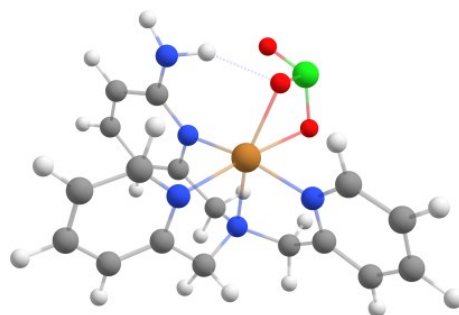


## XYZ coordinates

**<sup>2</sup>1b<sup>+</sup>**

N	-2.146585000	-1.502003000	-1.825005000
C	-2.488948000	-1.197328000	-0.539639000
N	-1.514787000	-0.752328000	0.282147000
C	-1.808617000	-0.378998000	1.552574000
C	-0.614757000	0.008633000	2.391768000
N	0.379665000	0.753567000	1.585262000
C	0.025079000	2.176655000	1.367326000
C	-0.855871000	2.414054000	0.154605000
C	-1.833828000	3.405961000	0.149052000
C	-2.556743000	3.632608000	-1.024299000
C	-2.281819000	2.857016000	-2.149696000
C	-1.296967000	1.875112000	-2.054120000
N	-0.597560000	1.663322000	-0.930484000
Cu	0.349101000	-0.241602000	-0.276884000
O	0.703292000	-1.816990000	-1.462174000
Cl	0.962666000	-3.072836000	-0.438899000
O	-0.345226000	-3.795974000	-0.316018000
O	1.331534000	-2.369969000	0.867358000
C	1.774424000	0.596733000	2.054149000
C	2.728681000	0.761687000	0.892491000
N	2.257413000	0.357663000	-0.304566000
C	3.050668000	0.372898000	-1.384883000
C	4.367732000	0.817372000	-1.318691000
C	4.863759000	1.255017000	-0.089900000
C	4.032756000	1.227905000	1.031808000
C	-3.094298000	-0.418416000	2.052945000
C	-4.119542000	-0.880729000	1.207259000
C	-3.825315000	-1.271786000	-0.082234000
H	-2.823456000	-2.041404000	-2.349842000
H	-1.178789000	-1.795225000	-1.966187000
H	-0.130801000	-0.912455000	2.731465000
H	-0.924348000	0.580528000	3.275776000
H	-0.444243000	2.593768000	2.267159000
H	0.960287000	2.724574000	1.208128000
H	-2.027051000	3.989310000	1.044361000
H	-3.325605000	4.398767000	-1.054450000
H	-2.822569000	2.996983000	-3.079680000
H	-1.065330000	1.226327000	-2.892796000
H	1.883889000	-0.422408000	2.436959000
H	2.014154000	1.293410000	2.868060000
H	2.608391000	0.006494000	-2.305305000
H	4.985066000	0.817196000	-2.210371000
H	5.885527000	1.611909000	-0.003919000
H	4.392178000	1.555059000	2.002502000
H	-3.299391000	-0.112340000	3.072896000
H	-5.141736000	-0.933371000	1.569692000
H	-4.597601000	-1.636928000	-0.751437000



### Color code

White: Hydrogen

Grey: Carbon

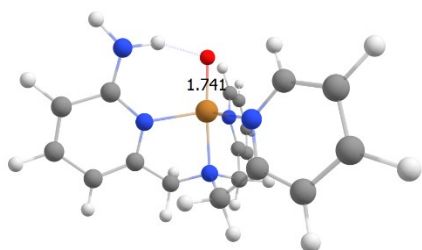
Blue: Nitrogen

Red: Oxygen

Green: Chloride

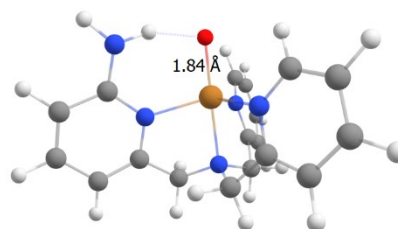
Orange: Copper

**<sup>1</sup>2b<sup>+</sup>**



C	3.954133000	-1.704489000	0.534327000
C	4.043372000	-2.080511000	-0.785554000
C	2.943248000	-1.901618000	-1.654004000
C	1.792865000	-1.357649000	-1.124670000
N	1.695347000	-0.967894000	0.172265000
C	2.746929000	-1.124106000	1.019107000
N	-0.030790000	1.982117000	0.360435000
C	-0.216346000	2.866180000	1.345532000
C	-0.270594000	4.234763000	1.084715000
C	-0.138983000	4.670688000	-0.234484000
C	0.051846000	3.734166000	-1.255652000
C	0.109407000	2.386122000	-0.915813000
N	-1.872283000	-0.952556000	0.444651000
C	-2.411566000	-0.931704000	-0.788817000
C	-3.596881000	-1.604727000	-1.065975000
C	-4.231520000	-2.292101000	-0.026240000
C	-3.666853000	-2.286143000	1.249979000
C	-2.469324000	-1.601258000	1.449815000
C	0.518279000	-1.195108000	-1.917518000
N	-0.227035000	0.002642000	-1.445727000
C	-1.673180000	-0.063374000	-1.783029000
C	0.399485000	1.273637000	-1.899506000
N	2.583699000	-0.692125000	2.276199000
Cu	-0.067379000	-0.058085000	0.583908000
O	-0.034558000	-0.075995000	2.324569000
H	4.787889000	-1.834838000	1.216680000
H	4.964075000	-2.515974000	-1.162260000
H	2.994633000	-2.190501000	-2.697915000
H	-0.314715000	2.428939000	2.335887000
H	-0.418025000	4.937434000	1.897804000
H	-0.185595000	5.729497000	-0.470679000
H	0.157780000	4.047698000	-2.289754000
H	-4.019001000	-1.588508000	-2.066121000
H	-5.158316000	-2.825535000	-0.214644000
H	-4.138416000	-2.806130000	2.076850000
H	-1.947561000	-1.535294000	2.401317000
H	0.714899000	-1.134662000	-2.995484000
H	-0.129873000	-2.061657000	-1.744339000
H	-1.817127000	-0.408044000	-2.815017000
H	-2.069547000	0.956192000	-1.718110000
H	0.071451000	1.528636000	-2.915162000
H	1.481304000	1.105573000	-1.935194000
H	1.610819000	-0.409211000	2.551027000
H	3.297300000	-0.873085000	2.967164000

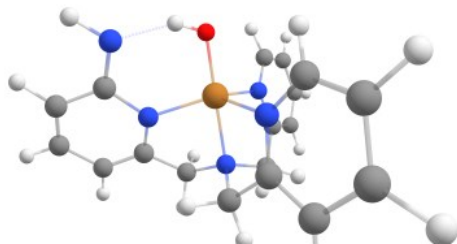
**<sup>3</sup>2b<sup>+</sup>**



C	4.028082000	-1.676727000	0.430748000
C	4.065885000	-2.057323000	-0.892648000
C	2.928403000	-1.891797000	-1.708614000
C	1.793447000	-1.361266000	-1.128314000
N	1.740415000	-0.979477000	0.170223000
C	2.833943000	-1.116476000	0.958041000
N	-0.069684000	2.028447000	0.382678000
C	-0.286498000	2.970058000	1.313617000
C	-0.355967000	4.323645000	0.992905000
C	-0.205007000	4.701673000	-0.341668000
C	0.015817000	3.718092000	-1.308155000
C	0.085687000	2.386270000	-0.906520000
N	-1.911806000	-0.986522000	0.470221000
C	-2.418047000	-0.949184000	-0.775714000
C	-3.582254000	-1.635021000	-1.111574000
C	-4.242023000	-2.361465000	-0.117040000
C	-3.718590000	-2.380148000	1.176347000
C	-2.541782000	-1.678523000	1.429908000
C	0.494677000	-1.202670000	-1.885525000
N	-0.234629000	-0.002200000	-1.419060000
C	-1.674651000	-0.056005000	-1.746209000
C	0.398945000	1.256440000	-1.864871000
N	2.744928000	-0.679279000	2.231954000
Cu	-0.057285000	-0.045104000	0.694637000
O	0.023627000	-0.109560000	2.532287000
H	4.894913000	-1.787010000	1.074422000
H	4.975804000	-2.479939000	-1.308229000
H	2.937269000	-2.177877000	-2.754684000
H	-0.404546000	2.612226000	2.331679000
H	-0.530146000	5.057837000	1.772120000
H	-0.261511000	5.747254000	-0.628877000
H	0.134779000	3.980166000	-2.355135000
H	-3.966988000	-1.598980000	-2.126339000
H	-5.152181000	-2.905229000	-0.351432000
H	-4.205741000	-2.930129000	1.974364000
H	-2.076209000	-1.645577000	2.410348000
H	0.670457000	-1.166116000	-2.969231000
H	-0.148743000	-2.066891000	-1.684287000
H	-1.834791000	-0.374877000	-2.785288000
H	-2.070919000	0.961778000	-1.653633000
H	0.101005000	1.512811000	-2.890635000
H	1.482264000	1.092919000	-1.871948000
H	1.827271000	-0.383825000	2.593647000
H	3.495291000	-0.868267000	2.879979000

