	-0.16387800	-2.11558300
O	1.98795800	0.59761400	-1.68541400
C	3.99868600	0.50985000	-2.97218600
H	3.54888400	1.34525700	-3.50912000
H	4.45270300	-0.18750200	-3.67661400
H	4.79035900	0.89450000	-2.31982500
O	-0.75614900	-0.20600000	-2.30281900
H	-1.46872400	-0.94121600	-2.19383700
H	-0.19516800	-0.27403000	-3.09419600
N	4.89724400	-1.75325300	1.22779400
C	5.64754200	-0.90972100	0.49580100
H	6.58352600	-1.29190400	0.11718800
N	5.36574300	0.38443400	0.19592400
C	4.20673800	0.93354300	0.63447000
N	3.96274900	2.24630300	0.39300600

H	4.67223300	2.79405900	-0.06851500
H	3.12235700	2.67512800	0.74508700
C	3.30612900	0.11114500	1.34974800
N	2.04523200	0.34620600	1.91160500
C	1.74920800	-0.78149300	2.54843800
H	0.84559900	-0.95415000	3.10508100
N	2.73950500	-1.73870300	2.42507300
H	2.74423700	-2.66772800	2.81780700
C	3.74122400	-1.19007400	1.64241900
N	-2.88439300	-1.46289900	-1.63322300
C	-3.50172200	-2.58451700	-1.21239700
H	-3.04732000	-3.52649300	-1.47938800
N	-4.64163800	-2.65122700	-0.49317100
C	-5.28025900	-1.50371900	-0.13293900
N	-6.42471400	-1.57848600	0.57950500
H	-6.81146500	-2.48680900	0.78824000
H	-6.93683000	-0.73821400	0.80326700
C	-4.70628600	-0.26780000	-0.51622300
N	-5.08449200	1.05844000	-0.30013000
C	-4.14908900	1.77721200	-0.90790600
H	-4.13029500	2.85160200	-0.94758400
N	-3.17475800	0.98678500	-1.50774300
H	-2.32552500	1.25581100	-1.99563900
C	-3.52136000	-0.32319300	-1.26058500
C	-2.57521400	3.38142800	2.13124500
H	-2.96101100	4.33680700	2.46518700
C	-3.11898300	2.21446400	2.59523600
H	-3.94565700	2.23470000	3.29418100
H	-1.23474000	5.51011000	0.93396200
H	0.60683000	5.27275600	-0.73542500
H	-3.96187500	-0.34957000	3.27694800
H	-2.93681000	-2.46109200	2.41708200

A04A_sp

Atom	X	Y	Z
Cu	0.59573800	0.13748200	-0.42557700
N	-0.92784700	-0.18478500	0.87082400
C	-1.43009500	-1.35274800	1.27476400
H	-0.91391900	-2.23767900	0.92780500
C	-2.58093200	-1.41153000	2.09129700
C	-3.21938300	-0.24309200	2.50732400
C	-2.65921400	1.00759300	2.10003100
C	-1.52210600	0.97322800	1.27232300
C	-0.94413700	2.19429500	0.78060300
C	-1.47987600	3.43966700	1.15772000
C	-0.85210100	4.59759300	0.62755300
C	0.22851200	4.46060200	-0.23501500
C	0.69112800	3.16541600	-0.57494200
H	1.51655500	2.99205100	-1.25287000
N	0.11266500	2.07583600	-0.06996600
C	2.48656000	-3.69046100	-0.73637400
H	3.40027100	-3.78343400	-0.13983700
H	2.65320100	-4.22248600	-1.67530900
H	1.65242500	-4.14299900	-0.20175200

C	2.20411800	-2.23298100	-0.99008200
O	1.16114100	-1.72627900	-0.38783900
C	3.07575400	-1.50934500	-1.82757700
H	3.90425100	-2.04816600	-2.26506600
C	2.97108000	-0.13572700	-2.10707800
O	2.02951400	0.64107700	-1.63339700
C	4.00459100	0.53010900	-2.97340000
H	3.56693800	1.39347900	-3.47483300
H	4.41773300	-0.16078700	-3.70872200
H	4.82547200	0.87183300	-2.33332900
O	-0.79302700	-0.04014300	-2.16984500
H	-1.45900300	-0.81677900	-2.07511100
H	-0.26421900	-0.03914800	-2.98643300
N	4.95193100	-1.86265200	1.15626900
C	5.71504800	-1.02444700	0.43122300
H	6.63521100	-1.42373600	0.03212200
N	5.46463500	0.28273600	0.16141200
C	4.32631000	0.85300800	0.62606600
N	4.11208600	2.17580300	0.41285700
H	4.82928800	2.71540400	-0.04630700
H	3.28517400	2.61686200	0.78160500
C	3.41362700	0.04022200	1.33648500
N	2.16562900	0.29696600	1.91690100
C	1.84725900	-0.83424300	2.53641400
H	0.94436500	-0.99361000	3.09785400
N	2.81075400	-1.81441500	2.38320500
H	2.79521000	-2.75085000	2.75756100
C	3.81721500	-1.27742200	1.59819800
N	-2.84789500	-1.45847000	-1.54104000
C	-3.37990100	-2.63941600	-1.16794600
H	-2.83972300	-3.53211100	-1.44434400
N	-4.53115800	-2.82112200	-0.48842300
C	-5.27525700	-1.74206600	-0.11966800
N	-6.43625000	-1.93605400	0.54350900
H	-6.75291600	-2.88047600	0.70559600
H	-7.03093200	-1.15116000	0.76351800
C	-4.79203000	-0.45192800	-0.44379600
N	-5.28211900	0.83216600	-0.19899000
C	-4.39258900	1.64310100	-0.75892700
H	-4.45874800	2.71621100	-0.76345900
N	-3.34260700	0.95353700	-1.35425000
H	-2.50691300	1.30736400	-1.80964100
C	-3.58655400	-0.38775400	-1.15430000
C	-2.62629800	3.46016200	2.03394900
H	-3.03721400	4.41734000	2.33103300
C	-3.19671800	2.29558200	2.47371600
H	-4.06932800	2.33247200	3.11206100
H	-1.22185700	5.57984800	0.89493200
H	0.71786900	5.32671400	-0.65696400
H	-2.97515100	-2.37803200	2.37466500
C	-4.47430100	-0.29089400	3.33349700
H	-4.33498700	0.20912400	4.29613900
H	-5.29040500	0.21439600	2.80747800
H	-4.77664700	-1.32015500	3.52418200

A05A_sp			
Atom	X	Y	Z
Cu	0.58055500	0.09659900	-0.44545300
N	-0.94455700	-0.25970800	0.84951500
C	-1.41868900	-1.44403800	1.24092300
H	-0.88955500	-2.31301100	0.87377900
C	-2.55417300	-1.53058200	2.07862700
C	-3.18297800	-0.36444600	2.50275400
C	-2.67844100	0.90094100	2.10365200
C	-1.54722900	0.88837900	1.26465900
C	-0.98731300	2.11870100	0.77770700
C	-1.54537400	3.34711300	1.17315800
C	-0.93998000	4.52077500	0.65191900
C	0.13847300	4.41128500	-0.21836100
C	0.62301000	3.12931600	-0.57585300
H	1.44815500	2.97890900	-1.25925700
N	0.06550500	2.02441900	-0.07898600
C	2.54464700	-3.69542300	-0.73443400
H	3.46115800	-3.77233300	-0.14001300
H	2.71717000	-4.22742000	-1.67239500
H	1.71894200	-4.15981200	-0.19687000
C	2.23802700	-2.24357800	-0.99225800
O	1.17983400	-1.75550700	-0.40066500
C	3.10384400	-1.50477300	-1.82224000
H	3.94653200	-2.02830000	-2.25095600
C	2.97592500	-0.13349100	-2.10434700
O	2.01581000	0.62571300	-1.63985700
C	4.00404500	0.55154300	-2.96188200
H	3.55187100	1.40065800	-3.47477200
H	4.44377200	-0.13362300	-3.68698900
H	4.80725800	0.91798900	-2.31311800
O	-0.78231400	-0.10175600	-2.20454000
H	-1.47075800	-0.85960000	-2.11751800
H	-0.24316700	-0.11489500	-3.01416100
N	4.96233300	-1.82033700	1.17189900
C	5.70974100	-0.96344500	0.45244200
H	6.64060000	-1.34097900	0.05691000
N	5.43125900	0.33838500	0.18425700
C	4.27815700	0.88202700	0.64476800
N	4.03548700	2.20007600	0.43385800
H	4.74176500	2.75652500	-0.02207600
H	3.19573900	2.62117100	0.79698300
C	3.38053800	0.04708000	1.34904900
N	2.12444400	0.27416100	1.92431600
C	1.82883800	-0.86546700	2.53955800
H	0.92779500	-1.04634000	3.09757400
N	2.81460400	-1.82352400	2.38806100
H	2.81907500	-2.76069900	2.76091900
C	3.81258400	-1.26179500	1.60953600
N	-2.87911200	-1.45553800	-1.58516200
C	-3.44846500	-2.61641700	-1.20499900
H	-2.94562400	-3.52802400	-1.48981900
N	-4.59465700	-2.75673800	-0.50685300
C	-5.29237700	-1.65159800	-0.12546000
N	-6.44263200	-1.80148400	0.56649000
H	-6.78746600	-2.73326000	0.74319300

H	-7.00334700	-0.99495200	0.79730900
C	-4.77143500	-0.37981100	-0.46330500
N	-5.21166700	0.92085700	-0.21102600
C	-4.30168000	1.69966900	-0.78381100
H	-4.32875600	2.77440900	-0.78764400
N	-3.28558300	0.97327800	-1.39342200
H	-2.44179500	1.29765700	-1.85609200
C	-3.57473100	-0.35859700	-1.19045200
C	-2.69286800	3.33957400	2.04833600
H	-3.12055000	4.29135700	2.34192100
C	-3.26356900	2.17483700	2.49490900
H	-1.32438300	5.49417000	0.93084900
H	0.60995500	5.29071400	-0.63318800
H	-2.93070800	-2.50228700	2.36488500
H	-4.06152300	-0.42249500	3.13167900
C	-4.50169100	2.18267500	3.35220200
H	-5.32912900	1.69844500	2.82370000
H	-4.34151300	1.65479000	4.29632100
H	-4.80451300	3.20276700	3.58739600

A06A_sp

Atom	X	Y	Z
Cu	0.59478100	0.13466800	-0.42986900
N	-0.92610100	-0.18670900	0.86738200
C	-1.42684000	-1.35606700	1.26831500
H	-0.91283400	-2.23942300	0.91416200
C	-2.57359500	-1.41891700	2.09037600
C	-3.20809600	-0.25205900	2.51543700
C	-2.64769000	1.00000900	2.11244800
C	-1.51602900	0.97112500	1.27769300
C	-0.93897000	2.19402500	0.78718700
C	-1.46707100	3.44009700	1.17145300
C	-0.84468700	4.61639100	0.64692700
C	0.22920400	4.45095200	-0.22568200
C	0.68518800	3.15906000	-0.57488500
H	1.50542100	2.99054000	-1.26031900
N	0.11111500	2.06702300	-0.07167400
C	2.48677700	-3.69430800	-0.74009200
H	3.40212700	-3.78804700	-0.14625100
H	2.65006300	-4.22669000	-1.67945100
H	1.65363300	-4.14586400	-0.20307100
C	2.20476900	-2.23656600	-0.99353000
O	1.16173900	-1.72969900	-0.39192900
C	3.07707700	-1.51319200	-1.83055700
H	3.90605300	-2.05200000	-2.26717400
C	2.97262700	-0.13940800	-2.10980000
O	2.03057800	0.63717000	-1.63741100
C	4.00759800	0.52658800	-2.97441500
H	3.57043600	1.38964400	-3.47684500
H	4.42252300	-0.16431700	-3.70874300
H	4.82696800	0.86880900	-2.33266200
O	-0.78617200	-0.06249100	-2.18258200
H	-1.45016600	-0.83916700	-2.08449100
H	-0.25136900	-0.06841800	-2.99516400
N	4.95436300	-1.86920500	1.15260400
C	5.71544900	-1.02691500	0.43020500