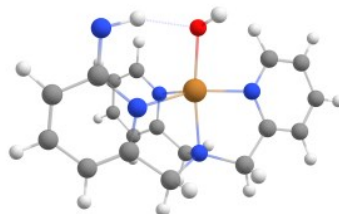
13b'+

33b'+



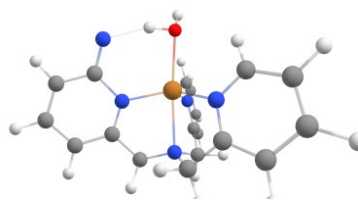
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C	-1.770540298	-0.387330906	2.840047209
N	-1.654101298	0.249610094	1.644152209
C	-2.718502298	0.305686094	0.742239209
N	0.664032702	2.667007094	1.386020209
C	1.060125702	3.539035094	0.452469209
C	1.282848702	4.884095094	0.746284209
C	1.091053702	5.320403094	2.057770209
C	0.676726702	4.406167094	3.030318209
C	0.464521702	3.083959094	2.647472209
N	2.027158702	-0.352793906	1.315323209
C	2.545223702	-0.393868906	2.557980209
C	3.699883702	-1.120327906	2.830426209
C	4.326753702	-1.797734906	1.780728209
C	3.780150702	-1.736489906	0.498049209
C	2.611299702	-1.004574906	0.301819209
C	-0.502162298	-0.404592906	3.661737209
N	0.405073702	0.674360094	3.188758209
C	1.825914702	0.457174094	3.576688209
C	-0.071528298	2.027553094	3.589186209
N	-2.494579298	0.848848094	-0.423779791
Cu	0.223741702	0.515390094	1.192712209
O	0.131918702	0.227465094	-0.566547791
H	-4.797020298	-0.284951906	0.484522209
H	-5.019850298	-1.319692906	2.721112209
H	-3.038959298	-1.332896906	4.285877209
H	1.190252702	3.133175094	-0.546826791
H	1.599952702	5.567508094	-0.034221791
H	1.261519702	6.359301094	2.323487209
H	0.516636702	4.717643094	4.058294209
H	4.102375702	-1.154336906	3.838153209
H	5.229919702	-2.370921906	1.966697209
H	4.240309702	-2.253558906	-0.336877791
H	2.100535702	-0.921078906	-0.653362791
H	-0.707600298	-0.294624906	4.734648209
H	0.022487702	-1.356188906	3.517772209
H	1.884395702	0.026322094	4.583673209
H	2.308899702	1.439335094	3.611710209
H	0.209919702	2.228177094	4.630663209
H	-1.163452298	2.017802094	3.532621209
H	-3.338450298	0.876498094	-0.994905791
H	-0.797687298	0.490703094	-0.817035791

C	3.809343000	-1.915855000	-0.071845000
C	4.108613000	-1.420562000	1.186626000
C	3.081140000	-0.865531000	1.951815000
C	1.774733000	-0.825859000	1.422051000
N	1.473767000	-1.285383000	0.214489000
C	2.468705000	-1.847616000	-0.567373000
N	-2.422405000	-0.523065000	-0.271225000
C	-3.270038000	-0.633793000	-1.303749000
C	-4.635447000	-0.399917000	-1.145735000
C	-5.113936000	-0.035223000	0.112890000
C	-4.218945000	0.077615000	1.181357000
C	-2.872418000	-0.184784000	0.950073000
N	0.540713000	1.358810000	-0.823028000
C	0.559003000	2.112519000	0.286301000
C	1.378213000	3.232736000	0.402600000
C	2.184721000	3.581834000	-0.685806000
C	2.146459000	2.802742000	-1.842538000
C	1.309002000	1.685834000	-1.866417000
C	0.634107000	-0.315174000	2.282563000
N	-0.502007000	0.214730000	1.503699000
C	-0.432973000	1.691012000	1.346880000
C	-1.823587000	-0.191679000	2.041874000
N	2.089770000	-2.301970000	-1.759018000
Cu	-0.402177000	-0.603403000	-0.518928000
O	-0.541178000	-1.176821000	-2.270255000
H	4.576851000	-2.359501000	-0.698379000
H	5.122834000	-1.461934000	1.571462000
H	3.274107000	-0.467095000	2.942899000
H	-2.803508000	-0.914831000	-2.243583000
H	-5.302968000	-0.497745000	-1.995232000
H	-6.170842000	0.162342000	0.264867000
H	-4.562135000	0.358613000	2.172572000
H	1.381085000	3.824819000	1.313174000
H	2.831385000	4.452395000	-0.628448000
H	2.753410000	3.049055000	-2.707592000
H	1.232921000	1.024592000	-2.725656000
H	0.281321000	-1.163806000	2.880151000
H	1.008668000	0.432057000	2.993527000
H	-0.216412000	2.171755000	2.310374000
H	-1.427238000	2.026253000	1.031226000
H	-2.128849000	0.439800000	2.887365000
H	-1.728273000	-1.216347000	2.416474000
H	0.199883000	-1.778076000	-2.460148000
H	2.891267000	-2.700717000	-2.257928000

**13b<sup>+</sup>****33b<sup>+</sup>**

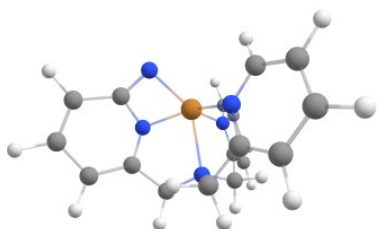
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C	1.667700000	-0.331070000	1.641540000
N	1.348625000	-1.280572000	0.720752000
C	2.394681000	-1.802999000	-0.085821000
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C	-4.467977000	-0.324931000	-1.347540000
C	-5.007096000	0.440157000	-0.313302000
C	-4.212759000	0.756822000	0.793033000
C	-2.905507000	0.285909000	0.832454000
N	0.545409000	0.853451000	-1.151615000
C	0.689191000	1.884012000	-0.304971000
C	1.640628000	2.881531000	-0.500534000
C	2.467141000	2.800229000	-1.624897000
C	2.317839000	1.727374000	-2.503130000
C	1.343703000	0.767927000	-2.223045000
C	0.483348000	0.178282000	2.416239000
N	-0.566212000	0.583478000	1.440932000
C	-0.309059000	1.922243000	0.834116000
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N	2.206354000	-2.629779000	-1.065574000
Cu	-0.449305000	-0.873490000	-0.040670000
O	-0.559414000	-2.244471000	-1.316400000
H	4.515087000	-1.761441000	-0.486926000
H	5.049150000	-0.105385000	1.326579000
H	3.140424000	0.776976000	2.721898000
H	-2.645247000	-1.350267000	-2.003947000
H	-5.053970000	-0.584054000	-2.222671000
H	-6.031926000	0.794599000	-0.367017000
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H	1.736077000	3.701418000	0.205314000
H	3.220670000	3.560975000	-1.805475000
H	2.946054000	1.625004000	-3.381663000
H	1.198256000	-0.101515000	-2.857587000
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H	0.750908000	1.004062000	3.085957000
H	0.005390000	2.627241000	1.613063000
H	-1.264312000	2.278181000	0.434473000
H	-2.207962000	1.404175000	2.556867000
H	-1.996667000	-0.348821000	2.659939000
H	-0.976156000	-3.045997000	-0.955304000
H	1.196787000	-2.756430000	-1.239595000

C	-3.886490000	-1.508182000	0.417933000
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C	-3.062595000	-1.174303000	-1.807075000
C	-1.765042000	-1.085301000	-1.278215000
N	-1.505041000	-1.201794000	0.023097000
C	-2.553048000	-1.388807000	0.920031000
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C	3.250702000	-0.236589000	1.403207000
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C	2.893248000	-0.298239000	-0.900848000
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C	-0.578294000	1.895316000	-0.621793000
C	-1.517302000	2.875478000	-0.930297000
C	-2.296043000	3.401750000	0.105966000
C	-2.112156000	2.927233000	1.403695000
C	-1.155811000	1.932765000	1.619752000
C	-0.569453000	-0.909771000	-2.191531000
N	0.525191000	-0.167021000	-1.529512000
C	0.368577000	1.311321000	-1.647933000
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N	-2.357905000	-1.439359000	2.230987000
Cu	0.430275000	-0.662755000	0.545782000
O	0.457343000	-1.134202000	2.360373000
H	-4.674358000	-1.670211000	1.144628000
H	-5.147559000	-1.481148000	-1.325312000
H	-3.217720000	-1.067909000	-2.876089000
H	2.783996000	-0.344544000	2.377656000
H	5.235618000	0.230083000	2.087078000
H	6.126009000	0.475159000	-0.247186000
H	4.570656000	0.137419000	-2.178869000
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H	-3.037564000	4.167219000	-0.102346000
H	-2.700382000	3.306635000	2.232564000
H	-0.984467000	1.505564000	2.603995000
H	-0.194547000	-1.906415000	-2.448879000
H	-0.868280000	-0.425767000	-3.130302000
H	0.061086000	1.576456000	-2.667678000
H	1.357429000	1.750146000	-1.478787000
H	2.153840000	-0.103069000	-2.928391000
H	1.849435000	-1.665727000	-2.160928000
H	0.787750000	-2.032168000	2.524350000
H	-1.344589000	-1.331933000	2.445716000

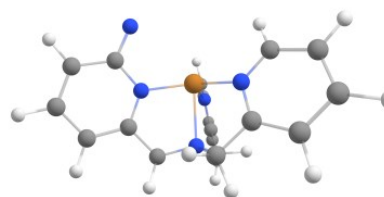
**<sup>1</sup>4b<sup>+</sup>****<sup>3</sup>4b<sup>+</sup>**

C	3.407941197	1.462998352	-1.670273421
C	3.673270197	1.401111352	-3.027152421
C	2.701838197	0.831686352	-3.856961421
C	1.478679197	0.362544352	-3.328796421
N	1.138001197	0.565846352	-2.059369421
C	2.099773197	1.120460352	-1.163420421
N	-2.364966803	0.917135352	-1.785641421
C	-3.232718803	1.255280352	-0.817174421
C	-4.450072803	1.873642352	-1.092497421
C	-4.776436803	2.145019352	-2.420483421
C	-3.869956803	1.797314352	-3.423912421
C	-2.665638803	1.191529352	-3.072353421
N	-0.890413803	-2.144759648	-1.635437421
C	-1.228489803	-2.611733648	-2.852994421
C	-1.275850803	-3.979213648	-3.124288421
C	-0.982971803	-4.887657648	-2.106578421
C	-0.642080803	-4.399311648	-0.845262421
C	-0.604073803	-3.020003648	-0.658490421
C	0.510070197	-0.386006648	-4.242258421
N	-0.865991803	-0.345228648	-3.783611421
C	-1.615551803	-1.588576648	-3.910339421
C	-1.604411803	0.869877352	-4.110999421
N	1.796355197	1.360571352	0.068267579
Cu	-0.625364803	-0.066600648	-1.446663421
O	-0.610871803	0.380937352	0.785905579
H	4.139624197	1.802332352	-0.945481421
H	4.626638197	1.723470352	-3.434681421
H	2.884644197	0.730859352	-4.923542421
H	-2.914618803	1.025571352	0.193821579
H	-5.121799803	2.131043352	-0.280502421
H	-5.719898803	2.618949352	-2.673983421
H	-4.090784803	1.996926352	-4.468235421
H	-1.541173803	-4.324473648	-4.119307421
H	-1.016324803	-5.956096648	-2.297184421
H	-0.403519803	-5.066968648	-0.024125421
H	-0.334126803	-2.587252648	0.300121579
H	0.619364197	-0.004594648	-5.270917421
H	0.831798197	-1.434564648	-4.266045421
H	-1.520771803	-2.037577648	-4.911609421
H	-2.676531803	-1.348370648	-3.774066421
H	-2.062479803	0.827397352	-5.112277421
H	-0.884920803	1.697804352	-4.125699421
H	0.242051197	0.907261352	0.687177579
H	-0.533121803	-0.138506648	1.601388579

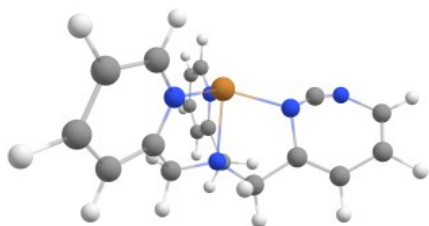
C	4.058077000	1.544866000	-0.540465000
C	4.197140000	1.823508000	0.800711000
C	3.086281000	1.678153000	1.655556000
C	1.862539000	1.256844000	1.135974000
N	1.694411000	0.972879000	-0.170389000
C	2.777470000	1.114298000	-1.022081000
N	-0.086503000	-1.967305000	-1.327531000
C	-0.324955000	-2.881872000	-1.282365000
C	-0.500094000	-4.233905000	-0.996692000
C	-0.433251000	-4.648169000	0.333125000
C	-0.184457000	-3.697226000	1.324077000
C	-0.006162000	-2.363821000	0.958820000
N	-1.817226000	1.005200000	-0.418052000
C	-2.304422000	1.035823000	0.840325000
C	-3.420692000	1.803589000	1.171081000
C	-4.061630000	2.544508000	0.177828000
C	-3.559064000	2.502766000	-1.122535000
C	-2.432050000	1.724934000	-1.371637000
C	0.626871000	1.146624000	2.018278000
N	-0.198294000	0.002332000	1.650513000
C	-1.630303000	0.149981000	1.877529000
C	0.352092000	-1.304341000	1.990905000
N	2.579303000	0.827556000	-2.294280000
Cu	-0.000322000	0.073100000	-0.670968000
O	0.054879000	-0.200090000	-3.086984000
H	4.878871000	1.632702000	-1.243321000
H	5.152923000	2.150238000	1.198519000
H	3.172155000	1.897888000	2.714890000
H	-0.367178000	-2.496524000	-2.295857000
H	-0.689708000	-4.938023000	-1.800000000
H	-0.574032000	-5.692055000	0.596909000
H	-0.125518000	-3.984468000	2.369830000
H	-3.781439000	1.817506000	2.195327000
H	-4.933003000	3.146556000	0.416943000
H	-4.020760000	3.065006000	-1.927287000
H	-1.991008000	1.669230000	-2.361701000
H	0.928745000	1.134631000	3.077653000
H	0.023025000	2.049965000	1.867638000
H	-1.862027000	0.522726000	2.887942000
H	-2.076879000	-0.848913000	1.802746000
H	0.048908000	-1.643687000	2.993979000
H	1.444563000	-1.208115000	2.010083000
H	0.970995000	0.107419000	-3.241378000
H	-0.450487000	0.034722000	-3.881389000

**15b<sup>+</sup>**

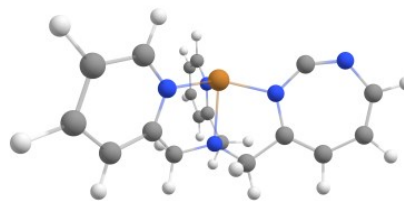
C	-3.089682000	-2.490949000	-1.088016000
C	-3.297729000	-2.973818000	0.175458000
C	-2.400531000	-2.647941000	1.257752000
C	-1.216101000	-2.015052000	0.977125000
N	-0.851807000	-1.863610000	-0.336857000
C	-1.876179000	-1.735913000	-1.276878000
N	-0.610807000	1.795060000	-0.474410000
C	-0.674406000	2.749419000	-1.415543000
C	-0.991299000	4.070113000	-1.110620000
C	-1.247299000	4.403149000	0.219017000
C	-1.188618000	3.405212000	1.193956000
C	-0.877412000	2.101214000	0.816459000
N	1.982065000	-0.279316000	-0.548200000
C	2.458429000	-0.178411000	0.706463000
C	3.776831000	-0.504186000	1.019537000
C	4.628644000	-0.934394000	0.000844000
C	4.132538000	-1.033273000	-1.298896000
C	2.799205000	-0.701001000	-1.526415000
C	-0.200213000	-1.437171000	1.933881000
N	0.120038000	-0.058408000	1.481728000
C	1.498330000	0.362527000	1.751332000
C	-0.894091000	0.951277000	1.810164000
N	-1.531574000	-0.706113000	-2.006966000
Cu	-0.154504000	-0.136225000	-0.773156000
H	-3.833540000	-2.562559000	-1.873927000
H	-4.210365000	-3.516230000	0.403817000
H	-2.662383000	-2.913753000	2.277126000
H	-0.472652000	2.430082000	-2.432894000
H	-1.033828000	4.812860000	-1.899770000
H	-1.491248000	5.424274000	0.495777000
H	-1.388480000	3.632963000	2.236421000
H	4.128824000	-0.422551000	2.043625000
H	5.659480000	-1.194738000	0.221147000
H	4.756901000	-1.369316000	-2.119805000
H	2.360176000	-0.778589000	-2.516870000
H	-0.551389000	-1.461477000	2.973847000
H	0.728137000	-2.015320000	1.876054000
H	1.527916000	1.457540000	1.709467000
H	1.826955000	0.073687000	2.759537000
H	-1.874148000	0.460788000	1.751507000
H	-0.787633000	1.334744000	2.835699000

**35b<sup>+</sup>**

C	4.251458560	-1.047798697	1.029789181
C	4.578685560	-0.914765697	2.368582181
C	3.620594560	-0.423375697	3.267789181
C	2.349283560	-0.063848697	2.797719181
N	2.013695560	-0.189888697	1.509033181
C	2.938349560	-0.678418697	0.614406181
N	-1.289844440	-1.267158697	1.267079181
C	-2.080564440	-1.781208697	0.308701181
C	-3.124170440	-2.660793697	0.584019181
C	-3.363603440	-3.014716697	1.911017181
C	-2.544984440	-2.481806697	2.907998181
C	-1.509666440	-1.618608697	2.554445181
N	-0.530234440	2.105949303	1.215266181
C	-0.885349440	2.450831303	2.474009181
C	-1.163067440	3.772859303	2.816994181
C	-1.092951440	4.764757303	1.837526181
C	-0.736635440	4.403209303	0.539162181
C	-0.458787440	3.064555303	0.275021181
C	1.303272560	0.546583303	3.725472181
N	-0.060246440	0.256830303	3.293315181
C	-1.032166440	1.329800303	3.493694181
C	-0.539652440	-1.088914697	3.601603181
N	2.529105560	-0.787614697	-0.648023819
Cu	0.119538560	0.177282303	1.036814181
H	4.952329560	-1.426387697	0.294165181
H	5.566920560	-1.192517697	2.721827181
H	3.854407560	-0.316091697	4.322384181
H	-1.860726440	-1.471011697	-0.707941819
H	-3.732710440	-3.049500697	-0.225492819
H	-4.173725440	-3.690376697	2.167842181
H	-2.703702440	-2.735049697	3.951990181
H	-1.433773440	4.019511303	3.839331181
H	-1.308095440	5.799424303	2.086497181
H	-0.666378440	5.138262303	-0.255530819
H	-0.165033440	2.737835303	-0.717663819
H	1.496091560	0.227239303	4.761386181
H	1.435920560	1.635058303	3.701088181
H	-2.029681440	0.891506303	3.369454181
H	-0.995608440	1.747342303	4.511731181
H	0.334464560	-1.751515697	3.614647181
H	-1.000579440	-1.153544697	4.599692181

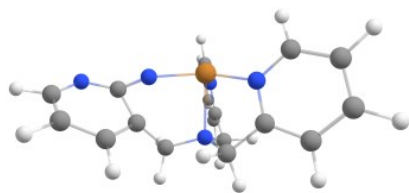
**16b<sup>+</sup>**

C	-4.062811000	-2.508905000	-0.765728000
C	-3.478527000	-3.125359000	0.284955000
C	-2.390877000	-2.601787000	1.127459000
C	-1.371161000	-1.791249000	0.755973000
N	-3.668622000	-1.154130000	-1.120625000
C	-2.443402000	-1.131461000	-1.009655000
N	-0.409896000	1.982241000	-0.513255000
C	-0.462078000	3.010333000	-1.381216000
C	-0.753915000	4.313788000	-0.992064000
C	-0.988431000	4.568118000	0.358908000
C	-0.930191000	3.507013000	1.262314000
C	-0.649600000	2.223139000	0.796918000
N	2.152008000	-0.542511000	-0.650600000
C	2.569983000	-0.480711000	0.635728000
C	3.807735000	-0.987478000	1.025208000
C	4.646310000	-1.560661000	0.067782000
C	4.214629000	-1.616735000	-1.256546000
C	2.960657000	-1.099351000	-1.569978000
C	-0.212949000	-1.390994000	1.641481000
N	0.240600000	-0.032472000	1.345688000
C	1.654095000	0.214475000	1.632932000
C	-0.675324000	1.033220000	1.746888000
N	-1.266416000	-1.327055000	-0.622332000
Cu	0.265525000	0.117337000	-0.901069000
H	-4.862500000	-2.936750000	-1.359241000
H	-3.887696000	-4.088050000	0.580975000
H	-2.374024000	-2.966255000	2.152190000
H	-0.260902000	2.767812000	-2.419696000
H	-0.787863000	5.105431000	-1.732893000
H	-1.209608000	5.573270000	0.704560000
H	-1.105065000	3.668985000	2.321766000
H	4.109343000	-0.931799000	2.066843000
H	5.614569000	-1.960075000	0.353520000
H	4.828803000	-2.056130000	-2.035280000
H	2.579701000	-1.128639000	-2.585722000
H	-0.479641000	-1.536254000	2.699270000
H	0.628035000	-2.061415000	1.423155000
H	1.932017000	-0.076312000	2.657922000
H	1.818616000	1.296045000	1.552912000
H	-0.493193000	1.378399000	2.776124000
H	-1.689381000	0.614093000	1.734307000