H	6.63699700	-1.42262900	0.03068900
N	5.46134500	0.28009000	0.16281600
C	4.32109400	0.84600300	0.62834300
N	4.10098000	2.16772200	0.41569400
H	4.81351700	2.71034000	-0.04698900
H	3.26704300	2.60259100	0.77601500
C	3.41173900	0.02955800	1.33883000
N	2.16393400	0.28234000	1.92104300
C	1.84763700	-0.85141300	2.53661700
H	0.94505700	-1.01433800	3.09757700
N	2.81287000	-1.82957700	2.37960400
H	2.79891400	-2.76739500	2.75047200
C	3.81815900	-1.28799700	1.59629500
N	-2.84645500	-1.47124500	-1.54223300
C	-3.39437000	-2.64430500	-1.16784600
H	-2.86629900	-3.54455400	-1.44300800
N	-4.54829500	-2.80987600	-0.48835000
C	-5.27804800	-1.72056700	-0.12145000
N	-6.44206600	-1.89831000	0.54134600
H	-6.77078600	-2.83826800	0.70512500
H	-7.02637500	-1.10530600	0.75991600
C	-4.77772900	-0.43737800	-0.44700400
N	-5.25005500	0.85355400	-0.20338600
C	-4.34825400	1.65140400	-0.76286000
H	-4.39877200	2.72529200	-0.76714500
N	-3.30796800	0.94715000	-1.35714500
H	-2.46410400	1.28721100	-1.80906100
C	-3.57089000	-0.39032400	-1.15671900
C	-2.60759000	3.45158300	2.05658600
H	-3.02238000	4.40142400	2.36762300
C	-3.17857800	2.28607200	2.49483100
H	0.72176700	5.31459000	-0.65137600
H	-2.96760900	-2.38659600	2.36997400
C	-1.33912000	5.98721400	1.02441900
H	-2.38737800	6.12030200	0.74294900
H	-1.26451900	6.14541300	2.10384200
H	-0.75602200	6.76247300	0.52850400
C	-4.46007600	-0.30191200	3.34599000
H	-4.31717100	0.19454900	4.30989900
H	-5.27728300	0.20607200	2.82428600
H	-4.76281000	-1.33158600	3.53376800
H	-4.04697800	2.32312000	3.13897900
A07A_sp			
Atom	X	Y	Z
Cu	0.59828500	0.10397300	-0.43794700
N	-0.92034500	-0.23238600	0.86469000
C	-1.40256600	-1.41156900	1.26118500
H	-0.88288100	-2.28674700	0.89572300
C	-2.53583700	-1.48065700	2.10159100
C	-3.15242600	-0.30598800	2.52067300
C	-2.63964900	0.95609800	2.11637600
C	-1.51208600	0.92152300	1.27750900
C	-0.94786300	2.14650800	0.78677500
C	-1.49364200	3.37970800	1.18477900
C	-0.87060700	4.53815900	0.64536000

C	0.20129000	4.41254100	-0.23178900
C	0.66998500	3.12643700	-0.58439000
H	1.48923600	2.95870700	-1.27082800
N	0.09870400	2.03458300	-0.07498900
C	2.52513000	-3.70706200	-0.73743500
H	3.44057900	-3.79141200	-0.14231400
H	2.69424800	-4.23994300	-1.67546100
H	1.69548000	-4.16500700	-0.20042900
C	2.23052900	-2.25253800	-0.99425700
O	1.18270700	-1.75350100	-0.39400000
C	3.09652600	-1.52305600	-1.83240900
H	3.93005100	-2.05538700	-2.26823000
C	2.98049000	-0.15060700	-2.11365600
O	2.03206300	0.61867100	-1.64184700
C	4.00912100	0.52304800	-2.97974700
H	3.56359700	1.38005500	-3.48521400
H	4.43142200	-0.16593400	-3.71164300
H	4.82454000	0.87572200	-2.33863300
O	-0.77106100	-0.08947600	-2.19364800
H	-1.46572700	-0.84153000	-2.09953100
H	-0.23451400	-0.11176200	-3.00471500
N	4.97299000	-1.85570500	1.15245800
C	5.72703400	-1.00990300	0.42678800
H	6.65111600	-1.39985700	0.02745300
N	5.46301100	0.29447600	0.15633100
C	4.31898800	0.85324500	0.62127900
N	4.09027400	2.17319100	0.40651600
H	4.79996600	2.71971300	-0.05602900
H	3.25592100	2.60456200	0.77000800
C	3.41555600	0.03157200	1.33348900
N	2.16585700	0.27605000	1.91543000
C	1.85935200	-0.85818200	2.53527800
H	0.95890100	-1.02641100	3.09812800
N	2.83228800	-1.82891500	2.38089900
H	2.82651200	-2.76536700	2.75548100
C	3.83266400	-1.28188000	1.59506700
N	-2.87470400	-1.42253200	-1.56054900
C	-3.45415300	-2.57758500	-1.17827600
H	-2.96044000	-3.49417000	-1.46299300
N	-4.60034300	-2.70627800	-0.47782900
C	-5.28677700	-1.59417300	-0.09649700
N	-6.43699600	-1.73240400	0.59813300
H	-6.78932200	-2.66070000	0.77813200
H	-6.98895400	-0.92030100	0.83032500
C	-4.75479100	-0.32779900	-0.43703800
N	-5.18191300	0.97727100	-0.18505100
C	-4.26435400	1.74660700	-0.75848100
H	-4.28094000	2.82158100	-0.76298300
N	-3.25653200	1.01009400	-1.36934000
H	-2.40957000	1.32523800	-1.83279100
C	-3.55880300	-0.31868000	-1.16545500
C	-2.64731100	3.41547900	2.07791700
C	-3.21933100	2.23623900	2.51162200
H	0.67716000	5.28639900	-0.65352000
H	-2.92259000	-2.44626200	2.39505800
H	-1.23014100	5.52301800	0.90918100

H	-4.02854600	-0.36045400	3.15172400
C	-3.15354900	4.78806800	2.45891900
H	-2.35200500	5.38028100	2.90981400
H	-3.51356100	5.33310500	1.58028000
H	-3.96667000	4.75443900	3.17633400
C	-4.46409200	2.16362400	3.36321200
H	-5.24716100	1.62300600	2.82178600
H	-4.26955000	1.63615900	4.30150400
H	-4.86418900	3.13995900	3.61626000
A08A_sp			
Atom	X	Y	Z
Cu	0.56285000	0.08809500	-0.48105700
N	-0.95247000	-0.24736600	0.82318800
C	-1.43559200	-1.41648700	1.24428500
H	-0.92422600	-2.29716800	0.87657000
C	-2.55277200	-1.51410200	2.11169800
C	-3.17185800	-0.33248100	2.54736300
C	-2.62866600	0.92088300	2.12848500
C	-1.52754300	0.90665200	1.25648200
C	-0.96745000	2.13272800	0.75864100
C	-1.47899700	3.37754500	1.16320700
C	-0.87668200	4.55922400	0.63009100
C	0.18033400	4.42139400	-0.28106800
C	0.61201200	3.11708800	-0.63532100
H	1.41707300	2.95397900	-1.34128000
N	0.05696700	2.01771800	-0.12808700
C	2.54061900	-3.70538300	-0.70856500
H	3.45084700	-3.77000100	-0.10295100
H	2.72551500	-4.24977000	-1.63699100
H	1.71056200	-4.16481300	-0.17338300
C	2.23126000	-2.25810200	-0.98949700
O	1.17039200	-1.76400800	-0.40989400
C	3.09998500	-1.52980800	-1.82618100
H	3.94546900	-2.05766500	-2.24402800
C	2.97206800	-0.16211300	-2.12472300
O	2.00972800	0.60202200	-1.67446800
C	4.00527500	0.51267300	-2.98510600
H	3.55755400	1.36037100	-3.50427100
H	4.44258600	-0.17947000	-3.70516800
H	4.80955300	0.87901000	-2.33762900
O	-0.76508100	-0.14523100	-2.26221200
H	-1.45420200	-0.90013400	-2.16682300
H	-0.21234600	-0.17595100	-3.06175700
N	4.94877200	-1.81380800	1.18050200
C	5.70221000	-0.96737300	0.45505400
H	6.63509300	-1.35146400	0.07069500
N	5.42733500	0.33111400	0.16695600
C	4.27206800	0.88214500	0.61313900
N	4.02841900	2.19594900	0.37821300
H	4.73334400	2.74505000	-0.08819400
H	3.17629400	2.61590600	0.71297500
C	3.37156900	0.05982900	1.32799800
N	2.11499100	0.29900400	1.89638200
C	1.81128900	-0.83259100	2.52171100

H	0.90558700	-1.00430500	3.07498000
N	2.79428300	-1.79648400	2.38542500
H	2.79178900	-2.73028700	2.76630900
C	3.79796700	-1.24723900	1.60553500
N	-2.86773800	-1.47476100	-1.61707600
C	-3.46395100	-2.62382800	-1.24528800
H	-2.98375100	-3.54541100	-1.53685700
N	-4.61558100	-2.74065200	-0.55052300
C	-5.28313400	-1.62148200	-0.15829400
N	-6.44135200	-1.75105800	0.52795200
H	-6.82197700	-2.67470000	0.67126900
H	-6.97967400	-0.93224600	0.76883500
C	-4.72869800	-0.36058200	-0.48040600
N	-5.13733900	0.94853500	-0.22097100
C	-4.20926100	1.70761200	-0.79151100
H	-4.20795300	2.78267400	-0.78538300
N	-3.21420800	0.96094800	-1.40986800
H	-2.35878600	1.26444000	-1.86677100
C	-3.53364200	-0.36402000	-1.21187300
C	-2.58967600	3.37655700	2.08806800
H	-2.99702200	4.32108900	2.42351600
C	-3.14388900	2.20743100	2.53696200
H	-3.98709900	2.24388700	3.21325800
C	0.87886900	5.60612400	-0.90509100
H	0.18327400	6.22600900	-1.47641600
H	1.34271400	6.24225200	-0.14681400
H	1.66233500	5.27416300	-1.58790900
C	-1.38879600	5.91128800	1.05579800
H	-2.44919300	6.02228000	0.81125700
H	-1.28622800	6.03928700	2.13733700
H	-0.84971400	6.72232600	0.57207900
C	-4.39560500	-0.35095800	3.42356600
H	-4.18035100	0.07977200	4.40644700
H	-5.19181100	0.24415700	2.96655000
H	-4.77395800	-1.35953500	3.57230600
C	-3.03352600	-2.88503500	2.52250000
H	-3.06030100	-2.99000800	3.60996700
H	-4.03538700	-3.08755900	2.13496800
H	-2.37291500	-3.65730300	2.12500400
A09A_sp			
Atom	X	Y	Z
Cu	0.51060200	0.09841600	-0.51637800
N	-1.02991200	-0.35801100	0.73170400
C	-1.47551000	-1.57067500	1.06641800
H	-0.94860300	-2.40861900	0.63079000
C	-2.56694200	-1.72493900	1.95162000
C	-3.19002600	-0.59792000	2.47748300
C	-2.72866500	0.69745700	2.12267400
C	-1.62721400	0.75380800	1.24483700
C	-1.06559500	2.01733900	0.85601100
C	-1.59356400	3.21118700	1.37944500
C	-0.98291400	4.42136600	0.95644500
C	0.07856400	4.38021500	0.06083900
C	0.54337100	3.12993600	-0.41735000

H	1.36471900	3.03394500	-1.11469200
N	-0.02313600	1.99060500	-0.01879900
C	2.52146300	-3.64911200	-0.99352000
H	3.37686100	-3.76317500	-0.31903700
H	2.79603300	-4.10013500	-1.94900600
H	1.65757300	-4.16604300	-0.57766200
C	2.21366900	-2.18419900	-1.15886200
O	1.13119100	-1.74541500	-0.57198700
C	3.10354800	-1.38252400	-1.89951500
H	3.96474200	-1.86895200	-2.33493500
C	2.97705100	0.00582600	-2.08428000
O	1.99445300	0.72407500	-1.60318800
C	4.03321700	0.75516900	-2.84897900
H	3.59795600	1.64149500	-3.31084700
H	4.49975600	0.12756700	-3.60855400
H	4.81250700	1.06928800	-2.14579000
O	-0.74858400	0.00886200	-2.34788500
H	-1.38897000	-0.79791500	-2.33479500
H	-0.17426900	0.08309600	-3.12919200
N	4.83168700	-1.90587600	1.14379100
C	5.60094800	-1.00415300	0.50721300
H	6.54380600	-1.35602000	0.11648300
N	5.33041000	0.31293500	0.31824000
C	4.16374200	0.82700000	0.77899300
N	3.92757900	2.15658600	0.64947300
H	4.64772700	2.74103600	0.25441100
H	3.07594900	2.55382000	1.01178600
C	3.24511800	-0.05113600	1.39891400
N	1.97382400	0.14019200	1.95350900
C	1.66077000	-1.03731100	2.48248800
H	0.74729400	-1.25211100	3.00733000
N	2.64908000	-1.98619300	2.29296900
H	2.64222000	-2.94643500	2.60175400
C	3.66899000	-1.37568600	1.58276500
N	-2.73985700	-1.51641200	-1.85962900
C	-3.21230900	-2.73910100	-1.54763700
H	-2.64522600	-3.58959900	-1.89431200
N	-4.33325800	-3.00999800	-0.84720300
C	-5.10733300	-1.98748300	-0.39075800
N	-6.22973700	-2.26986600	0.30525600
H	-6.49431800	-3.23537100	0.43237700
H	-6.84518800	-1.52711900	0.60013100
C	-4.69099500	-0.66091100	-0.65625200
N	-5.22174400	0.58460700	-0.31519200
C	-4.37762400	1.46568400	-0.83900100
H	-4.48407100	2.53352400	-0.76884000
N	-3.31890300	0.85785500	-1.50219900
H	-2.50243000	1.27220400	-1.94152700
C	-3.50915100	-0.50227800	-1.38946100
C	-2.71543200	3.13745400	2.28035300
C	-3.28879500	1.94050700	2.63552300
H	0.55565000	5.28818400	-0.27949200
H	-2.90813200	-2.71852000	2.20532500
H	-1.34988600	5.36871500	1.33221700
H	-4.02020600	-0.69767000	3.16408100
H	-3.13824000	4.05927300	2.66315400