**36b<sup>+</sup>**

C	-3.692478286	-1.184018357	-0.993080943
C	-3.462843286	-1.359336357	0.346940057
C	-2.193459286	-1.421400357	1.018501057
C	-0.927228286	-1.318761357	0.496039057
N	-2.744997286	-1.060417357	-1.985491943
C	-1.482444286	-1.064515357	-1.811606943
N	1.846964714	1.352497643	-0.892100943
C	2.360385714	2.184426643	-1.815243943
C	2.841709714	3.453105643	-1.503338943
C	2.797836714	3.872953643	-0.174624943
C	2.268064714	3.010731643	0.786404057
C	1.791428714	1.760680643	0.395917057
N	2.796240714	-1.969657357	-0.907434943
C	3.188406714	-2.113206357	0.379030057
C	4.048175714	-3.138387357	0.769234057
C	4.533491714	-4.028619357	-0.189734943
C	4.134673714	-3.870907357	-1.516304943
C	3.261473714	-2.832436357	-1.828300943
C	0.273325714	-1.492826357	1.417788057
N	1.362958714	-0.580888357	1.082147057
C	2.706898714	-1.072718357	1.380478057
C	1.129496714	0.826253643	1.399355057
N	-0.581240286	-1.115963357	-0.838587943
Cu	1.307529714	-0.600854357	-1.161358943
H	-4.717589286	-1.142406357	-1.350348943
H	-4.341300286	-1.455944357	0.979516057
H	-2.245589286	-1.572163357	2.093963057
H	2.382098714	1.811579643	-2.834431943
H	3.244455714	4.087362643	-2.285801943
H	3.171787714	4.851398643	0.110998057
H	2.220519714	3.304132643	1.830882057
H	4.334507714	-3.234612357	1.812310057
H	5.205511714	-4.832013357	0.096128057
H	4.482550714	-4.539225357	-2.296733943
H	2.913374714	-2.679027357	-2.844921943
H	-0.043192286	-1.408854357	2.468312057
H	0.650936714	-2.513702357	1.274511057
H	2.788686714	-1.475446357	2.401885057
H	3.386803714	-0.214043357	1.325486057
H	1.451400714	1.088124643	2.419152057
H	0.046691714	0.996934643	1.357548057

**16b'+**



C	4.238509707	-1.934000358	0.365840309
C	3.400234707	-2.888125358	1.062419309
C	2.253570707	-2.487233358	1.707652309
C	1.770949707	-1.131807358	1.500667309
N	3.868245707	-0.709522358	0.051323309
C	2.578097707	-0.555563358	0.386724309
N	-2.186604293	-0.972882358	0.263719309
C	-3.188739293	-1.103933358	-0.624611691
C	-4.427442293	-1.644235358	-0.290659691
C	-4.641580293	-2.056875358	1.023579309
C	-3.605033293	-1.920954358	1.948262309
C	-2.386262293	-1.385164358	1.537401309
N	-0.382942293	2.042114642	0.470111309
C	-0.502476293	2.293540642	1.793604309
C	-0.288869293	3.567543642	2.316645309
C	0.041138707	4.615586642	1.455962309
C	0.154365707	4.354184642	0.091334309
C	-0.061724293	3.053244642	-0.355784691
C	1.059750707	-0.314459358	2.568479309
N	-0.363096293	-0.134465358	2.252669309
C	-0.935887293	1.139429642	2.685936309
C	-1.202757293	-1.306657358	2.490440309
N	1.381387707	-0.682929358	0.003291309
Cu	-0.474454293	0.050796642	-0.007247691
H	5.266027707	-2.206096358	0.134340309
H	3.798147707	-3.884985358	1.222752309
H	1.817436707	-3.123137358	2.476492309
H	-2.980232293	-0.761150358	-1.632948691
H	-5.201479293	-1.730529358	-1.045716691
H	-5.597156293	-2.474205358	1.325970309
H	-3.736986293	-2.230310358	2.980748309
H	-0.381896293	3.734278642	3.385648309
H	0.211188707	5.614520642	1.845833309
H	0.411933707	5.134754642	-0.616571691
H	0.026116707	2.800850642	-1.407939691
H	1.208580707	-0.788267358	3.551490309
H	1.512347707	0.680020642	2.621369309
H	-0.703100293	1.372876642	3.736276309
H	-2.026752293	1.048816642	2.616846309
H	-1.559145293	-1.367501358	3.530937309
H	-0.581732293	-2.193229358	2.316193309



17b+

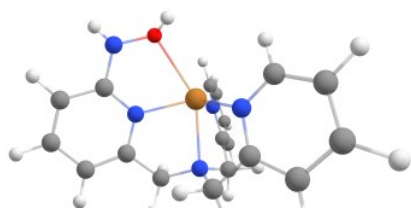
37b+



C	2.551908000	-0.310112000	0.639163000
C	3.786926000	-0.172571000	1.267287000
C	4.930528000	0.115191000	0.523357000
C	4.814619000	0.207827000	-0.876953000
N	3.692719000	-0.032594000	-1.530176000
C	2.528320000	-0.234965000	-0.815989000
N	1.438403000	-0.326011000	-1.566723000
Cu	-0.219282000	0.016435000	-0.980058000
N	-1.273863000	1.655580000	-0.523589000
C	-0.943951000	2.191417000	0.675336000
C	-1.547041000	3.359771000	1.133948000
C	-2.497531000	3.998747000	0.335738000
C	-2.827482000	3.442937000	-0.899716000
C	-2.193227000	2.267262000	-1.289960000
N	-1.375545000	-1.596462000	-0.460243000
C	-1.803156000	-2.545670000	-1.310410000
C	-2.421040000	-3.713566000	-0.872588000
C	-2.583679000	-3.906831000	0.499288000
C	-2.124191000	-2.926878000	1.380258000
C	-1.527639000	-1.776980000	0.866854000
C	-1.061289000	-0.645652000	1.767852000
N	0.112729000	0.040370000	1.222130000
C	0.136030000	1.481456000	1.475700000
C	1.360934000	-0.681535000	1.495742000
H	3.854965000	-0.263078000	2.348891000
H	5.894193000	0.246013000	1.005371000
H	5.687404000	0.435691000	-1.485745000
H	-1.272777000	3.763348000	2.103765000
H	-2.974827000	4.912276000	0.676777000
H	-3.562230000	3.903316000	-1.551237000
H	-2.416781000	1.792819000	-2.240061000
H	-1.634150000	-2.355818000	-2.365597000
H	-2.754359000	-4.452718000	-1.593027000
H	-3.051618000	-4.809907000	0.879111000
H	-2.223670000	-3.051222000	2.454389000
H	-0.874847000	-1.028017000	2.782938000
H	-1.874709000	0.084146000	1.847443000
H	0.028871000	1.723353000	2.544995000
H	1.115342000	1.856810000	1.156067000
H	1.141159000	-1.745724000	1.342365000
H	1.641876000	-0.573166000	2.555982000

C	2.442854000	-0.863356000	0.602164000
C	3.669296000	-0.952645000	1.252969000
C	4.858426000	-0.851817000	0.528117000
C	4.778663000	-0.663878000	-0.864230000
N	3.638255000	-0.557404000	-1.528252000
C	2.469283000	-0.641524000	-0.825031000
N	1.340541000	-0.481068000	-1.521487000
Cu	-0.326174000	0.004007000	-1.009866000
N	-0.816655000	1.950573000	-0.511473000
C	-0.368488000	2.308940000	0.711431000
C	-0.629390000	3.570936000	1.242164000
C	-1.352410000	4.492866000	0.484443000
C	-1.803722000	4.121319000	-0.781986000
C	-1.517066000	2.838199000	-1.238291000
N	-1.820582000	-1.317248000	-0.502936000
C	-2.494990000	-2.141216000	-1.322831000
C	-3.307677000	-3.167964000	-0.849290000
C	-3.411800000	-3.352641000	0.528828000
C	-2.703814000	-2.503112000	1.381151000
C	-1.920734000	-1.490341000	0.832864000
C	-1.187100000	-0.486017000	1.702369000
N	0.103854000	-0.080351000	1.118438000
C	0.479286000	1.296689000	1.462619000
C	1.161379000	-1.083293000	1.370666000
H	3.698584000	-1.111681000	2.328298000
H	5.823348000	-0.921090000	1.019229000
H	5.685420000	-0.595707000	-1.461431000
H	-0.266568000	3.826895000	2.233047000
H	-1.561788000	5.482669000	0.878417000
H	-2.369711000	4.805008000	-1.405457000
H	-1.852165000	2.499845000	-2.213734000
H	-2.369336000	-1.967069000	-2.386801000
H	-3.835213000	-3.807736000	-1.548491000
H	-4.027567000	-4.148920000	0.935692000
H	-2.757118000	-2.624200000	2.458788000
H	-1.058988000	-0.884235000	2.719356000
H	-1.810671000	0.411265000	1.785174000
H	0.419127000	1.482135000	2.545674000
H	1.527109000	1.432785000	1.171398000
H	0.732495000	-2.053760000	1.091648000
H	1.392226000	-1.130779000	2.446505000