C	-4.46936700	1.91849700	3.54152100
C	-4.38279500	2.49625400	4.81950900
C	-5.68901000	1.36345100	3.10942200
C	-5.49945900	2.50876200	5.66599000
H	-3.44222400	2.91913100	5.15434800
C	-6.80423200	1.38374300	3.95634400
H	-5.77054900	0.96617100	2.10282800
C	-6.71152300	1.95057300	5.23663100
H	-5.42380800	2.94944500	6.65183300
H	-7.74655300	0.97326800	3.61540300
H	-7.57564700	1.96351200	5.88870400
A10A_sp			
Atom	X	Y	Z
Cu	0.52719100	0.03806300	-0.52385000
N	-0.98787100	-0.30870600	0.76838400
C	-1.46624500	-1.49349400	1.15159500
H	-0.97347000	-2.36292500	0.73869100
C	-2.53548200	-1.58715400	2.06441700
C	-3.12527200	-0.43565500	2.59454900
C	-2.63443900	0.83605200	2.15302500
C	-1.55550900	0.83332000	1.24786600
C	-1.00885900	2.06960000	0.75231400
C	-1.52111200	3.30738300	1.18695100
C	-0.91457700	4.49289400	0.65921100
C	0.09626900	4.34369100	-0.29441000
C	0.52504800	3.06157200	-0.69660200
H	1.30996200	2.90553500	-1.42470000
N	-0.01216700	1.95924300	-0.17024600
C	2.60551700	-3.70461400	-0.67654000
H	3.50832700	-3.73966800	-0.05756600
H	2.81726500	-4.25322700	-1.59669300
H	1.78003600	-4.17977400	-0.14805000
C	2.26337800	-2.26874100	-0.97625800
O	1.18599300	-1.79435100	-0.41109700
C	3.12116000	-1.52753600	-1.81343700
H	3.98428600	-2.03813700	-2.21628400
C	2.96278600	-0.16668000	-2.12810700
O	1.97439600	0.57699400	-1.69998100
C	3.98993000	0.52640600	-2.98078100
H	3.52687500	1.35468100	-3.51756000
H	4.45813800	-0.16173700	-3.68501300
H	4.77258900	0.92355500	-2.32502500
O	-0.76819600	-0.31130500	-2.29851300
H	-1.51865200	-1.00303300	-2.17742600
H	-0.22279800	-0.41853500	-3.09603700
N	4.91215700	-1.73523700	1.22012400
C	5.65081400	-0.87736600	0.49303600
H	6.59366900	-1.24368300	0.11570500
N	5.34958600	0.41295800	0.19542000
C	4.18125600	0.94270000	0.63371600
N	3.91404700	2.25069600	0.39250800
H	4.61070000	2.81070900	-0.07353100
H	3.05993300	2.66123700	0.73358700
C	3.29392600	0.10508600	1.34789400
N	2.02865800	0.31960100	1.90724400

C	1.74482900	-0.81636100	2.53444400
H	0.83942000	-1.00649300	3.08251100
N	2.74952700	-1.75880600	2.40972400
H	2.76276500	-2.69186900	2.79233000
C	3.74651800	-1.19139400	1.63459700
N	-2.99568500	-1.43195200	-1.65514400
C	-3.74399300	-2.49955200	-1.31388700
H	-3.34520400	-3.47539800	-1.54572100
N	-4.95418800	-2.47349800	-0.71701000
C	-5.52991500	-1.27760000	-0.40978900
N	-6.76070600	-1.25933900	0.14497100
H	-7.25851800	-2.12900200	0.26176700
H	-7.20233200	-0.37937500	0.36641600
C	-4.80789100	-0.09353300	-0.69188300
N	-5.09119600	1.25857700	-0.49368800
C	-4.04426400	1.89803900	-0.99915600
H	-3.92932300	2.96708500	-1.01773100
N	-3.08974100	1.03135200	-1.52028400
H	-2.18292700	1.22664500	-1.93629500
C	-3.56586000	-0.24516700	-1.32194200
C	-2.66623600	3.28935300	2.06766100
C	-3.20254000	2.11324000	2.51759900
H	0.57896100	5.21840500	-0.70835400
H	-2.87851600	-2.56276900	2.38006800
H	-3.13281100	4.22846300	2.33140400
H	-4.09604200	2.12825500	3.12598800
C	-1.31862400	5.85071500	1.09765800
C	-1.41014400	6.16489800	2.46683800
C	-1.56327200	6.85419800	0.14237700
C	-1.74928300	7.46060800	2.87207900
H	-1.18372100	5.40989600	3.21099700
C	-1.91321600	8.14713000	0.54941100
H	-1.50195200	6.61960200	-0.91446600
C	-2.00780300	8.45289600	1.91470400
H	-1.80453700	7.69723000	3.92680300
H	-2.11177300	8.91027200	-0.19201200
H	-2.27472900	9.45356300	2.22907600
C	-4.21215000	-0.56888200	3.59339200
C	-4.18557800	0.16446100	4.79491300
C	-5.25344100	-1.48834700	3.37035400
C	-5.19266600	-0.00996700	5.75074500
H	-3.36399800	0.84149600	4.99838200
C	-6.26468600	-1.65424900	4.32328700
H	-5.28255400	-2.05552900	2.44702300
C	-6.23804300	-0.91499700	5.51468400
H	-5.15778000	0.54827900	6.67735800
H	-7.06674000	-2.35803400	4.14102800
H	-7.01769100	-1.04767000	6.25385400
AllA_sp			
Atom	X	Y	Z
Cu	0.55452800	0.07664100	-0.49935400
N	-0.96434800	-0.25324100	0.81208900
C	-1.44450900	-1.42571600	1.23030300
H	-0.94574000	-2.30652100	0.84964100
C	-2.54502500	-1.48936000	2.11932600

C	-3.12972700	-0.31243200	2.57261000
C	-2.61533900	0.93731700	2.13965200
C	-1.52939000	0.90557900	1.24748700
C	-0.97550600	2.13060400	0.73948400
C	-1.49526600	3.37707300	1.13911800
C	-0.89182600	4.53592200	0.58594500
C	0.15555300	4.39721800	-0.31740500
C	0.60841300	3.10462500	-0.67471400
H	1.41466800	2.93124600	-1.37513700
N	0.04718200	2.01467600	-0.14991400
C	2.54999700	-3.70264200	-0.67012200
H	3.45297700	-3.75536600	-0.05247900
H	2.75104300	-4.25317000	-1.59146400
H	1.71697500	-4.16435400	-0.14170000
C	2.23488700	-2.26039800	-0.96634300
O	1.16633100	-1.76692700	-0.39763100
C	3.10466500	-1.53379200	-1.80310800
H	3.95466000	-2.06153000	-2.21167700
C	2.97487400	-0.16897200	-2.11364200
O	2.00602400	0.59540500	-1.67510100
C	4.00951000	0.50388600	-2.97257000
H	3.55873200	1.33842900	-3.51009900
H	4.46286900	-0.19404500	-3.67674500
H	4.80175300	0.89012900	-2.32184800
O	-0.76268700	-0.16716300	-2.27241900
H	-1.48070700	-0.89885400	-2.16565900
H	-0.21654100	-0.22521400	-3.07508800
N	4.91430200	-1.77288100	1.20884000
C	5.66176400	-0.92592600	0.47789900
H	6.59432000	-1.30747800	0.09033400
N	5.38116900	0.37120100	0.18991300
C	4.22652800	0.91990300	0.64000000
N	3.98607300	2.23602800	0.41230500
H	4.69756100	2.78578900	-0.04394300
H	3.15571300	2.66778500	0.78406600
C	3.32735000	0.09359600	1.35260100
N	2.06971400	0.32659600	1.92286900
C	1.77610800	-0.80467900	2.55464100
H	0.87605800	-0.97924900	3.11644300
N	2.76413700	-1.76242300	2.41934500
H	2.77094100	-2.69331500	2.80775700
C	3.76203900	-1.21030700	1.63419400
N	-2.89070000	-1.42572900	-1.61166400
C	-3.49659200	-2.55567100	-1.19583400
H	-3.03208700	-3.49166200	-1.46644800
N	-4.63604800	-2.63712500	-0.47785100
C	-5.28715400	-1.49781800	-0.11332700
N	-6.43119600	-1.58715400	0.59744400
H	-6.80973400	-2.50024600	0.80089600
H	-6.95404600	-0.75342700	0.82163100
C	-4.72508400	-0.25443900	-0.49064400
N	-5.11822900	1.06647300	-0.26991700
C	-4.19247200	1.79860000	-0.87630100
H	-4.18934900	2.87342000	-0.91546800
N	-3.20840100	1.02086500	-1.47852400
H	-2.36660100	1.30283700	-1.97120500

C	-3.53976700	-0.29416000	-1.23517800
C	-2.60447300	3.36893900	2.06490400
C	-3.14887800	2.21451500	2.54373400
H	-3.99317700	2.24760200	3.22014000
H	-1.25156200	5.51646100	0.86814800
H	0.62695600	5.26507200	-0.75573900
H	-3.97703300	-0.34180900	3.24616100
H	-2.92526500	-2.45405000	2.42346900
Cl	-3.29930800	4.94217900	2.56454800
A12A_sp			
Atom	X	Y	Z
Cu	0.56892700	0.05236700	-0.52645000
N	-0.95548200	-0.26977300	0.77550700
C	-1.43090900	-1.44606400	1.19139300
H	-0.93007900	-2.32245400	0.80262100
C	-2.52289400	-1.52147900	2.08963900
C	-3.10330300	-0.34857500	2.55729000
C	-2.59065300	0.90184000	2.12607800
C	-1.51684900	0.88568700	1.22086300
C	-0.96598400	2.11796100	0.71714700
C	-1.47894600	3.37095700	1.11621100
C	-0.83940500	4.52111300	0.56941600
C	0.21153400	4.36042800	-0.32558500
C	0.64053000	3.06505600	-0.69270000
H	1.44624400	2.87748800	-1.38998800
N	0.05622800	1.98649400	-0.17135200
C	2.58498600	-3.71524200	-0.65788100
H	3.48993500	-3.75994000	-0.04258400
H	2.78573100	-4.27173600	-1.57575500
H	1.75532500	-4.17685500	-0.12415000
C	2.26333500	-2.27686300	-0.96434500
O	1.18737900	-1.78625600	-0.40573100
C	3.13400200	-1.54995700	-1.79972000
H	3.98983400	-2.07545200	-2.19882900
C	2.99929900	-0.18793700	-2.12051300
O	2.02211800	0.57359900	-1.69446100
C	4.03544700	0.48590100	-2.97616300
H	3.58161900	1.30906400	-3.52849900
H	4.50421300	-0.21494700	-3.66710100
H	4.81596700	0.88898600	-2.32144900
O	-0.73311700	-0.22935600	-2.30684600
H	-1.47669200	-0.92928000	-2.19374400
H	-0.18449300	-0.32322100	-3.10430000
N	4.91550700	-1.75204500	1.21566100
C	5.65235500	-0.89537300	0.48538900
H	6.58862500	-1.26540400	0.09565900
N	5.35660000	0.39921700	0.20123300
C	4.19736500	0.93453100	0.65507900
N	3.94579800	2.25028200	0.43560000
H	4.65517300	2.80849300	-0.01401300
H	3.12230300	2.67774400	0.82700300
C	3.30661200	0.09564100	1.36400300
N	2.04659700	0.31214400	1.93613900
C	1.76744900	-0.82427300	2.56547600
H	0.87135000	-1.01062100	3.13007300

N	2.76647000	-1.76970000	2.42697200
H	2.78667400	-2.70034300	2.81579500
C	3.75701100	-1.20385900	1.64237000
N	-2.91998200	-1.38852900	-1.62012200
C	-3.56430800	-2.47966700	-1.15946100
H	-3.15238300	-3.44208600	-1.42276200
N	-4.68328100	-2.49279500	-0.40518200
C	-5.26936000	-1.31717700	-0.04650000
N	-6.39117900	-1.33692200	0.70404000
H	-6.80861100	-2.22662200	0.93433900
H	-6.87244700	-0.47568700	0.91793800
C	-4.66263600	-0.10988900	-0.47004200
N	-4.98914200	1.23215800	-0.26931500
C	-4.05551600	1.90787200	-0.92790200
H	-4.01111700	2.98034100	-1.00195800
N	-3.12757700	1.07248400	-1.54121100
H	-2.29083000	1.30777800	-2.06586100
C	-3.50664700	-0.22047600	-1.25290700
C	-2.58395200	3.33290300	2.05686700
C	-3.11733600	2.17130500	2.53833300
H	-3.95136400	2.21629400	3.22656300
H	-1.17622600	5.50916800	0.83691800
H	0.70044000	5.22449200	-0.75206700
H	-3.94412300	-0.38102500	3.23874500
H	-2.89874200	-2.48922300	2.38842100
N	-3.23438900	4.57284200	2.51492900
O	-3.91278700	4.52436000	3.57344900
O	-3.09648200	5.61108400	1.80842300
A13A_sp			
Atom	X	Y	Z
Cu	0.70899300	-0.26115800	-0.81094900
N	-0.84874000	-0.71526400	0.49346100
C	-1.48636900	-1.86982100	0.70840800
H	-1.18197400	-2.72302200	0.11742800
C	-2.52924000	-1.98749500	1.65599800
C	-2.89460800	-0.87493200	2.40286600
C	-2.23090100	0.36031800	2.19130500
C	-1.22232400	0.39158600	1.20550700
C	-0.57045900	1.63409300	0.89138000
C	-0.89326200	2.80549800	1.60233000
C	-0.22204100	3.99812600	1.21979500
C	0.68215700	3.97058100	0.16737900
C	0.93216900	2.74952500	-0.50764900
H	1.61762300	2.67667200	-1.33915600
N	0.32410500	1.62164600	-0.13671500
C	2.37420300	-2.00242600	-2.40383100
H	2.36535600	-2.70593400	-3.23554500
C	2.47569600	-0.57219900	-2.95184800
O	2.00717700	0.36208800	-2.11446000
O	-0.78940200	-0.24599500	-2.56151100
H	-1.68463000	-0.74657400	-2.56595900
H	-0.42179100	0.02939700	-3.41958000
N	4.70947200	0.60724600	3.39414500
C	5.42394800	1.47685100	2.65231800

H	6.25449300	1.96579900	3.13790300
N	5.21312900	1.79800700	1.35758100
C	4.19071200	1.23015600	0.66071500
N	4.04761100	1.56855700	-0.63785900
H	4.75155400	2.18281600	-1.02337700
H	3.34003300	1.14710500	-1.24569400
C	3.35052100	0.31377100	1.35890900
N	2.22068000	-0.45274800	1.01254700
C	1.91294700	-1.13830900	2.10945500
H	1.08928200	-1.82419800	2.19896800
N	2.76861000	-0.86980000	3.15266100
H	2.75573300	-1.26491600	4.08128200
C	3.69418800	0.05921700	2.70009500
N	-3.13851800	-1.11818800	-1.97705200
C	-3.92490900	-2.18843500	-1.73910400
H	-3.67160000	-3.10839000	-2.24429500
N	-5.00929000	-2.22672500	-0.93921100
C	-5.41048900	-1.09716400	-0.29142500
N	-6.50307200	-1.13928500	0.49879400
H	-7.03513000	-1.99540000	0.55250500
H	-6.84371600	-0.29578700	0.93609900
C	-4.64928100	0.08286600	-0.47049100
N	-4.77795700	1.37402400	0.04285900
C	-3.76922200	2.04981000	-0.49015800
H	-3.56703000	3.09170800	-0.31716500
N	-2.98247600	1.26135200	-1.32516300
H	-2.12622900	1.50379900	-1.81007100
C	-3.53695500	0.00043700	-1.31771300
C	-1.89081300	2.73955300	2.64362700
C	-2.54359200	1.56872700	2.91515200
H	-3.31349300	1.53140900	3.67545200
H	-0.42523500	4.92167700	1.74776600
H	1.20243300	4.86326600	-0.14800200
H	-3.68844800	-0.93923900	3.13658600
H	-3.02889500	-2.93731900	1.78184800
H	-2.12937400	3.64182200	3.19308500
N	1.18152600	-2.15535500	-1.51201700
H	0.35563700	-2.41860400	-2.04786000
H	1.35991500	-2.82179900	-0.76440000
O	3.00264000	-0.35140700	-4.05053700
H	3.27537400	-2.17818500	-1.81234000

A14A_sp

Atom	X	Y	Z
Cu	0.68271400	-0.26572600	-0.83779300
N	-0.87788700	-0.69699500	0.46815200
C	-1.50288600	-1.85260800	0.71038800
H	-1.19125900	-2.71524400	0.13709200
C	-2.54258400	-1.96025400	1.66301400
C	-2.91615200	-0.83537700	2.38639100
C	-2.26423400	0.40115200	2.14589200
C	-1.26010700	0.42286900	1.15601000
C	-0.62212200	1.66435600	0.80901200
C	-0.94808600	2.85046700	1.49319700
C	-0.28973600	4.05597600	1.08791200
C	0.60127200	3.98235200	0.02079100

C	0.85618200	2.75140200	-0.62694400
H	1.53657500	2.66835500	-1.46169700
N	0.26401100	1.62548000	-0.22668800
C	2.38842300	-2.03324800	-2.35502100
H	2.39752700	-2.76692200	-3.16032000
C	2.46568900	-0.62225400	-2.95452500
O	1.98620300	0.33341200	-2.14859700
O	-0.78906700	-0.37568900	-2.61746800
H	-1.68855200	-0.86773100	-2.60320200
H	-0.42794700	-0.12300300	-3.48518100
N	4.58720200	0.85380000	3.39413100
C	5.28763500	1.71749200	2.63215400
H	6.09141700	2.25272700	3.11413300
N	5.09363300	1.98068700	1.32168900
C	4.10497800	1.35132700	0.62825700
N	3.97805700	1.63108200	-0.68555000
H	4.66888900	2.25251700	-1.08304100
H	3.29173300	1.16746600	-1.28759100
C	3.28070400	0.43626400	1.34650400
N	2.18438400	-0.38044400	1.00797500
C	1.87710600	-1.03417000	2.12393800
H	1.07464800	-1.74351100	2.22366800
N	2.70168800	-0.69716500	3.17290900
H	2.68348100	-1.05808900	4.11521200
C	3.60489800	0.24493700	2.70271500
N	-3.14792100	-1.20460900	-2.00369500
C	-3.94481200	-2.25843800	-1.73007000
H	-3.69943300	-3.19767000	-2.20263900
N	-5.03054000	-2.25864700	-0.93094000
C	-5.42120800	-1.10371200	-0.32300300
N	-6.51529100	-1.10799700	0.46653800
H	-7.05563700	-1.95656600	0.54868100
H	-6.84766800	-0.24678000	0.87463600
C	-4.64856500	0.06218600	-0.54177700
N	-4.76616600	1.37212300	-0.07505700
C	-3.75038600	2.01884200	-0.63022200
H	-3.53843900	3.06416000	-0.49411400
N	-2.97021200	1.19462800	-1.43575700
H	-2.10753100	1.41172600	-1.92138900
C	-3.53628900	-0.06008300	-1.38433000
C	-1.93941000	2.79143700	2.54157400
C	-2.58180500	1.62151700	2.84314300
H	-3.34706200	1.59637600	3.60874300
H	1.11525700	4.86879400	-0.32412400
H	-3.70681400	-0.89099500	3.12426300
H	-3.03246600	-2.91201500	1.81081000
H	-2.18920100	3.69587700	3.07999700
N	1.19341700	-2.17478100	-1.46480800
H	0.37399600	-2.46457900	-1.99670300
H	1.37686200	-2.81245200	-0.69385900
O	2.98383400	-0.43271400	-4.06349300
H	3.28899000	-2.16973900	-1.75224400
C	-0.55792400	5.35930200	1.79139800
H	-1.61450500	5.63473600	1.72906900
H	-0.29511800	5.29156100	2.85067700
H	0.02711200	6.16568900	1.35102300

A15A_sp			
Atom	X	Y	Z
Cu	0.70208400	-0.26312300	-0.82373300
N	-0.86917800	-0.67468100	0.47146200
C	-1.50871600	-1.82226400	0.71679900
H	-1.20240800	-2.69300200	0.15308400
C	-2.55708700	-1.90872700	1.66151400
C	-2.92598000	-0.77327400	2.37177800
C	-2.25909200	0.45433000	2.12748400
C	-1.24608600	0.45197500	1.14798700
C	-0.59567000	1.68733000	0.80515700
C	-0.92477600	2.88075200	1.47737200
C	-0.24600800	4.05599900	1.05446500
C	0.66489800	3.99365200	0.00860500
C	0.91918700	2.75254900	-0.62303300
H	1.61023100	2.64910100	-1.44662700
N	0.30596700	1.64009400	-0.21581500
C	2.37545400	-2.05427700	-2.35219100
H	2.36318700	-2.78047400	-3.16414700
C	2.48042800	-0.64007200	-2.93989100
O	2.02054500	0.31867700	-2.12603800
O	-0.76609200	-0.32397200	-2.60460500
H	-1.66604000	-0.81620400	-2.59733700
H	-0.39455800	-0.07807500	-3.46984500
N	4.63469100	0.74458000	3.41506700
C	5.35996200	1.59091700	2.65681600
H	6.18097200	2.09801100	3.14010600
N	5.17112600	1.86817500	1.34851500
C	4.16212600	1.27418100	0.65361600
N	4.04019100	1.56715900	-0.65797000
H	4.74835100	2.17050600	-1.05274500
H	3.34243400	1.12413900	-1.26214900
C	3.31191800	0.37977400	1.36780800
N	2.18962900	-0.39994400	1.02728700
C	1.86380000	-1.04962000	2.14052800
H	1.03946200	-1.73359600	2.23831500
N	2.70088000	-0.74494600	3.18921100
H	2.67236600	-1.10949900	4.12987900
C	3.63253900	0.17079500	2.72232200
N	-3.12989100	-1.15255900	-2.01268600
C	-3.92977000	-2.20635200	-1.74796700
H	-3.68008500	-3.14530100	-2.21884500
N	-5.02337400	-2.20691400	-0.95973100
C	-5.41990800	-1.05240000	-0.35473800
N	-6.52190000	-1.05707900	0.42359300
H	-7.06272000	-1.90583100	0.50050000
H	-6.85748500	-0.19637700	0.83013700
C	-4.64501400	0.11355100	-0.56499300
N	-4.76726000	1.42328200	-0.09889600
C	-3.74581800	2.07017400	-0.64315600
H	-3.53560600	3.11567600	-0.50543800
N	-2.95748500	1.24613700	-1.44111900
H	-2.09245700	1.46369700	-1.92210600
C	-3.52424900	-0.00853500	-1.39609000

C	-1.93281200	2.86160500	2.52594800
C	-2.57263700	1.68324000	2.81130700
H	-3.34813000	1.66253500	3.56778700
H	1.18693400	4.87619100	-0.33168000
H	-3.72471400	-0.81497000	3.10178800
H	-3.05894200	-2.85354500	1.81366200
N	1.18345300	-2.17891300	-1.45526700
H	0.35814500	-2.46242000	-1.98128500
H	1.36316500	-2.81552200	-0.68251600
O	3.00148500	-0.45180100	-4.04760100
H	3.27711600	-2.21635100	-1.75756900
C	-2.27039300	4.13651800	3.25598800
H	-3.03891300	3.95962800	4.00773000
H	-1.39264800	4.54583000	3.76416000
H	-2.64541700	4.90219000	2.57040600
H	-0.44364100	5.00029900	1.54418100

A16A_sp

Atom	X	Y	Z
Cu	0.71201700	-0.20046700	-0.76300700
N	-0.85009500	-0.60742700	0.53354100
C	-1.49065200	-1.75479200	0.77316100
H	-1.14759900	-2.63533400	0.24671700
C	-2.58797000	-1.83484200	1.65528800
C	-3.03267700	-0.69977600	2.33050300
C	-2.33640000	0.52707300	2.10196800
C	-1.27214300	0.52437800	1.17719500
C	-0.60973200	1.75694400	0.83739500
C	-0.96429700	2.96129700	1.47384700
C	-0.27331600	4.15337600	1.08373900
C	0.67714300	4.05115900	0.07253200
C	0.95514000	2.80519700	-0.53559300
H	1.67664900	2.70108400	-1.33268300
N	0.33192800	1.69281000	-0.14681300
C	2.31627000	-2.00369400	-2.35345600
H	2.27860200	-2.72398100	-3.16986700
C	2.43122700	-0.58686400	-2.93296900
O	1.99609300	0.37198100	-2.10683700
O	-0.83065700	-0.16567700	-2.49409100
H	-1.68535400	-0.72522900	-2.51460100
H	-0.44981900	0.10792300	-3.34699600
N	4.81176200	0.63878300	3.34729400
C	5.54791000	1.45888500	2.57086400
H	6.40702900	1.92404400	3.02920400
N	5.32616900	1.75774900	1.27251100
C	4.26808500	1.21648900	0.60852400
N	4.10958700	1.53360400	-0.69345200
H	4.82543800	2.11498000	-1.10668000
H	3.36910600	1.13293100	-1.27536600
C	3.40769800	0.34845600	1.34289800
N	2.24342900	-0.38080800	1.03405900
C	1.92494900	-1.02351500	2.15333400
H	1.07443300	-1.67062500	2.27360100
N	2.80795500	-0.76299200	3.17606500
H	2.79308200	-1.13149300	4.11543900

C	3.76289700	0.11512000	2.68465100
N	-3.13738000	-1.19919000	-1.94422100
C	-3.87103200	-2.31213100	-1.73642300
H	-3.54280500	-3.21775500	-2.22414700
N	-4.98954500	-2.40916500	-0.99033400
C	-5.48502500	-1.30312200	-0.36920300
N	-6.62159900	-1.40473100	0.35249100
H	-7.10846500	-2.28874600	0.37304500
H	-7.04121500	-0.58037700	0.75603400
C	-4.77705700	-0.08517400	-0.50602900
N	-4.99454500	1.19547600	0.00401500
C	-3.99916700	1.92474400	-0.48401600
H	-3.85385500	2.97281300	-0.29301000
N	-3.13888600	1.18300200	-1.28625700
H	-2.27433200	1.46934200	-1.73250600
C	-3.62500400	-0.10597900	-1.30356900
C	-2.01365000	2.92890900	2.46277100
C	-2.68150200	1.76870700	2.74872100
H	-3.48886200	1.77761500	3.46804400
H	1.21787600	4.92622800	-0.26048900
H	-3.08823300	-2.78414600	1.79051900
N	1.13986300	-2.11719700	-1.43475300
H	0.30014400	-2.38742700	-1.94477200
H	1.32554000	-2.76225300	-0.67034600
O	2.94050400	-0.39931400	-4.04657800
H	3.22627300	-2.18256400	-1.77658400
H	-2.28768300	3.84473400	2.96945100
C	-4.22655200	-0.75174500	3.24175100
H	-3.96197700	-0.45745900	4.26117200
H	-5.00053300	-0.06509700	2.88496100
H	-4.64906500	-1.75534200	3.27511000
C	-0.57140100	5.47288600	1.74407400
H	-1.61839200	5.75791200	1.60798600
H	-0.37819800	5.42349700	2.81915400
H	0.04985300	6.26443300	1.32696600
A17A_sp			
Atom	X	Y	Z
Cu	0.72627600	-0.22782700	-0.78388900
N	-0.85856400	-0.64226100	0.48851900
C	-1.49302400	-1.79734100	0.70917600
H	-1.14133300	-2.67003700	0.17587500
C	-2.59117700	-1.88278800	1.59007300
C	-3.02033300	-0.73908500	2.25313600
C	-2.36064400	0.50030900	2.04009500
C	-1.28549400	0.48720400	1.12805300
C	-0.62318000	1.71931200	0.80146300
C	-0.99772400	2.91135600	1.44665600
C	-0.30454400	4.08635300	1.04163200
C	0.66012900	4.02059200	0.04544000
C	0.95770900	2.77695300	-0.55857300
H	1.68863100	2.67015500	-1.34642200
N	0.33019800	1.66649400	-0.16978900
C	2.37882000	-2.01840400	-2.33733500
H	2.37003900	-2.73633900	-3.15667600
C	2.50509200	-0.59937100	-2.90876400