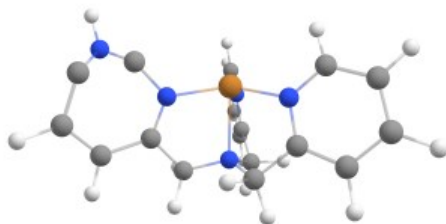
**18b<sup>+</sup>**



C	-3.284585044	1.095485793	0.468923664
C	-3.493572044	0.876513793	1.820194664
C	-2.467556044	0.320445793	2.597488664
C	-1.270742044	-0.011717207	1.979983664
N	-1.053690044	0.218113793	0.663552664
C	-2.028804044	0.760519793	-0.067951336
N	2.325509956	1.116820793	0.189646664
C	3.106436956	1.625702793	-0.780644336
C	4.206175956	2.439436793	-0.525065336
C	4.521199956	2.732167793	0.801402664
C	3.721652956	2.199025793	1.812546664
C	2.627234956	1.402672793	1.477235664
N	1.315391956	-2.233506207	0.055387664
C	1.787702956	-2.638792207	1.255961664
C	2.016324956	-3.985379207	1.534215664
C	1.768786956	-4.941493207	0.548163664
C	1.287590956	-4.519021207	-0.690430336
C	1.071666956	-3.157960207	-0.890017336
C	-0.168504044	-0.732597207	2.743527664
N	1.160955956	-0.449860207	2.220723664
C	2.106493956	-1.558644207	2.280091664
C	1.698467956	0.862394793	2.554501664
N	-1.771608044	1.088826793	-1.408947336
Cu	0.838231956	-0.256707207	-0.046129336
O	-0.685369044	0.380928793	-1.990755336
H	-4.053948044	1.533337793	-0.159712336
H	-4.446186044	1.135368793	2.272100664
H	-2.605576044	0.139268793	3.658514664
H	2.837923956	1.358103793	-1.798339336
H	4.800466956	2.823045793	-1.347682336
H	5.375705956	3.355867793	1.045465664
H	3.941605956	2.397266793	2.857372664
H	2.384735956	-4.278349207	2.512928664
H	1.942592956	-5.994666207	0.746911664
H	1.075323956	-5.224483207	-1.486870336
H	0.685686956	-2.782235207	-1.832717336
H	-0.258736044	-0.507911207	3.818403664
H	-0.340711044	-1.810272207	2.633643664
H	2.171800956	-2.009048207	3.283672664
H	3.100349956	-1.155588207	2.050325664
H	2.218281956	0.875023793	3.526446664
H	0.847862956	1.549457793	2.643004664
H	-0.145465044	1.087806793	-2.383105336
H	-2.580929044	0.939989793	-2.007639336

19b<sup>+</sup>

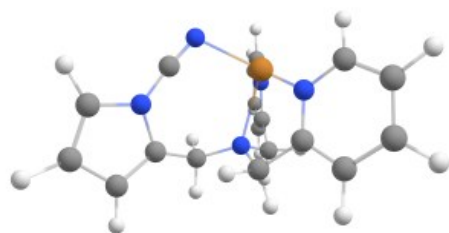
39b<sup>+</sup>



C	-4.239057000	-0.586718000	-0.592527000
C	-4.561426000	-0.693382000	0.727440000
C	-3.359844000	-0.775632000	1.522497000
C	-2.082685000	-0.700279000	0.987914000
C	-0.843347000	-0.876948000	1.843843000
N	0.239569000	0.015918000	1.426900000
C	1.588871000	-0.499192000	1.647543000
C	1.966140000	-1.583257000	0.647684000
C	2.808694000	-2.632377000	1.010877000
C	3.193219000	-3.568074000	0.049631000
C	2.712928000	-3.429373000	-1.251850000
C	1.863731000	-2.363454000	-1.536390000
N	1.494544000	-1.456895000	-0.614116000
Cu	0.079218000	-0.005222000	-0.819751000
C	0.049545000	1.427861000	1.746800000
C	0.674123000	2.345678000	0.705114000
N	0.645681000	1.936120000	-0.584492000
C	1.132681000	2.755648000	-1.533653000
C	1.666028000	4.009889000	-1.250139000
C	1.706095000	4.430782000	0.078508000
C	1.206027000	3.582237000	1.066884000
N	-1.834761000	-0.509495000	-0.389296000
C	-2.976553000	-0.500998000	-1.012816000
N	-3.962673000	-0.506713000	-2.067125000
H	-5.551657000	-0.698743000	1.168795000
H	-3.455535000	-0.902491000	2.596736000
H	-1.103827000	-0.759663000	2.907155000
H	-0.476253000	-1.902924000	1.717252000
H	2.284298000	0.338654000	1.515155000
H	1.735195000	-0.873423000	2.673043000
H	3.159449000	-2.711732000	2.035539000
H	3.850107000	-4.390906000	0.314602000
H	2.980581000	-4.132466000	-2.033403000
H	1.456742000	-2.222693000	-2.532740000
H	-1.031132000	1.616090000	1.760588000
H	0.429254000	1.690520000	2.746777000
H	1.091384000	2.382638000	-2.552173000
H	2.044766000	4.632038000	-2.054089000
H	2.122777000	5.397928000	0.342655000
H	1.225440000	3.874709000	2.112531000
H	-4.166450000	0.406887000	-2.492910000

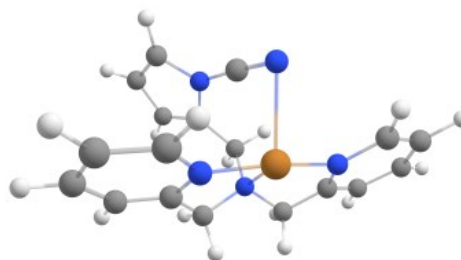
C	-3.682845000	2.301833000	-0.825332000
C	-3.956617000	2.365725000	0.593595000
C	-3.147905000	1.635774000	1.413629000
C	-1.988296000	0.923221000	0.903988000
C	-1.108533000	0.174934000	1.898566000
N	0.265515000	0.018054000	1.437411000
C	0.871694000	-1.289638000	1.680274000
C	0.348436000	-2.353241000	0.726307000
C	0.186329000	-3.674021000	1.140816000
C	-0.229221000	-4.635785000	0.218667000
C	-0.478105000	-4.242650000	-1.095377000
C	-0.306690000	-2.902059000	-1.431187000
N	0.096718000	-1.973445000	-0.547013000
Cu	0.107918000	0.067076000	-0.816878000
C	1.133807000	1.169147000	1.680835000
C	2.222391000	1.316962000	0.627521000
N	1.905478000	0.990968000	-0.646772000
C	2.823299000	1.179189000	-1.611409000
C	4.090973000	1.695762000	-1.357211000
C	4.425473000	2.022005000	-0.043845000
C	3.476693000	1.824466000	0.960569000
N	-1.622417000	0.933181000	-0.356417000
C	-2.443668000	1.584836000	-1.268063000
N	-3.743179000	1.078950000	-1.574554000
H	-4.718854000	3.028281000	0.995193000
H	-3.294277000	1.652269000	2.490324000
H	-1.162659000	0.666345000	2.882410000
H	-1.547715000	-0.822314000	2.028149000
H	1.950346000	-1.185461000	1.512781000
H	0.743376000	-1.627112000	2.720302000
H	0.385738000	-3.943743000	2.173658000
H	-0.359982000	-5.669650000	0.523320000
H	-0.804871000	-4.952650000	-1.847681000
H	-0.499140000	-2.548834000	-2.439511000
H	0.503514000	2.065712000	1.639856000
H	1.590714000	1.145468000	2.682750000
H	2.522131000	0.902629000	-2.616809000
H	4.794412000	1.830324000	-2.171964000
H	5.406861000	2.418924000	0.197107000
H	3.703978000	2.064726000	1.994859000
H	-4.081274000	1.117195000	-2.537901000

**<sup>1</sup>10b<sup>+</sup>**



C	1.903882000	3.631837000	-1.155823000
C	2.330574000	4.218447000	-0.001205000
C	1.640348000	3.598200000	1.095526000
C	0.791482000	2.642642000	0.606413000
N	0.946962000	2.662343000	-0.803427000
C	0.350606000	1.812879000	-1.635874000
N	1.309089000	-1.723180000	-0.442644000
C	1.771056000	-2.805526000	-1.103121000
C	2.772979000	-3.626325000	-0.599844000
C	3.313800000	-3.325129000	0.650621000
C	2.837287000	-2.209800000	1.336549000
C	1.842164000	-1.417534000	0.762347000
N	-2.197375000	-0.657646000	-0.371406000
C	-2.301185000	-0.448155000	0.961578000
C	-3.535055000	-0.242092000	1.572690000
C	-4.694085000	-0.258574000	0.793276000
C	-4.580519000	-0.472405000	-0.579419000
C	-3.311872000	-0.663370000	-1.121996000
C	-0.179148000	1.747094000	1.302048000
N	0.056547000	0.300428000	1.098074000
C	-1.004121000	-0.491320000	1.745889000
C	1.401674000	-0.140995000	1.463792000
N	-0.193655000	0.997763000	-2.274269000
Cu	-0.304277000	-0.716295000	-1.010024000
H	2.161523000	3.783832000	-2.193272000
H	3.061255000	5.012136000	0.067223000
H	1.755730000	3.842984000	2.143246000
H	1.311025000	-3.007769000	-2.064707000
H	3.110574000	-4.482506000	-1.173848000
H	4.090233000	-3.947612000	1.084665000
H	3.234712000	-1.946717000	2.312343000
H	-3.586032000	-0.070837000	2.643547000
H	-5.665807000	-0.100653000	1.251056000
H	-5.452451000	-0.487759000	-1.224504000
H	-3.170379000	0.823065000	-2.185999000
H	-0.148490000	2.007875000	2.372728000
H	-1.201230000	1.946175000	0.956529000
H	-1.178579000	-0.163796000	2.783215000
H	-0.661436000	-1.531777000	1.788202000
H	1.515670000	-0.269648000	2.552667000
H	2.097522000	0.654495000	1.172627000

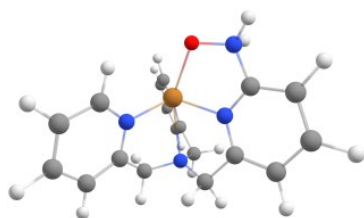
**<sup>3</sup>10b<sup>+</sup>**



C	2.652057000	1.834030000	-1.661958000
C	3.187363000	2.583896000	-0.654602000
C	2.226232000	2.661117000	0.405587000
C	1.108662000	1.952794000	0.047692000
N	1.358299000	1.454363000	-1.258472000
C	0.542417000	0.646336000	-1.928081000
N	1.244968000	-1.400734000	0.079040000
C	2.096902000	-2.076423000	-0.751217000
C	3.444322000	-2.180538000	-0.487646000
C	3.978991000	-1.561084000	0.664017000
C	3.111083000	-0.860594000	1.506140000
C	1.758994000	-0.797330000	1.211891000
N	-2.419200000	-0.533605000	-0.244259000
C	-2.804420000	0.165531000	0.879518000
C	-4.090493000	0.667264000	1.007242000
C	-5.024245000	0.448085000	-0.009793000
C	-4.618735000	-0.263631000	-1.157482000
C	-3.322068000	-0.725357000	-1.247333000
C	-0.177784000	1.738667000	0.760182000
N	-0.403979000	0.350476000	1.299514000
C	-1.750117000	0.250272000	1.941176000
C	0.730964000	-0.179173000	2.109001000
N	-0.208474000	-0.085255000	-2.449748000
Cu	-0.585816000	-1.022573000	-0.227628000
H	3.026422000	1.530736000	-2.627958000
H	4.167358000	3.039900000	-0.665771000
H	2.351607000	3.185746000	1.343694000
H	1.648311000	-2.520022000	-1.634170000
H	4.078505000	-2.732150000	-1.173392000
H	5.037348000	-1.626925000	0.890002000
H	3.483637000	-0.364215000	2.397539000
H	-4.361650000	1.220302000	1.901827000
H	-6.037040000	0.824985000	0.080233000
H	-5.304702000	-0.441346000	-1.978515000
H	-2.955816000	-1.247996000	-2.124368000
H	-0.206371000	2.432858000	1.609841000
H	-1.040419000	1.963071000	0.124141000
H	-1.924139000	1.089597000	2.625659000
H	-1.734492000	-0.675607000	2.534691000
H	0.296762000	-0.948129000	2.765628000
H	1.161273000	0.603933000	2.743592000