O	2.03951900	0.35482900	-2.09330900
O	-0.78104300	-0.20122700	-2.53250900
H	-1.67104500	-0.70723900	-2.55516500
H	-0.39944700	0.07793500	-3.38316800
N	4.72107400	0.62278000	3.42890800
C	5.46907100	1.45233800	2.67415800
H	6.31263800	1.92295800	3.15533500
N	5.27690500	1.75431200	1.37191800
C	4.24001400	1.20715400	0.67999100
N	4.11236900	1.52678300	-0.62479900
H	4.83439300	2.11419500	-1.01828400
H	3.39042900	1.12174400	-1.22628800
C	3.36801100	0.33035500	1.38984000
N	2.21689900	-0.40651700	1.05021500
C	1.87799200	-1.05755600	2.15871100
H	1.03128100	-1.71341800	2.25622400
N	2.73412000	-0.79470800	3.20320000
H	2.70023000	-1.16816100	4.14014900
C	3.69304300	0.09361000	2.73871500
N	-3.14102000	-1.11124900	-2.01446800
C	-3.89080800	-2.21209900	-1.80026400
H	-3.58282800	-3.12212600	-2.29294800
N	-5.00073200	-2.29229300	-1.03942000
C	-5.46864000	-1.17959500	-0.40901800
N	-6.58823500	-1.26460400	0.33997900
H	-7.08647700	-2.14172800	0.37537300
H	-6.98354300	-0.43447900	0.75601300
C	-4.74722600	0.02857700	-0.56053400
N	-4.94040900	1.31227700	-0.04806200
C	-3.94079000	2.02714000	-0.54752300
H	-3.78074600	3.07432000	-0.36331500
N	-3.09968200	1.27213200	-1.35867000
H	-2.24074800	1.55292300	-1.81659300
C	-3.60492400	-0.00981000	-1.37043800
C	-2.06591900	2.90688100	2.44011900
C	-2.75275000	1.73893700	2.70259000
H	1.18946400	4.90549900	-0.27715400
H	-3.09099000	-2.83061500	1.73072500
N	1.17458000	-2.13900600	-1.45662300
H	0.34914100	-2.39459400	-1.99698100
H	1.33348300	-2.79810900	-0.69821700
O	3.04785200	-0.40498300	-4.00499000
H	3.27072900	-2.19524800	-1.73218400
H	-3.86513800	-0.79777700	2.92470600
H	-0.53166100	5.03830800	1.50057200
C	-3.94574000	1.65341600	3.62454300
H	-4.81993100	1.31048200	3.06205100
H	-3.76711000	0.95071400	4.44370400
H	-4.20772700	2.60907300	4.06640300
C	-2.36577200	4.22752200	3.11114300
H	-1.45224300	4.66014500	3.52770100
H	-2.77924600	4.94883100	2.39873900
H	-3.07242900	4.13337000	3.92910700

A18A_sp
Atom

X

Y

Z

Cu	0.67155900	-0.23229000	-0.79956500
N	-0.86970600	-0.63378200	0.52808800
C	-1.48923700	-1.78144100	0.81627400
H	-1.15414700	-2.66716800	0.29062100
C	-2.55443300	-1.88620000	1.74299800
C	-2.97510500	-0.72557600	2.40847000
C	-2.30149600	0.50261900	2.13119700
C	-1.27402000	0.50293500	1.16831600
C	-0.63386100	1.73457100	0.79081300
C	-0.96353000	2.94598000	1.42307100
C	-0.28901400	4.13625600	1.00367600
C	0.63677300	4.04789000	-0.04352400
C	0.87217700	2.78187500	-0.64075800
H	1.56336600	2.67110300	-1.46426200
N	0.26935700	1.66925500	-0.22501900
C	2.32510900	-2.05898600	-2.31057300
H	2.30738000	-2.80444200	-3.10495500
C	2.42947300	-0.65957500	-2.93309100
O	1.96158300	0.31846200	-2.14968000
O	-0.84364900	-0.29013700	-2.53985800
H	-1.71285500	-0.82857900	-2.53781400
H	-0.47298000	-0.03182500	-3.40166500
N	4.63843400	1.00664800	3.33104600
C	5.33462900	1.84068600	2.53334400
H	6.14454000	2.38934900	2.98931700
N	5.12911700	2.06025800	1.21634800
C	4.13254900	1.40984300	0.55396000
N	3.99187300	1.64613600	-0.76719700
H	4.68388600	2.24529400	-1.19527500
H	3.29106100	1.16992800	-1.34268900
C	3.31449000	0.52011000	1.31007900
N	2.21558900	-0.30697700	1.00861300
C	1.91396600	-0.91872000	2.14910300
H	1.10795500	-1.61895600	2.27894900
N	2.74697300	-0.54605100	3.17977000
H	2.73350300	-0.87146300	4.13488600
C	3.64851400	0.37638400	2.66959300
N	-3.16154700	-1.25620900	-1.94076000
C	-3.90906700	-2.35314600	-1.70369700
H	-3.60965500	-3.26931500	-2.19011800
N	-5.01034200	-2.42154900	-0.92815100
C	-5.46635800	-1.30087000	-0.30390900
N	-6.58013500	-1.37678000	0.45762100
H	-7.09171900	-2.24645000	0.48830200
H	-6.96832300	-0.54099800	0.86923600
C	-4.74363000	-0.09677200	-0.47514400
N	-4.92809200	1.19377400	0.02231700
C	-3.93389100	1.89975300	-0.50086400
H	-3.76736700	2.94791300	-0.32881300
N	-3.10699600	1.13387300	-1.31542000
H	-2.24397100	1.39859500	-1.77745500
C	-3.61334300	-0.14681000	-1.30222200
C	-1.97789100	2.91452600	2.45038000
C	-2.62731900	1.75388600	2.77394100
N	1.13995300	-2.16009200	-1.40287900
H	0.30770400	-2.45129800	-1.91346500

H	1.32271000	-2.77962700	-0.61716600
O	2.96058500	-0.50032700	-4.04134900
H	3.23055900	-2.20724800	-1.71807500
C	1.40641900	5.23771400	-0.56194200
H	0.73982700	6.02277300	-0.92757000
H	2.03625300	5.67059400	0.21951800
H	2.05894400	4.94270700	-1.38426900
C	-0.58951900	5.44328400	1.69106300
H	-1.64353100	5.71359600	1.57703100
H	-0.38118600	5.37286600	2.76240500
H	0.00783700	6.25817300	1.28979000
C	-4.12528900	-0.73780800	3.37883500
H	-3.79440600	-0.45652100	4.38311200
H	-4.88559600	-0.01577900	3.06583300
H	-4.59559500	-1.71617200	3.44097100
C	-3.19239300	-3.23510500	1.97094800
H	-3.14869700	-3.52531900	3.02359200
H	-4.24080200	-3.23615600	1.66166900
H	-2.68474100	-4.00705000	1.38973900
H	-2.24067100	3.83240700	2.95899300
H	-3.40452600	1.77061900	3.52530700
A19A_sp			
Atom	X	Y	Z
Cu	0.48800800	0.09012500	-0.51519500
N	-1.05528900	-0.17289200	0.82054500
C	-1.74848000	-1.27896700	1.11302600
H	-1.43867300	-2.20156500	0.64048200
C	-2.83946700	-1.26819200	2.00070900
C	-3.23646000	-0.08037200	2.61777100
C	-2.52450000	1.11595500	2.28551800
C	-1.44495100	1.01335500	1.38079800
C	-0.72880600	2.19465400	0.97002900
C	-1.06704800	3.45828400	1.49372600
C	-0.31118500	4.58985400	1.04409200
C	0.66142600	4.37721200	0.06761500
C	0.91108600	3.08202100	-0.42973200
H	1.65467100	2.89759800	-1.19125600
N	0.24360700	2.02160400	0.02981900
C	1.55681000	-1.83218300	-2.37893300
H	1.31617200	-2.50349400	-3.20346000
C	1.83545400	-0.43394600	-2.94218500
O	1.51985400	0.57055400	-2.10512700
O	-1.25903700	0.65728800	-2.38272400
H	-1.46439400	-0.19154900	-2.84008400
H	-0.46072500	1.10524800	-2.72990000
N	5.18091800	0.23881800	2.82730700
C	5.91146800	0.95071100	1.94591800
H	6.90122600	1.24633900	2.25773200
N	5.53379900	1.33323500	0.70683400
C	4.30479800	1.00498000	0.22486000
N	3.98939700	1.40769500	-1.02491000
H	4.71550600	1.88423000	-1.54188900
H	3.11250300	1.15861200	-1.48433400
C	3.44379200	0.25783200	1.08140200

N	2.13756500	-0.25537700	0.96967000
C	1.89575600	-0.86895200	2.12472200
H	0.97446400	-1.36089100	2.38092700
N	2.96380200	-0.79412400	2.98494700
H	3.03687500	-1.17985800	3.91498400
C	3.96501300	-0.07697600	2.34462300
N	-2.46814100	-1.87652200	-2.30221700
C	-2.71732900	-3.18829100	-2.52924100
H	-1.98825800	-3.73028700	-3.11468900
N	-3.78115600	-3.89847600	-2.10944800
C	-4.75333400	-3.28671300	-1.37729500
N	-5.82303300	-4.00125700	-0.97306100
H	-5.89309000	-4.97076000	-1.24463100
H	-6.57566000	-3.55165300	-0.47394100
C	-4.59573600	-1.91184200	-1.07737400
N	-5.39588800	-1.00738900	-0.37935500
C	-4.75214200	0.15152100	-0.47550800
H	-5.09696900	1.08000100	-0.05543500
N	-3.57035800	0.04781100	-1.19222000
H	-2.87792500	0.75977200	-1.43879600
C	-3.45270600	-1.27014400	-1.57935900
C	-2.19708700	3.54313300	2.38660200
C	-2.89576000	2.42719400	2.75924100
N	0.48623100	-1.79536000	-1.33767100
H	-0.45422500	-1.88912700	-1.74389500
H	0.64045200	-2.51216900	-0.63156600
O	2.35078300	-0.28846200	-4.05684900
H	2.48612100	-2.17650900	-1.91946800
H	-2.51476900	4.51872300	2.72768400
H	-3.76620500	2.51976500	3.39389700
C	-0.53204700	5.95486500	1.57939800
C	-0.54565400	6.19149800	2.96715500
C	-0.67310900	7.03790500	0.69295600
C	-0.70555500	7.49211800	3.45835000
H	-0.39334900	5.37071400	3.65888500
C	-0.84401500	8.33671600	1.18639700
H	-0.67206500	6.86284500	-0.37685400
C	-0.86062000	8.56653700	2.56969300
H	-0.69924500	7.66874800	4.52612500
H	-0.96282100	9.16299300	0.49775400
H	-0.98629800	9.57169900	2.95083700
C	-4.37457200	-0.09008900	3.56792300
C	-4.23487200	0.44135200	4.86404500
C	-5.59422700	-0.67679700	3.18184900
C	-5.30401000	0.38575500	5.76492400
H	-3.28770800	0.86586900	5.17776800
C	-6.66548700	-0.71710900	4.08329500
H	-5.71346000	-1.06453000	2.17559100
C	-6.52280900	-0.18983300	5.37467600
H	-5.18706500	0.78201600	6.76532000
H	-7.60712500	-1.15478800	3.77812900
H	-7.35087800	-0.22817600	6.07063900
H	-3.35993900	-2.19008300	2.21996300
H	1.25584300	5.20439900	-0.29444300