**<sup>1</sup>11b<sup>+</sup>**

**<sup>3</sup>11b<sup>+</sup>**

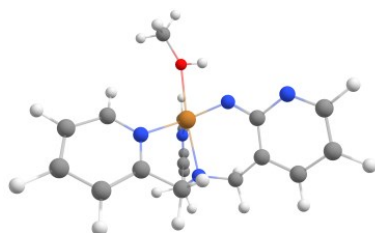


C	3.414027985	-1.972301867	1.354072582
C	3.800733985	-1.777730867	2.687042582
C	3.004074985	-0.999256867	3.525106582
C	1.835137985	-0.420241867	3.017019582
N	1.461715985	-0.635966867	1.749826582
C	2.229015985	-1.372081867	0.968551582
N	-2.027814015	-0.150714867	1.181338582
C	-2.950717015	-0.283078867	0.210066582
C	-4.300668015	-0.499870867	0.472032582
C	-4.716869015	-0.576152867	1.800715582
C	-3.763560015	-0.436953867	2.810101582
C	-2.426434015	-0.233839867	2.470124582
N	0.335375985	2.412286133	1.003022582
C	0.084443985	3.009843133	2.187092582
C	0.501319985	4.314196133	2.450047582
C	1.182374985	5.027310133	1.461655582
C	1.436573985	4.406243133	0.239472582
C	0.999393985	3.096035133	0.055938582
C	0.980103985	0.536526133	3.842779582
N	-0.310780015	0.812280133	3.245335582
C	-0.711748015	2.212451133	3.208576582
C	-1.356816015	-0.151872867	3.547767582
N	1.682626985	-1.509438867	-0.420956418
Cu	-0.131554015	0.424736133	0.793614582
O	1.001233985	-0.402684867	-0.882069418
H	4.015791985	-2.562160867	0.668469582
H	4.718594985	-2.223167867	3.057609582
H	3.291341985	-0.828539867	4.558612582
H	-2.579050015	-0.208093867	-0.807335418
H	-5.002912015	-0.598642867	-0.349093418
H	-5.762026015	-0.735103867	2.048268582
H	-4.051250015	-0.484387867	3.856267582
H	0.291187985	4.764377133	3.415922582
H	1.512053985	6.045279133	1.646670582
H	1.966739985	4.918295133	-0.556778418
H	1.184332985	2.558503133	-0.869552418
H	0.897573985	0.153065133	4.873369582
H	1.536047985	1.479419133	3.914224582
H	-0.643274015	2.702569133	4.193724582
H	-1.767614015	2.243105133	2.915174582
H	-1.840529015	0.037137133	4.521550582
H	-0.878215015	-1.136804867	3.621084582
H	2.466121985	-1.726552867	-1.053571418
H	1.057673985	-2.333662867	-0.436452418

C	4.225357000	-0.311974000	-0.617208000
C	4.591319000	-0.244754000	0.757589000
C	3.558204000	-0.065010000	1.726981000
C	2.241694000	-0.079231000	1.343592000
N	1.899572000	-0.392054000	0.030302000
C	2.892002000	-0.373362000	-0.905804000
N	-1.255872000	-1.611445000	-1.483256000
C	-1.996303000	-2.149968000	-1.483256000
C	-2.887205000	-3.198274000	-1.260662000
C	-3.016376000	-3.693857000	0.037410000
C	-2.251497000	-3.128681000	1.059172000
C	-1.372352000	-2.091529000	0.747990000
N	-1.048379000	1.723223000	-0.445965000
C	-1.521741000	1.948949000	0.797854000
C	-2.160657000	3.143266000	1.122794000
C	-2.320620000	4.117389000	0.135514000
C	-1.828710000	3.874335000	-1.147290000
C	-1.188857000	2.663411000	-1.394898000
C	1.057787000	0.442160000	2.125802000
N	-0.213444000	-0.042715000	1.503991000
C	-1.381982000	0.812998000	1.794369000
C	-0.462271000	-1.471027000	1.788106000
N	2.286233000	-0.453265000	-2.248531000
Cu	0.162803000	0.093757000	-0.571479000
O	1.042997000	0.229328000	-2.352496000
H	4.980285000	-0.310138000	-1.399066000
H	5.633986000	-0.237317000	1.048354000
H	3.818296000	0.153195000	2.759659000
H	-1.862955000	-1.719518000	-2.472123000
H	-3.465475000	-3.607391000	-2.082370000
H	-3.705706000	-4.504528000	0.253565000
H	-2.332713000	-3.487848000	2.080810000
H	-2.524067000	3.308249000	2.132515000
H	-2.815400000	5.055358000	0.368482000
H	-1.926669000	4.608558000	-1.939562000
H	-0.762252000	2.424554000	-2.364270000
H	1.098391000	0.180174000	3.192090000
H	1.022087000	1.537890000	2.054724000
H	-1.345155000	1.200669000	2.820706000
H	-2.278471000	0.187079000	1.719829000
H	-0.876671000	-1.605729000	2.796876000
H	0.510738000	-1.973480000	1.762235000
H	2.920064000	-0.062932000	-2.954487000
H	2.102902000	-1.435652000	-2.501097000

112+

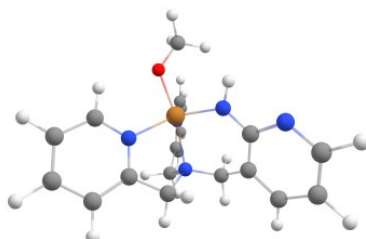
312+



C	3.192153560	0.365594612	-1.384580462	C	2.629450000	0.875977000	-0.591380000
C	4.481334560	0.188726612	-1.880984462	C	3.903445000	0.980174000	-1.141027000
C	5.540745560	-0.087171388	-1.016895462	C	5.029508000	0.774152000	-0.341590000
C	5.284434560	-0.129750388	0.366947538	C	4.833547000	0.472719000	1.019551000
N	4.102697560	0.134459612	0.894681538	N	3.642504000	0.366698000	1.587044000
C	3.018993560	0.324744612	0.059832538	C	2.525382000	0.548249000	0.811131000
N	1.854038560	0.409805612	0.688384538	N	1.353004000	0.397129000	1.432747000
Cu	0.211658560	0.152584612	-0.013208462	Cu	-0.310098000	0.012029000	0.699079000
N	-0.848145440	-1.437494388	-0.597325462	N	-0.820118000	-1.925108000	-0.027050000
C	-0.402789440	-2.018228388	-1.735454462	C	-0.206353000	-2.215478000	-1.192032000
C	-1.007703440	-3.167122388	-2.240504462	C	-0.409625000	-3.430118000	-1.846201000
C	-2.081915440	-3.734488388	-1.551804462	C	-1.257945000	-4.376900000	-1.270589000
C	-2.531055440	-3.129185388	-0.377948462	C	-1.888598000	-4.074416000	-0.062936000
C	-1.886214440	-1.977110388	0.063210538	C	-1.643774000	-2.833730000	0.519728000
N	-0.787534440	1.787863612	-0.724589462	N	-1.752079000	1.383136000	0.051112000
C	-1.286497440	2.752261612	0.068030538	C	-2.499397000	2.178781000	0.831940000
C	-1.826901440	3.925779612	-0.452732462	C	-3.234677000	3.244849000	0.316645000
C	-1.834902440	4.102353612	-1.836846462	C	-3.175055000	3.495410000	-1.054563000
C	-1.307447440	3.099174612	-2.652288462	C	-2.387069000	2.672325000	-1.863210000
C	-0.794412440	1.945974612	-2.061379462	C	-1.691183000	1.619669000	-1.273638000
C	-0.270616440	0.782965612	-2.889688462	C	-0.869689000	0.632687000	-2.077831000
N	0.809595560	0.067478612	-2.209421462	N	0.332318000	0.184616000	-1.341406000
C	0.800008560	-1.379665388	-2.413352462	C	0.749120000	-1.170522000	-1.735268000
C	2.102916560	0.737454612	-2.367273462	C	1.419334000	1.188492000	-1.433835000
H	4.658422560	0.242283612	-2.952577462	H	4.019924000	1.227280000	-2.193733000
H	6.545609560	-0.245819388	-1.395287462	H	6.031674000	0.848323000	-0.750667000
H	6.089559560	-0.341837388	1.067743538	H	5.689298000	0.315725000	1.673231000
H	-0.640469440	-3.610312388	-3.161043462	H	0.090672000	-3.629667000	-2.789072000
H	-2.562996440	-4.631032388	-1.930618462	H	-1.427509000	-5.331219000	-1.759807000
H	-3.365367440	-3.533295388	0.185088538	H	-2.560033000	-4.778364000	0.417015000
H	-2.193980440	-1.459918388	0.966354538	H	-2.117697000	-2.547011000	1.452760000
H	-1.235521440	2.553461612	1.134105538	H	-2.486070000	1.942836000	1.891420000
H	-2.222310440	4.682456612	0.216463538	H	-3.829164000	3.865286000	0.978769000
H	-2.238957440	5.009238612	-2.276500462	H	-3.726316000	4.323613000	-1.489449000
H	-1.291661440	3.207811612	-3.732697462	H	-2.312665000	2.845991000	-2.932455000
H	0.039985560	1.142072612	-3.883017462	H	-0.595398000	1.058764000	-3.053206000
H	-1.096948440	0.081636612	-3.050648462	H	-1.488396000	-0.250118000	-2.272311000
H	0.815631560	-1.657658388	-3.479732462	H	0.839484000	-1.265337000	-2.827644000
H	1.713916560	-1.783444388	-1.961374462	H	1.744926000	-1.343927000	-1.312757000
H	1.906059560	1.812558612	-2.265560462	H	0.980532000	2.142820000	-1.118473000
H	2.488888560	0.590581612	-3.389825462	H	1.730193000	1.305244000	-2.483571000
O	-0.373072440	0.739370612	2.380163538	O	-0.958819000	0.116555000	2.887102000
C	-0.839971440	-0.005445388	3.508616538	C	-1.518126000	-0.876374000	3.758184000
H	-1.931640440	-0.010332388	3.456257538	H	-2.551066000	-1.029811000	3.437649000
H	-0.535159440	0.466787612	4.449815538	H	-1.517747000	-0.524919000	4.795303000
H	0.604541560	0.760044612	2.378530538	H	-0.025302000	0.283334000	3.121263000
H	-0.471505440	-1.039540388	3.485982538	H	-0.965116000	-1.821093000	3.690024000