A20A_sp

Atom	X	Y	Z
Cu	0.73785800	-0.23577200	-0.77777100
N	-0.83091600	-0.68836100	0.51519800
C	-1.45970900	-1.84691000	0.73473300
H	-1.12972000	-2.70653900	0.16737700
C	-2.52486000	-1.96124800	1.65776000
C	-2.92710800	-0.83987700	2.37112500
C	-2.27373800	0.39901700	2.15005800
C	-1.23715800	0.42531400	1.19522800
C	-0.59231800	1.67222000	0.87860100
C	-0.95553200	2.86144700	1.54188500
C	-0.28540900	4.05211900	1.15504600
C	0.65972000	4.00534100	0.13996800
C	0.94952100	2.77198400	-0.49215100
H	1.66379300	2.68487800	-1.29759100
N	0.33985200	1.64776100	-0.11303000
C	2.39601200	-1.96405100	-2.39187400
H	2.38832900	-2.65965100	-3.23023100
C	2.50171200	-0.52903000	-2.92593400
O	2.02918800	0.39796200	-2.08205900
O	-0.77813700	-0.18310700	-2.50641800
H	-1.67468100	-0.68170100	-2.52001600
H	-0.41120300	0.10911200	-3.35924700
N	4.84855600	0.42125200	3.36820800
C	5.57471600	1.28784800	2.63444500
H	6.43843900	1.72665500	3.10959300
N	5.33692400	1.66263600	1.35887900
C	4.27246900	1.16026700	0.67598600
N	4.10352300	1.55138900	-0.60507700
H	4.81868200	2.15357500	-0.98910800
H	3.37521000	1.16382200	-1.21006100
C	3.41819200	0.25213700	1.36812800
N	2.24648700	-0.45530600	1.03382500
C	1.94332300	-1.16306200	2.11830100
H	1.09506200	-1.81739600	2.21296400
N	2.84130900	-0.96540400	3.14099400
H	2.83857100	-1.38752100	4.05783900
C	3.79128300	-0.06122500	2.68896100
N	-3.13040700	-1.07540700	-1.96142500
C	-3.88247900	-2.17303800	-1.73661800
H	-3.59177700	-3.08173800	-2.24217600
N	-4.97403600	-2.25163400	-0.94998200
C	-5.42112700	-1.13927200	-0.30247900
N	-6.52081300	-1.22121000	0.47404100
H	-7.02587100	-2.09421900	0.51657500
H	-6.89613200	-0.39114200	0.90905900
C	-4.69743800	0.06638800	-0.46719200
N	-4.87609000	1.34936400	0.05109300
C	-3.88753900	2.06372900	-0.46890900
H	-3.72631100	3.11215900	-0.29055300
N	-3.06459800	1.30652200	-1.29931100
H	-2.22109900	1.58820400	-1.78384400
C	-3.57429500	0.02628700	-1.30307600
C	-1.99573300	2.78167800	2.54050200
C	-2.63686300	1.61490000	2.83144600
N	1.20028100	-2.12329700	-1.50473300

H	0.37400000	-2.37312700	-2.04665700
H	1.37352100	-2.80447500	-0.76913900
O	3.03546500	-0.29777400	-4.01878100
H	3.29509100	-2.14723800	-1.79937800
H	-3.43500900	1.59521800	3.56216800
H	-3.74114100	-0.90004900	3.08239700
H	-0.51992200	4.98565200	1.64861500
Cl	-2.48295100	4.28406000	3.38035400
H	1.18051500	4.89678100	-0.17786000
H	-3.01463700	-2.91535800	1.78969100
A21A_sp			
Atom	X	Y	Z
Cu	0.70505900	-0.24009200	-0.80434400
N	-0.85191300	-0.64759400	0.51388000
C	-1.45347300	-1.80815900	0.79359000
H	-1.11778800	-2.68182400	0.25153600
C	-2.49318700	-1.91132600	1.74636700
C	-2.89838400	-0.77174600	2.42776700
C	-2.27370500	0.46709000	2.13854200
C	-1.26423100	0.48482600	1.15737600
C	-0.64917600	1.73272000	0.77773900
C	-1.01750100	2.95156400	1.38917200
C	-0.34398300	4.12398200	0.93547500
C	0.58438500	4.02429500	-0.09082100
C	0.86268600	2.76793500	-0.67656000
H	1.55897200	2.64300100	-1.49253500
N	0.26434700	1.66338500	-0.22967600
C	2.40981400	-2.00606200	-2.32181400
H	2.41638500	-2.74814700	-3.11929300
C	2.46501400	-0.60085600	-2.93599600
O	1.98639100	0.35800400	-2.13037200
O	-0.79992000	-0.37066200	-2.54944100
H	-1.71211100	-0.83539500	-2.51422700
H	-0.45543600	-0.13004700	-3.42745700
N	4.67842200	0.87054200	3.37341000
C	5.37193200	1.73040200	2.60091900
H	6.19007900	2.25662100	3.06809300
N	5.15349100	1.99845800	1.29512000
C	4.14512900	1.38203200	0.62053800
N	3.99860700	1.66494500	-0.69151700
H	4.69104600	2.27822500	-1.09922200
H	3.31059800	1.19548300	-1.28538500
C	3.32275000	0.47646300	1.35321300
N	2.20741600	-0.32469600	1.03771000
C	1.91875900	-0.97910900	2.15927700
H	1.11285000	-1.68187000	2.27567600
N	2.77115200	-0.65654400	3.18898000
H	2.77094600	-1.01979200	4.13088400
C	3.67493300	0.27635900	2.70144300
N	-3.17727200	-1.13826100	-1.90017900
C	-3.95182700	-2.19404500	-1.57119200
H	-3.70927600	-3.14300600	-2.02561100
N	-5.01117900	-2.18510200	-0.73805400
C	-5.39587400	-1.01933100	-0.14678700
N	-6.46243700	-1.01442800	0.67847900

H	-6.99571100	-1.86412900	0.79285700
H	-6.79968600	-0.14474400	1.06527200
C	-4.64309300	0.14868700	-0.42096100
N	-4.76442500	1.46958100	0.01238800
C	-3.78760600	2.11901700	-0.60623200
H	-3.59883100	3.17475100	-0.51985000
N	-3.02340900	1.28215300	-1.41589100
H	-2.19711600	1.50905500	-1.95548900
C	-3.56262700	0.01872400	-1.30302100
C	-2.03494100	2.86773500	2.41825300
C	-2.63970500	1.69828500	2.77673200
N	1.22547300	-2.15101600	-1.41575700
H	0.40512000	-2.45727200	-1.93728500
H	1.42693700	-2.78183200	-0.64342100
O	2.96527800	-0.41414200	-4.05236300
H	3.31861000	-2.12779100	-1.72833700
H	-3.40800800	1.70859100	3.53909900
H	-3.69082600	-0.81777200	3.16408900
H	-0.56721700	5.08362300	1.37278700
N	-2.52366400	4.07500900	3.10882000
O	-3.07067000	3.92365400	4.23163300
O	-2.39163400	5.18654700	2.52457700
H	-2.95988500	-2.86924200	1.92452600
H	1.09865100	4.90263700	-0.45255800
H	-3.40800800	1.70859100	3.53909900
H	-3.69082600	-0.81777200	3.16408900
H	-0.56721700	5.08362300	1.37278700
N	-2.52366400	4.07500900	3.10882000
O	-3.07067000	3.92365400	

A01A_sp				
1,2				
Cu	0	0.518299	0.04773	-0.492492
N	0	-0.978527	-0.284477	0.822151
C	0	-1.402338	-1.508754	1.183827
H	0	-0.847481	-2.338145	0.767736
C	0	-2.495628	-1.670089	2.044417
H	0	-2.83609	-2.660882	2.308615
C	0	-3.141147	-0.524852	2.529645
C	0	-2.681383	0.745863	2.154382
H	0	-3.183539	1.632561	2.511539
C	0	-1.588075	0.833495	1.288076
C	0	-1.018965	2.105692	0.780105
C	0	-1.430898	3.377079	1.190734
H	0	-2.199477	3.498396	1.94036
C	0	-0.818562	4.500851	0.617977
C	0	0.183471	4.329783	-0.347453
H	0	0.668359	5.178331	-0.808543
C	0	0.552722	3.027794	-0.708392
H	0	1.324578	2.804085	-1.432595
N	0	-0.043521	1.95896	-0.149412
C	0	2.621707	-3.681334	-0.610709
H	0	3.520567	-3.700011	0.014941
H	0	2.845664	-4.238783	-1.522496
H	0	1.797958	-4.158899	-0.081672

C	0	2.268657	-2.252611	-0.929043
O	0	1.193251	-1.775607	-0.360492
C	0	3.113614	-1.517877	-1.783878
H	0	3.974557	-2.029195	-2.190317
C	0	2.946889	-0.161037	-2.11065
O	0	1.959393	0.582701	-1.67889
C	0	3.961787	0.527245	-2.981227
H	0	3.4924	1.353446	-3.515617
H	0	4.418796	-0.16494	-3.688867
H	0	4.754984	0.926194	-2.339311
O	0	-0.759155	-0.31579	-2.278118
H	0	-1.503808	-1.015738	-2.160502
H	0	-0.199716	-0.42392	-3.065902
N	0	4.923816	-1.679648	1.238428
C	0	5.65809	-0.838469	0.487709
H	0	6.595196	-1.215432	0.106644
N	0	5.358646	0.447762	0.171383
C	0	4.197596	0.990179	0.612738
N	0	3.937311	2.296861	0.354489
H	0	4.638388	2.845542	-0.118769
H	0	3.099615	2.724753	0.714212
C	0	3.312355	0.167976	1.347204
N	0	2.052645	0.396004	1.914339
C	0	1.773495	-0.726782	2.567582
H	0	0.87462	-0.902986	3.130871
N	0	2.774578	-1.673575	2.451241
H	0	2.791983	-2.597503	2.855503
C	0	3.764617	-1.124039	1.654597
N	0	-2.952775	-1.46301	-1.605787
C	0	-3.633366	-2.546202	-1.180118
H	0	-3.22716	-3.513701	-1.432978
N	0	-4.780573	-2.544701	-0.470657
C	0	-5.36006	-1.361321	-0.125753
N	0	-6.509504	-1.368996	0.582157
H	0	-6.9432	-2.253952	0.799222
H	0	-6.977583	-0.501291	0.79745
C	0	-4.720703	-0.161611	-0.520533
N	0	-5.03029	1.185597	-0.324405
C	0	-4.054755	1.846608	-0.935424
H	0	-3.983955	2.9179	-0.99747
N	0	-3.117318	0.998864	-1.514417
H	0	-2.252217	1.216527	-2.000562
C	0	-3.53382	-0.287948	-1.253249
H	0	-1.118399	5.494333	0.92371
H	0	-3.996827	-0.616625	3.185098

A01C

1	2
Cu	-0.5696067216 0.2446811936 0.4800822725
N	0.8653847112 0.3046842308 -0.9451900364
C	1.3058583443 -0.7841994959 -1.6015765862
H	0.7945068564 -1.706987963 -1.3649542039
C	2.364181732 -0.6951424974 -2.5159129471
H	2.7173265581 -1.5827443093 -3.0206508447
C	2.9573834943 0.5540336346 -2.7377712809
C	2.4833385279 1.6828764855 -2.0525661782

H	2.9452740537	2.6462525798	-2.2094207936
C	1.4272644911	1.5230493157	-1.1518263506
C	0.8345647591	2.6202470012	-0.3458156671
C	1.2427321473	3.9566220965	-0.4023095407
H	2.0346924763	4.2686730048	-1.0678313886
C	0.6016205848	4.8924921236	0.4230987152
C	-0.4243528468	4.4750299887	1.2817224155
H	-0.9352971174	5.1739269024	1.9281023553
C	-0.7866805166	3.1220846571	1.2872203756
H	-1.5704900439	2.7172899904	1.913035675
N	-0.1652354876	2.234810926	0.4871309164
C	-1.7092182916	-3.8445724217	0.5795544814
H	-1.7996716346	-4.0010482328	-0.4986766232
H	-2.4956582716	-4.3921328461	1.0962170571
H	-0.736088924	-4.2383888899	0.886345639
C	-1.7639289939	-2.3676220902	0.8697582834
O	-0.9059743114	-1.6366017315	0.1883097583
C	-2.6999362475	-1.8630394046	1.7751114032
H	-3.4086179416	-2.5534096723	2.2074898615
C	-2.9100034571	-0.4853846544	2.0416206158
O	-2.1026582538	0.462239529	1.6513695749
C	-4.1385010872	-0.0763217394	2.7935298138
H	-4.0502742171	0.9519911425	3.1412109044
H	-4.3329831697	-0.7474591055	3.6322132844
H	-4.9845518024	-0.1618929868	2.1019674633
O	0.7485021401	-0.2010318993	2.2379601866
H	1.4435551978	-0.90205032	1.9477848036
H	0.191037871	-0.4548222244	2.9939701133
N	-4.7358368655	-2.4126636194	-1.651354211
C	-4.9014168879	-1.5117161671	-0.5691442937
N	-4.1212944887	-0.3718947634	-0.5972211241
C	-3.225786189	-0.1810490902	-1.5565701386
N	-2.4663133237	0.9599919452	-1.4721047038
H	-2.7328728869	1.6212074305	-0.7542571129
H	-1.891430721	1.2607994303	-2.2430314502
C	-3.028291568	-1.1038654846	-2.6484620654
C	-3.8280002694	-2.2101746271	-2.6559447655
N	2.8294790021	-1.2828251589	1.2068007359
C	3.4264817566	-2.2836626682	0.5299610338
H	2.9898290011	-3.2666786931	0.6185580705
N	4.5256002806	-2.1828000748	-0.2464753654
C	5.1390308837	-0.9762236283	-0.3951349526
N	6.2417724848	-0.8850928166	-1.1694610325
H	6.6229370763	-1.7262996964	-1.5763966899
H	6.7399440362	-0.010315611	-1.2395369001
C	4.5833496125	0.1450663013	0.2672261619
N	4.9437623782	1.4931182968	0.3145974389
C	4.0418633881	2.0537723975	1.111352044
H	4.028093881	3.0930249457	1.3872200691
N	3.1039572242	1.1415750614	1.5804202268
H	2.2847717553	1.2846368205	2.1648780552
C	3.4416107054	-0.0823019762	1.0457686749
H	0.8988893074	5.9322424792	0.3934448059
H	3.7846802716	0.6508941833	-3.4279842953
O	-5.7168136671	-1.7889240426	0.3333545524
H	-3.7812618871	-2.957630988	-3.4347202197

H	-2.298933628	-0.9286540633	-3.4234601315
H	-5.3463695206	-3.2201244577	-1.6387773887

A01G

1	2		
Cu	0.2109421318	-0.4920321741	-0.6361992258
N	-1.1553602467	-0.182565354	0.8375222314
C	-1.8331974948	-1.1641128842	1.4607772478
H	-1.569970769	-2.1716449299	1.1689158668
C	-2.8280539636	-0.8735964191	2.4020397494
H	-3.3748966456	-1.674662042	2.8783248838
C	-3.1097947814	0.469391268	2.6851474038
C	-2.3980998023	1.4831823924	2.0290428478
H	-2.6279040098	2.5202936193	2.2228845008
C	-1.4193636857	1.1222396244	1.0977138029
C	-0.6300421406	2.0902975727	0.2956964238
C	-0.6879122758	3.4770129162	0.4515115229
H	-1.3181267616	3.9285650365	1.2040032386
C	0.1006442425	4.2802568699	-0.3881457109
C	0.9200942929	3.6821907692	-1.3515023544
H	1.5448468207	4.2723336513	-2.0057890489
C	0.9353690793	2.2831862899	-1.4517325995
H	1.5642639566	1.7468582327	-2.1451990445
N	0.1720075443	1.528476487	-0.6431359372
C	1.0401786846	-4.6697291718	-0.3386424812
H	1.1280695571	-4.6691436134	0.7518023616
H	1.8189535948	-5.3018452717	-0.7616747723
H	0.0612981992	-5.087890206	-0.5860632886
C	1.1148938789	-3.2525618697	-0.847455431
O	0.1922073082	-2.4453681702	-0.3929770347
C	2.1316155319	-2.8883607192	-1.7489316442
H	2.853823546	-3.6435149018	-2.0212761674
C	2.233782671	-1.6279624659	-2.3813459867
O	1.4063359123	-0.644626165	-2.1814788546
C	3.330330497	-1.3655262044	-3.3776580376
H	2.8877158767	-1.1507123137	-4.3541492495
H	4.0146958471	-2.2074825209	-3.4706175522
H	3.8728577217	-0.4696746704	-3.0640261641
O	-1.4400297652	-0.6265858638	-2.251286246
H	-2.2342244662	-1.1767782047	-1.9535052928
H	-0.912900511	-0.9980162772	-2.9795251584
N	5.3549085378	-0.3934802603	2.3378896645
C	6.0314996792	0.3907282747	1.5116566016
N	5.4555802894	0.9540172364	0.3850162753
C	4.1059798307	0.7844129628	-0.0388090679
C	3.3831688651	-0.063250827	0.8668946425
N	2.0618858558	-0.5183923708	0.8587931874
C	1.9450619205	-1.2926154401	1.9260169971
H	1.0541649394	-1.8231917684	2.2086006814
N	3.131744752	-1.3633087585	2.6395082087
H	3.3096923147	-1.8844675999	3.4850301218
C	4.056953237	-0.5882421742	1.9763597963
N	-3.7363029286	-1.1761381263	-1.1174840839
C	-4.5960986009	-1.953198857	-0.4308492472
H	-4.479811613	-3.0215836063	-0.5313379523
N	-5.5997753814	-1.5341022158	0.3711456632

C	-5.8172926386	-0.2010878147	0.5346727681
N	-6.8243298937	0.2137515365	1.3363852707
H	-7.4311880698	-0.4759591442	1.7530967361
H	-7.031042901	1.1978148325	1.4184262296
C	-4.9653377599	0.7058745292	-0.1389823043
N	-4.9038879123	2.1000314933	-0.1727959852
C	-3.8860001072	2.3694565501	-0.9835155719
H	-3.5578175053	3.3586328719	-1.2479668317
N	-3.2775801862	1.2242610344	-1.4764705549
H	-2.4515092836	1.110678729	-2.062418107
C	-3.957219709	0.1523454031	-0.9401326331
H	0.0755733764	5.357032631	-0.2835351151
H	-3.8848886342	0.7270463505	3.3944953453
O	3.7240900405	1.3528619977	-1.0846047221
H	6.0019970983	1.5492226807	-0.2278921132
N	7.3397358956	0.6626594544	1.7633650933
H	7.9079348918	1.2488974052	1.17479014
H	7.7453327721	0.244497425	2.5863513962

C01G

1	2
Cu	-0.0356273439 -0.6981454003 0.5385371959
N	1.2960581312 -0.422778598 -0.9710376699
C	1.8155601699 -1.416338643 -1.7144140543
H	1.4674871605 -2.4117811419 -1.4795829355
C	2.7717966937 -1.1569126725 -2.7037824035
H	3.196414881 -1.9724612461 -3.2696803879
C	3.1827368216 0.1645675268 -2.9079668803
C	2.6458562791 1.1910420343 -2.1160814475
H	2.9718443927 2.2118887483 -2.253375848
C	1.7035150847 0.8609890215 -1.1384510446
C	1.1101445521 1.8319314648 -0.1852581087
C	1.3537457322 3.2073709701 -0.2021051491
H	1.9897331358 3.6517937249 -0.9540408622
C	0.744216786 4.0098021166 0.7759581138
C	-0.0871361189 3.4234052554 1.7363369249
H	-0.5800609377 4.0151959698 2.4937593627
C	-0.2957682974 2.0369954663 1.6925117215
H	-0.9501205962 1.5134400778 2.3719197718
N	0.2988619326 1.2827465332 0.7533161182
C	-1.4248455059 -4.6936704945 -0.0744324299
H	-1.5952871555 -4.5844229855 -1.1494539199
H	-2.2368072689 -5.2732950454 0.3613735174
H	-0.4836772144 -5.2341747277 0.0517777971
C	-1.2959974738 -3.3292780205 0.5534524972
O	-0.3092699153 -2.5991660639 0.1078215806
C	-2.208520448 -2.9282926674 1.5477202376
H	-3.0043476598 -3.6121257155 1.8027560765
C	-2.1156481902 -1.7275944854 2.286377566
O	-1.1804279507 -0.8389502767 2.121290666
C	-3.1177258668 -1.4222532894 3.3675714618
H	-2.6069444546 -1.3913473761 4.3339932038
H	-3.9187833171 -2.1587851884 3.4093698365
H	-3.5288690337 -0.4257578085 3.18587616
O	1.6852835116 -1.2700897306 1.9669105868
H	2.358032348 -1.8269104264 1.4588764265

H	1.2150572643	-1.7132447751	2.6928613123
N	-5.2694808064	0.344757769	-2.0421769789
C	-5.7762427668	1.143998854	-1.1152406901
N	-5.0518039205	1.5470319201	-0.0058800086
C	-3.7079634614	1.1798042035	0.295736566
C	-3.1722923422	0.3125279985	-0.7151725836
N	-1.9243473075	-0.3026784976	-0.8436862004
C	-1.984624835	-1.0017012115	-1.9659192058
H	-1.1923719524	-1.617443444	-2.3509858745
N	-3.2183338639	-0.8693701721	-2.5847938425
H	-3.5220172951	-1.2993103408	-3.4457210719
C	-3.9858880187	-0.0383639687	-1.7992904896
N	3.8262570238	0.2879034288	1.2746089942
C	4.317356776	-0.7669197024	0.4761304708
N	5.4315423924	-0.5354496009	-0.2750668264
C	6.0334402653	0.6599601644	-0.2417875622
N	7.1461881657	0.8100644041	-1.0045365955
H	7.4785363542	0.0036388196	-1.5131073405
H	7.6869111543	1.6591843486	-1.0022142898
C	5.5441197861	1.7572735324	0.5576653117
C	4.429305651	1.5117501552	1.310042127
H	0.9130655079	5.0787534536	0.7786912183
H	3.9275009387	0.3940394071	-3.658251815
O	3.6879951036	-1.8690663627	0.4926617873
H	6.0438579062	2.7127602345	0.5827469254
H	3.9869514234	2.256647667	1.9566464372
H	2.9790615357	0.068354742	1.8140858442
N	-7.0529485308	1.5956411618	-1.2422784157
H	-7.5671694071	1.2947232199	-2.0557361884
H	-7.497744166	2.1985778886	-0.570444168
H	-5.4698420836	2.1609280406	0.684567456
O	-3.1785234433	1.6243181989	1.3373168501

C01A

1	2		
Cu	-0.4225712679	0.8705879862	-0.0979065437
N	0.9825014015	0.0022787552	1.0931392678
C	1.5388447275	0.5952844878	2.1649953662
H	1.2203096288	1.6080721682	2.361089231
C	2.4840248082	-0.0731873319	2.9537098271
H	2.9357798475	0.4310752852	3.7948896826
C	2.8415934046	-1.3806751873	2.6090177603
C	2.2642750616	-1.9849655337	1.4814778207
H	2.5494076553	-2.9869297218	1.195627122
C	1.3367436389	-1.2567926045	0.7318304229
C	0.7152554699	-1.7421162767	-0.5250220712
C	0.9173359494	-3.0189579097	-1.0583386459
H	1.5114917051	-3.7520758847	-0.5327677936
C	0.3268750623	-3.3394148494	-2.2892007088
C	-0.4325448501	-2.3753680553	-2.9634714794
H	-0.8940769356	-2.5872834426	-3.9168924761
C	-0.6019682098	-1.1197797154	-2.3667337598
H	-1.1786608988	-0.3327617416	-2.8278594368
N	-0.0520789224	-0.8300245326	-1.1746085271
C	-0.9615577502	4.657955349	1.8262458857
H	-1.4551401273	4.3451986672	2.7503528124

H	-1.3925133992	5.6005425421	1.494016357
H	0.0979652663	4.7994817256	2.0523978204
C	-1.1102696466	3.5684008825	0.797831106
O	-0.549232804	2.4353910988	1.0829981621
C	-1.8460609242	3.8223501846	-0.3871818787
H	-2.2682961248	4.8093803779	-0.5032088507
C	-2.1488448334	2.8744208487	-1.3729660494
O	-1.7042819177	1.635772203	-1.3878462063
C	-3.0687562041	3.240145288	-2.5088332552
H	-2.6267967033	2.926466079	-3.4571936288
H	-3.2784747945	4.3078561087	-2.5393555149
H	-4.0153114438	2.7030680313	-2.3882815924
O	1.216815406	2.0611279245	-1.237687403
H	1.9650683649	2.2656355573	-0.5748811738
H	0.8412578923	2.8315752631	-1.6958106481
N	-4.7782165661	-2.5641185976	1.809262231
C	-5.3745329786	-2.6558134824	0.6052839496
H	-6.2186017995	-3.3235947103	0.5276633909
N	-5.0347912222	-1.9851797053	-0.521491318
C	-3.982976453	-1.1280321032	-0.5099001711
N	-3.7116344916	-0.4178774857	-1.6330003251
H	-4.3323779018	-0.5547433089	-2.4173198342
H	-3.0141039129	0.325067483	-1.6305460077
C	-3.237832868	-1.0083561702	0.6918270755
N	-2.1103871975	-0.2620941565	1.0679601251
C	-1.9438063351	-0.5070862808	2.3618291622
H	-1.1727721519	-0.0741869933	2.9732091384
N	-2.8880567825	-1.3842453494	2.8531511784
H	-2.982972454	-1.7185358209	3.800451592
C	-3.7222828638	-1.7261841137	1.7990948383
N	3.3226156763	0.2620895361	-1.3826537505
C	3.8689473854	0.8747709446	-0.2359812191
N	4.9834050462	0.3243159076	0.3164861722
C	5.5395171431	-0.7673127584	-0.2265895908
N	6.6562602299	-1.2498474242	0.3710893381
H	7.0278124017	-0.7363722118	1.1573249245
H	7.1637161429	-2.0382115518	0.0039642209
C	4.9939019247	-1.42030776	-1.3927906287
C	3.8774725879	-0.8542678958	-1.9411457673
H	0.4595411285	-4.3257842056	-2.7135428506
H	3.5732155579	-1.9195445609	3.1958274429
O	3.2781691531	1.9018871854	0.2257368273
H	5.4560634499	-2.2925827966	-1.8271583547
H	3.3972716645	-1.2507755161	-2.8246361276
H	2.4768656737	0.7065463464	-1.7569051441

G01G

1	2
Cu	0.3175193599 -0.1984987161 -0.7431949026
N	-1.0708473487 -0.3085997285 0.7375651069
C	-1.636181295 -1.4501616508 1.1723293782
H	-1.2866574264 -2.355896545 0.6946992683
C	-2.6202843799 -1.4378064005 2.1677732217
H	-3.0639678997 -2.3636616932 2.5055752123
C	-3.0252968238 -0.2052571614 2.6997109248