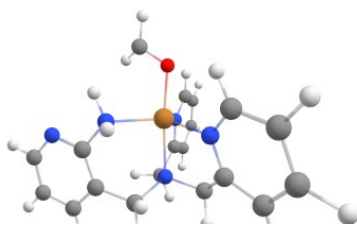
**113+**

**313+**



C	-2.439351000	-0.795772000	-0.864038000
C	-3.688768000	-0.551130000	-1.424084000
C	-4.806223000	-0.469433000	-0.589259000
C	-4.619856000	-0.635656000	0.791126000
N	-3.430005000	-0.839389000	1.355919000
C	-2.353070000	-0.935399000	0.548371000
N	-1.129081000	-1.230830000	1.109206000
Cu	0.104390000	0.165129000	0.744145000
N	0.778929000	1.986039000	0.216703000
C	0.364632000	2.398074000	-0.998140000
C	0.701234000	3.655393000	-1.487781000
C	1.472008000	4.501006000	-0.684203000
C	1.878635000	4.066982000	0.578612000
C	1.507244000	2.792007000	0.999613000
N	1.912760000	-1.338019000	0.146259000
C	2.505757000	-2.302670000	0.860077000
C	3.046383000	-3.453262000	0.281678000
C	2.953302000	-3.610382000	-1.099740000
C	2.324536000	-2.612867000	-1.849877000
C	1.823511000	-1.494363000	-1.186156000
C	1.169662000	-0.349529000	-1.919588000
N	-0.135683000	0.029849000	-1.301163000
C	-0.513858000	1.404721000	-1.718840000
C	-1.188011000	-0.973820000	-1.666030000
H	-3.793803000	-0.442550000	-2.501107000
H	-5.796343000	-0.281452000	-0.990575000
H	-5.467777000	-0.589929000	1.470343000
H	0.365817000	3.968527000	-2.471526000
H	1.748314000	5.488352000	-1.041411000
H	2.469440000	4.701529000	1.230131000
H	1.758835000	2.389561000	1.975313000
H	2.547841000	-2.148775000	1.933413000
H	3.521442000	-4.203550000	0.904977000
H	3.355050000	-4.493740000	-1.586695000
H	2.226026000	-2.703084000	-2.927556000
H	1.011722000	-0.592885000	-2.977675000
H	1.824531000	0.525159000	-1.872967000
H	-0.449029000	1.515663000	-2.809196000
H	-1.559940000	1.560622000	-1.430588000
H	-0.748066000	-1.953528000	-1.454593000
H	-1.393157000	-0.906345000	-2.742915000
O	0.217981000	0.558432000	2.523327000
H	-1.272125000	-1.251979000	2.121402000
C	0.842810000	-0.352948000	3.387218000
H	0.420456000	-1.370106000	3.330347000
H	1.929222000	-0.414678000	3.219865000
H	0.668486000	0.007730000	4.411952000

C	-2.491598000	-1.005003000	-0.690314000
C	-3.713172000	-1.174200000	-1.335060000
C	-4.903255000	-1.127040000	-0.605543000
C	-4.831298000	-0.910356000	0.788671000
N	-3.694959000	-0.733267000	1.435993000
C	-2.523665000	-0.766893000	0.727697000
N	-1.390547000	-0.558419000	1.409632000
Cu	0.394951000	0.081592000	0.796386000
N	0.630938000	2.045785000	0.150438000
C	0.067152000	2.358425000	-1.029654000
C	0.194876000	3.629474000	-1.584086000
C	0.912736000	4.598269000	-0.877245000
C	1.479715000	4.266581000	0.354259000
C	1.317911000	2.969124000	0.837797000
N	1.829549000	-1.326768000	0.049632000
C	2.602227000	-2.153384000	0.769727000
C	3.436241000	-3.099922000	0.176819000
C	3.458592000	-3.191309000	-1.214991000
C	2.653637000	-2.330168000	-1.964388000
C	1.857264000	-1.404589000	-1.293643000
C	1.021261000	-0.374284000	-2.017226000
N	-0.224181000	-0.067219000	-1.278535000
C	-0.754126000	1.256079000	-1.665416000
C	-1.203782000	-1.164097000	-1.457889000
H	-3.738051000	-1.353389000	-2.406789000
H	-5.865038000	-1.257737000	-1.090262000
H	-5.738665000	-0.879818000	1.387508000
H	-0.260123000	3.858440000	-2.543098000
H	1.026821000	5.598003000	-1.285412000
H	2.040864000	4.994207000	0.930727000
H	1.721012000	2.626906000	1.786598000
H	2.543490000	-2.042245000	1.846372000
H	4.046725000	-3.748676000	0.795765000
H	4.090270000	-3.921718000	-1.711343000
H	2.647018000	-2.373437000	-3.049333000
H	0.797430000	-0.698594000	-3.043709000
H	1.599108000	0.553848000	-2.087148000
H	-0.792906000	1.370667000	-2.758469000
H	-1.783219000	1.323667000	-1.296279000
H	-0.702078000	-2.083928000	-1.135123000
H	-1.439584000	-1.281846000	-2.526520000
O	1.064445000	0.507750000	2.494718000
H	-1.607174000	-0.412877000	2.399262000
C	1.098182000	-0.411370000	3.544770000
H	0.326704000	-1.199034000	3.449533000
H	2.074720000	-0.920211000	3.630012000
H	0.914533000	0.106810000	4.498950000

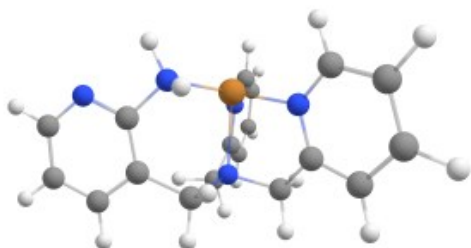
**14+****314+**

C	-2.008607000	-1.790212000	-0.661595000
C	-3.302807000	-1.955137000	-1.158466000
C	-4.394409000	-1.997917000	-0.288719000
C	-4.146549000	-1.859244000	1.075499000
N	-2.912628000	-1.727940000	1.582689000
C	-1.881442000	-1.709159000	0.740800000
N	-0.603629000	-1.546767000	1.354482000
Cu	0.390731000	0.243392000	0.713388000
N	-0.225976000	2.042514000	0.072934000
C	-0.728816000	2.102464000	-1.181594000
C	-0.952756000	3.321865000	-1.820810000
C	-0.671402000	4.513423000	-1.152294000
C	-0.161071000	4.448548000	0.144411000
C	0.049937000	3.195781000	0.711681000
N	2.166859000	-0.594576000	0.016106000
C	3.161052000	-1.058856000	0.793081000
C	4.218782000	-1.815268000	0.291453000
C	4.241329000	-2.106293000	-1.072643000
C	3.211188000	-1.622502000	-1.881793000
C	2.192516000	-0.862670000	-1.307523000
C	1.094166000	-0.235260000	-2.146696000
N	-0.214786000	-0.304891000	-1.494259000
C	-1.104843000	0.794337000	-1.858595000
C	-0.825647000	-1.642154000	-1.588787000
H	-3.454292000	-2.036304000	-2.232293000
H	-5.406285000	-2.124577000	-0.658410000
H	-4.958565000	-1.864024000	1.797827000
H	-1.345240000	3.332312000	-2.833325000
H	-0.842030000	5.470375000	-1.635845000
H	0.077931000	5.345624000	0.705767000
H	0.461319000	3.096893000	1.711141000
H	3.093635000	-0.803251000	1.846365000
H	4.999833000	-2.165973000	0.957984000
H	5.044004000	-2.699317000	-1.500445000
H	3.197411000	-1.827892000	-2.948038000
H	1.080445000	-0.691038000	-3.150301000
H	1.341474000	0.824552000	-2.281557000
H	-1.157544000	0.948672000	-2.949142000
H	-2.114184000	0.527828000	-1.527954000
H	-0.038218000	-2.365232000	-1.340082000
H	-1.139530000	-1.868342000	-2.622096000
O	1.241330000	0.519054000	3.069747000
C	0.706019000	0.968597000	4.064777000
H	-0.360272000	1.261314000	4.063835000
H	1.265731000	1.100279000	5.007400000
H	-0.722755000	-1.643302000	2.362280000
H	0.066559000	-2.249835000	1.043860000