C	-2.4304701816	0.9759469049	2.2371680974
H	-2.7616723498	1.9308154081	2.6159213597
C	-1.4453967659	0.8920676023	1.2476122604
C	-0.7529333826	2.0633828074	0.6554100293
C	-0.9439313794	3.3833875798	1.0698268353
H	-1.6256870303	3.6221983801	1.8732076049
C	-0.2295320905	4.4009985313	0.4183986919
C	0.6518005628	4.0761051713	-0.6190961774
H	1.2220314616	4.835756753	-1.1334710459
C	0.8005473839	2.7299424347	-0.9828722412
H	1.4838581437	2.3955918025	-1.7484042308
N	0.1054779742	1.7676199728	-0.3525606913
C	1.5438088598	-4.2562092053	-1.2127162965
H	1.5537274942	-4.4483721702	-0.1361564554
H	2.4224346483	-4.7095376915	-1.668422205
H	0.6449017669	-4.7270066826	-1.6192493566
C	1.4783469161	-2.7692008685	-1.4550621622
O	0.454231922	-2.1579707367	-0.9158113934
C	2.4774879654	-2.1456961786	-2.2226691842
H	3.2866441207	-2.7601211825	-2.5883744038
C	2.4566274561	-0.7870292818	-2.616718194
O	1.5212257248	0.0499082674	-2.2761813877
C	3.5375589808	-0.2352678143	-3.5046473309
H	3.0937950213	0.1145959509	-4.4407751583
H	4.3089836574	-0.9717059448	-3.7251589355
H	3.974475185	0.6350655981	-3.007827857
O	-1.2719862993	-0.1208369386	-2.4518281657
H	-2.0068558084	-0.786924058	-2.3101018207
H	-0.6550064215	-0.3018695483	-3.181805217
N	5.3523188155	-0.1718186507	2.4060841515
C	5.9772801851	0.7914756626	1.7445056807
N	5.3889268345	1.4685028019	0.6890974665
C	4.0792839825	1.2430978983	0.1762203313
C	3.411191673	0.20213724	0.9057916001
N	2.1413941996	-0.3641655314	0.7639886904
C	2.0634419175	-1.3023637003	1.6943033449
H	1.2166651838	-1.9443513778	1.854656882
N	3.2260588366	-1.3756900854	2.4458534287
H	3.4231571609	-2.0010437378	3.2129157178
C	4.0937842893	-0.4258206496	1.9546507127
N	-3.5455399123	-1.0874475383	-1.4907267771
C	-4.2697667019	-2.0656584585	-0.9693764376
N	-5.212039977	-1.8411527381	0.010399864
C	-5.5141813141	-0.5767786388	0.6264575535
C	-4.7729405075	0.4832971628	-0.0009390469
N	-4.7722852571	1.8578606087	0.2293771121
C	-3.869880436	2.3450984076	-0.6109417266
H	-3.62473267	3.3859197079	-0.7194127924
N	-3.2712637353	1.3479440866	-1.3735310176
H	-2.4832092087	1.397742338	-2.0173500991
C	-3.8424814683	0.1612327943	-0.9920329734
H	-0.3599783175	5.431099877	0.7230319539
H	-3.8122271495	-0.1587676951	3.4404593831
O	-6.3075794833	-0.5552469008	1.5818684313
N	-4.0820765701	-3.3489359852	-1.3906746184
H	-4.6422543069	-4.1176709908	-1.0611828371

H	-3.4218001035	-3.5082473057	-2.1347153759
H	-5.7560530506	-2.6100401887	0.3871227778
N	7.2420861926	1.1395833463	2.1006690766
H	7.7710344562	1.8600434899	1.6379236923
H	7.6563037782	0.6386703453	2.8715463743
O	3.6813597595	1.9280151562	-0.7910731514
H	5.8956434856	2.1999939192	0.2025128121

T01C

1	2			
Cu	0	0.927849	0.399205	0.131595
N	0	-0.893241	-0.04714	-0.919822
C	0	-1.510219	0.780604	-1.784017
H	0	-1.05129	1.751669	-1.910771
C	0	-2.693324	0.414052	-2.442081
H	0	-3.174532	1.105405	-3.119986
C	0	-3.24897	-0.841731	-2.168083
C	0	-2.620061	-1.686395	-1.243335
H	0	-3.073452	-2.633189	-0.989574
C	0	-1.433635	-1.256315	-0.631655
C	0	-0.727729	-2.050233	0.41094
C	0	-1.088237	-3.366987	0.736302
H	0	-1.876794	-3.872697	0.199699
C	0	-0.426893	-4.014603	1.784913
C	0	0.576074	-3.33362	2.489901
H	0	1.098311	-3.795649	3.315901
C	0	0.896223	-2.029394	2.095194
H	0	1.657272	-1.451078	2.600105
N	0	0.267893	-1.413948	1.074582
C	0	1.302873	4.726942	-0.802468
H	0	1.536644	4.423236	-1.827448
H	0	2.007044	5.496203	-0.487859
H	0	0.289995	5.136938	-0.805604
C	0	1.33855	3.504479	0.089362
O	0	0.487707	2.569754	-0.1795
C	0	2.290759	3.459512	1.143506
H	0	2.907277	4.33699	1.279985
C	0	2.536824	2.371504	2.000711
O	0	1.908333	1.222039	1.972766
C	0	3.637929	2.496244	3.032043
H	0	3.256713	2.175069	4.004121
H	0	4.018984	3.514004	3.108465
H	0	4.463551	1.830795	2.759077
O	0	-0.81796	1.732768	2.109089
H	0	-0.666646	2.184687	1.246646
H	0	0.059726	1.398178	2.398454
N	0	5.800633	-0.886059	-2.289293
C	0	6.377738	-1.254831	-1.13191
N	0	5.810755	-1.186911	0.107721
C	0	4.536907	-0.702471	0.242998
C	0	3.836452	-0.31059	-0.919763
C	0	4.51877	-0.428384	-2.153812
N	0	-4.428829	1.60213	0.139818
C	0	-5.453967	1.383955	-0.723419
N	0	-6.138373	0.209737	-0.885752
C	0	-5.806819	-0.865888	-0.103235

C	0	-4.755339	-0.743051	0.839143
C	0	-4.103939	0.509992	0.900795
H	0	-0.696972	-5.027518	2.052948
H	0	-4.176168	-1.147601	-2.635432
O	0	-5.857773	2.450005	-1.517118
H	0	-3.207192	0.265458	1.443168
H	0	-3.650129	1.744217	-0.606719
C	0	-3.831987	-1.643833	1.688608
H	0	-2.880431	-1.741565	1.188181
H	0	-3.690022	-1.206016	2.658728
H	0	-4.273318	-2.61756	1.80311
H	0	-6.054993	-0.306259	-1.799869
O	0	-6.493443	-2.063199	-0.273865
O	0	7.690343	-1.757386	-1.193772
H	0	3.884694	-1.409173	0.75677
H	0	5.852328	-2.157543	0.586952
N	0	3.834067	-1.087804	-3.082714
H	0	4.449455	-1.462566	-3.783268
H	0	3.289429	-1.831978	-2.68545
H	0	2.79703	-0.555026	-1.022983
T01G				
1	2			
Cu	0	-0.244849	0.809841	-0.46302
N	0	1.127203	0.517782	1.006854
C	0	1.503787	1.453969	1.897358
H	0	1.061469	2.431517	1.764972
C	0	2.428645	1.161033	2.908433
H	0	2.720485	1.928063	3.611296
C	0	2.968736	-0.130017	2.973328
C	0	2.579557	-1.09175	2.02935
H	0	3.005752	-2.084071	2.060543
C	0	1.6504	-0.734633	1.047467
C	0	1.180529	-1.640602	-0.029415
C	0	1.587332	-2.968376	-0.175207
H	0	2.272952	-3.421831	0.526347
C	0	1.08619	-3.709031	-1.257717
C	0	0.199603	-3.108687	-2.15801
H	0	-0.210549	-3.654751	-2.994882
C	0	-0.175745	-1.773245	-1.948892
H	0	-0.882923	-1.253143	-2.57546
N	0	0.315172	-1.07671	-0.910181
C	0	-1.94166	4.597075	0.54304
H	0	-1.967112	4.393151	1.61693
H	0	-2.864056	5.092734	0.245795
H	0	-1.098299	5.268336	0.360985
C	0	-1.717219	3.311625	-0.210304
O	0	-0.64792	2.640689	0.129499
C	0	-2.629081	2.917358	-1.208333
H	0	-3.499727	3.536291	-1.365418
C	0	-2.444432	1.815419	-2.071347
O	0	-1.410754	1.022538	-2.027229
C	0	-3.450118	1.512792	-3.148108
H	0	-2.980698	1.637117	-4.128035
H	0	-4.327123	2.155352	-3.087726
H	0	-3.742777	0.463196	-3.061082

O	0	1.309747	1.726877	-2.036383
H	0	1.829994	2.428556	-1.568885
H	0	0.607479	2.036467	-2.634716
N	0	-5.218073	-1.127046	2.036149
C	0	-5.621847	-1.904422	1.041576
N	0	-4.87193	-2.087238	-0.109041
C	0	-3.606613	-1.494514	-0.385379
C	0	-3.181048	-0.65799	0.700865
N	0	-2.035853	0.122909	0.87661
C	0	-2.174194	0.699335	2.06049
H	0	-1.473602	1.387213	2.4978
N	0	-3.359306	0.326902	2.673904
H	0	-3.704307	0.625146	3.57426
C	0	-4.012471	-0.534354	1.819931
N	0	3.505126	0.316774	-1.383956
C	0	3.862533	1.313117	-0.505481
N	0	4.835776	0.962864	0.406175
C	0	5.409481	-0.312775	0.566199
C	0	5.018563	-1.302322	-0.441867
C	0	4.09188	-0.939983	-1.366004
H	0	1.384173	-4.740917	-1.389136
H	0	3.7015	-0.383349	3.727765
O	0	3.329071	2.455496	-0.505412
H	0	3.753559	-1.623198	-2.132421
H	0	2.715088	0.55003	-1.998056
C	0	5.671324	-2.652344	-0.380904
H	0	5.553209	-3.093106	0.612778
H	0	5.249334	-3.32845	-1.127413
H	0	6.7465	-2.567625	-0.55465
H	0	5.127837	1.684446	1.057013
O	0	6.179042	-0.534381	1.522566
O	0	-3.040003	-1.746641	-1.470666
N	0	-6.812321	-2.553189	1.137538
H	0	-7.346746	-2.409427	1.980551
H	0	-7.17831	-3.152576	0.416514
H	0	-5.211279	-2.688579	-0.851853
T01A				
1	2			
Cu	0	-0.594534	0.888505	-0.215857
N	0	0.87182	0.338531	1.090118
C	0	1.266724	1.069603	2.149591
H	0	0.818983	2.049171	2.236128
C	0	2.205206	0.571229	3.063881
H	0	2.512093	1.176639	3.904789
C	0	2.732711	-0.710107	2.858604
C	0	2.319821	-1.457777	1.745448
H	0	2.735703	-2.439425	1.570514
C	0	1.384055	-0.899741	0.869372
C	0	0.914385	-1.554879	-0.375864
C	0	1.326236	-2.822822	-0.79629
H	0	1.980947	-3.425968	-0.184043
C	0	0.878621	-3.302784	-2.035342
C	0	0.049349	-2.500351	-2.828545
H	0	-0.30209	-2.835482	-3.793579
C	0	-0.337996	-1.247074	-2.33827

H	0	-0.983999	-0.583469	-2.892844
N	0	0.07547	-0.805786	-1.136958
C	0	-1.92892	4.592465	1.469867
H	0	-2.306607	4.227497	2.429178
H	0	-2.586441	5.380214	1.107367
H	0	-0.93064	4.999986	1.644632
C	0	-1.83645	3.438725	0.507502
O	0	-0.978352	2.512732	0.810846
C	0	-2.669981	3.415435	-0.637468
H	0	-3.349647	4.243895	-0.768567
C	0	-2.729773	2.381431	-1.581249
O	0	-1.959053	1.313596	-1.576441
C	0	-3.744306	2.438003	-2.692929
H	0	-3.266797	2.187049	-3.642546
H	0	-4.215971	3.41608	-2.76858
H	0	-4.52255	1.691203	-2.503327
O	0	0.774932	2.278058	-1.570958
H	0	1.393464	2.780681	-0.971458
H	0	0.166365	2.828742	-2.09197
N	0	-4.442724	-2.946086	1.986081
C	0	-4.939368	-3.297333	0.784856
H	0	-5.658087	-4.101977	0.76889
N	0	-4.640783	-2.735338	-0.411059
C	0	-3.743797	-1.720413	-0.479186
N	0	-3.519798	-1.132737	-1.681676
H	0	-4.052763	-1.48237	-2.464616
H	0	-2.958064	-0.287412	-1.756259
C	0	-3.105784	-1.316231	0.722102
N	0	-2.136854	-0.349316	1.034392
C	0	-2.015016	-0.39033	2.356278
H	0	-1.362817	0.242243	2.931362
N	0	-2.83546	-1.339067	2.927207
H	0	-2.93277	-1.559228	3.907384
C	0	-3.53704	-1.952006	1.899398
N	0	3.063237	0.757103	-1.407448
C	0	3.428255	1.530411	-0.331216
N	0	4.427288	1.003983	0.453981
C	0	5.029047	-0.26171	0.302119
C	0	4.627352	-1.001906	-0.898212
C	0	3.672084	-0.458656	-1.69445
H	0	1.178317	-4.284763	-2.375941
H	0	3.471616	-1.116797	3.535802
O	0	2.871283	2.62989	-0.057077
H	0	3.32777	-0.952747	-2.592314
H	0	2.259049	1.104048	-1.937457
C	0	5.304411	-2.3145	-1.163571
H	0	5.194271	-2.985639	-0.30747
H	0	4.894517	-2.796817	-2.053167
H	0	6.377617	-2.170534	-1.307088
H	0	4.730161	1.565332	1.243572
O	0	5.828126	-0.677765	1.162435