C	-2.005549000	-1.725691000	-0.720898000
C	-3.222624000	-1.902881000	-1.383819000
C	-4.414011000	-1.931377000	-0.657738000
C	-4.344004000	-1.760504000	0.725112000
N	-3.186303000	-1.616487000	1.385452000
C	-2.058387000	-1.621925000	0.682168000
N	-0.848718000	-1.442555000	1.420120000
Cu	0.371611000	0.174805000	0.747448000
N	-0.077732000	2.058487000	0.127427000
C	-0.562057000	2.155992000	-1.126260000
C	-0.757394000	3.393007000	-1.735015000
C	-0.457022000	4.552060000	-1.014772000
C	0.038222000	4.439690000	0.285141000
C	0.222511000	3.167932000	0.822461000
N	2.185652000	-0.739709000	0.181757000
C	3.116397000	-1.219943000	1.018245000
C	4.228795000	-1.919926000	0.552134000
C	4.360989000	-2.125794000	-0.822242000
C	3.388299000	-1.617875000	-1.688658000
C	2.313962000	-0.918336000	-1.144761000
C	1.253898000	-0.233396000	-1.979111000
N	-0.068850000	-0.256380000	-1.304180000
C	-0.931292000	0.846028000	-1.788467000
C	-0.707633000	-1.597169000	-1.475732000
H	-3.236670000	-2.003845000	-2.466496000
H	-5.370831000	-2.067148000	-1.150418000
H	-5.243078000	-1.746519000	1.335311000
H	-1.138780000	3.448532000	-2.750035000
H	-0.603736000	5.528464000	-1.466443000
H	0.285169000	5.316834000	0.873347000
H	0.618316000	3.003747000	1.819277000
H	2.944427000	-1.017247000	2.071670000
H	4.968289000	-2.294456000	1.251848000
H	5.210639000	-2.674107000	-1.217767000
H	3.467555000	-1.758034000	-2.762444000
H	1.185840000	-0.676914000	-2.981938000
H	1.540015000	0.817115000	-2.105105000
H	-0.890832000	0.932107000	-2.883229000
H	-1.963295000	0.600647000	-1.519454000
H	0.030648000	-2.333499000	-1.139696000
H	-0.882704000	-1.783837000	-2.545023000
O	0.934943000	0.557458000	2.506890000
C	-0.009541000	0.768893000	3.434052000
H	-0.979320000	1.174557000	3.125165000
H	0.352331000	1.013416000	4.433334000
H	-1.057859000	-1.262571000	2.408080000
H	-0.242073000	-2.262447000	1.373838000

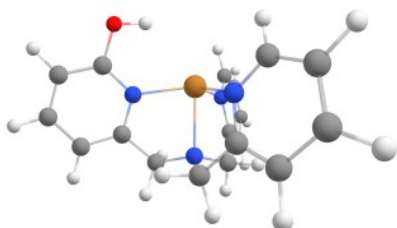


H	0.715676774	-1.945997815	-0.527457838
H	-0.258269226	-2.503444815	0.680392162

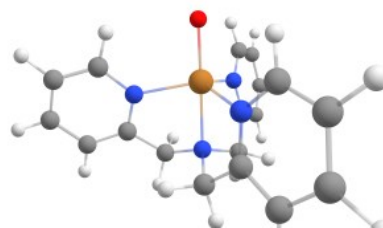


**15+**

C	1.626011774	-1.997185815	2.637159162
C	2.844075774	-2.225432815	3.282833162
C	4.010290774	-2.430453815	2.544177162
C	3.917831774	-2.388814815	1.154222162
N	2.758226774	-2.200691815	0.509264162
C	1.653238774	-2.024613815	1.227599162
N	0.461298774	-1.815685815	0.452696162
Cu	-0.437514226	0.008219185	0.970835162
N	0.257411774	1.833358185	1.397942162
C	0.653333774	1.999327185	2.682160162
C	0.949609774	3.260403185	3.196995162
C	0.858541774	4.380289185	2.369475162
C	0.465136774	4.204022185	1.043107162
C	0.170138774	2.917205185	0.602551162
N	-2.357820226	-0.596709815	1.493937162
C	-3.319170226	-1.063715815	0.677580162
C	-4.486858226	-1.661450815	1.147169162
C	-4.661882226	-1.786380815	2.525353162
C	-3.666958226	-1.302225815	3.376850162
C	-2.531148226	-0.705906815	2.830596162
C	-1.457873226	-0.085840815	3.706277162
N	-0.108692226	-0.310900815	3.176093162
C	0.835555774	0.750560185	3.531511162
C	0.378016774	-1.681898815	3.428825162
H	2.877144774	-2.228424815	4.369738162
H	4.963166774	-2.606779815	3.031593162
H	4.794817774	-2.520763815	0.526324162
H	1.251533774	3.359709185	4.235371162
H	1.087945774	5.369178185	2.754391162
H	0.380843774	5.042386185	0.359908162
H	-0.148411226	2.734299185	-0.418447838
H	-3.139207226	-0.946818815	-0.387183838
H	-5.233437226	-2.019521815	0.446155162
H	-5.554107226	-2.253181815	2.931315162
H	-3.769672226	-1.382397815	4.454833162
H	-1.558682226	-0.448491815	4.741572162
H	-1.627212226	0.997402185	3.728871162
H	0.782395774	1.016714185	4.599003162
H	1.845966774	0.370296185	3.348965162
H	-0.442247226	-2.358327815	3.157772162
H	0.575402774	-1.844050815	4.501265162

**12a<sup>+</sup>**

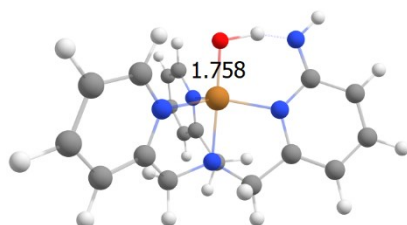
Cu	0.034711000	-0.004585000	-0.744065000
N	-1.821043000	-0.695060000	-0.273438000
C	-2.888201000	-0.724165000	-1.077494000
C	-4.177321000	-1.040330000	-0.625625000
C	-4.336878000	-1.317293000	0.721526000
C	-3.224934000	-1.277636000	1.578525000
C	-1.982234000	-0.974031000	1.047939000
C	-0.721621000	-0.989555000	1.895905000
N	0.388282000	1.991328000	-0.532769000
C	0.383893000	2.395131000	0.759195000
C	0.763558000	3.686234000	1.121707000
C	1.140586000	4.594459000	0.131735000
C	1.135251000	4.177889000	-1.198767000
C	0.757637000	2.868596000	-1.483086000
N	0.242345000	0.023554000	1.463267000
C	-0.108839000	1.401963000	1.801709000
C	1.646560000	-0.329849000	1.663877000
C	2.132069000	-1.355521000	0.649597000
C	3.107886000	-2.291912000	0.986198000
C	3.582274000	-3.169428000	0.010421000
C	3.056376000	-3.088471000	-1.278250000
C	2.073141000	-2.137191000	-1.535682000
N	1.616636000	-1.286036000	-0.599732000
H	-5.002350000	-1.050400000	-1.328060000
H	-5.320068000	-1.557876000	1.114087000
H	-3.329581000	-1.484752000	2.638334000
H	-0.240373000	-1.967503000	1.773895000
H	-0.986371000	-0.893722000	2.959979000
H	0.760500000	3.974592000	2.168615000
H	1.436907000	5.604908000	0.396158000
H	1.422410000	4.845984000	-2.003724000
H	0.749767000	2.498622000	-2.503467000
H	-1.203547000	1.460751000	1.834258000
H	0.254545000	1.697252000	2.798184000
H	2.236521000	0.584839000	1.528736000
H	1.849019000	-0.690266000	2.684362000
H	3.491172000	-2.329608000	2.001523000
H	4.343365000	-3.904219000	0.254484000
H	3.390528000	-3.750412000	-2.070060000
H	1.627965000	-2.046489000	-2.521433000
O	-2.716520000	-0.430481000	-2.379180000
H	-1.773624000	-0.224722000	-2.532450000

**33a<sup>+</sup>**

O	-0.035553000	-0.073012000	-2.620632000
Cu	-0.011711000	-0.013234000	-0.796344000
N	-1.904307000	-0.790631000	-0.431026000
C	-2.888016000	-0.865477000	-1.339394000
C	-4.164822000	-1.310161000	-1.002189000
C	-4.418702000	-1.672511000	0.321044000
C	-3.390359000	-1.586333000	1.263198000
C	-2.136835000	-1.146778000	0.846105000
C	-0.933138000	-1.090788000	1.764283000
N	0.261241000	2.025750000	-0.438072000
C	0.071092000	2.397701000	0.842375000
C	0.312758000	3.701484000	1.267895000
C	0.745602000	4.644828000	0.333066000
C	0.927635000	4.254768000	-0.993939000
C	0.677863000	2.928391000	-1.339029000
N	-0.007533000	-0.013191000	1.357625000
C	-0.482214000	1.326145000	1.759926000
C	1.384065000	-0.272827000	1.781506000
C	2.060745000	-1.263686000	0.856191000
C	3.075605000	-2.120736000	1.273733000
C	3.698709000	-2.934102000	0.323412000
C	3.287441000	-2.867070000	-1.008191000
C	2.254924000	-1.993356000	-1.344405000
N	1.660628000	-1.217249000	-0.427501000
H	-2.618210000	-0.556942000	-2.345046000
H	-4.938857000	-1.362924000	-1.760284000
H	-5.404967000	-2.014778000	0.619592000
H	-3.558515000	-1.858678000	2.300810000
H	-0.386297000	-2.037202000	1.681791000
H	-1.240274000	-0.982384000	2.813904000
H	0.161661000	3.974283000	2.307997000
H	0.939211000	5.668458000	0.639025000
H	1.261375000	4.958224000	-1.749134000
H	0.805233000	2.561734000	-2.352852000
H	-1.574916000	1.325419000	1.673950000
H	-0.238923000	1.541153000	2.809778000
H	1.925183000	0.678653000	1.724915000
H	1.428654000	-0.609880000	2.826439000
H	3.375984000	-2.148962000	2.316895000
H	4.493904000	-3.610695000	0.621622000
H	3.750400000	-3.481113000	-1.773252000
H	1.879070000	-1.886198000	-2.357828000

$^1\text{TS2/3}'^+$

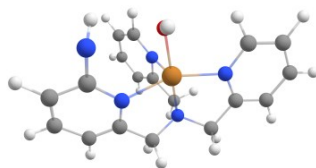
$^3\text{TS2/3}'^+$



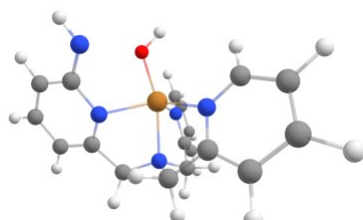
C	4.153288000	-1.160657000	0.592831000
C	4.325418000	-1.519653000	-0.717183000
C	3.229405000	-1.510152000	-1.622191000
C	2.003632000	-1.137408000	-1.129639000
N	1.827340000	-0.746903000	0.164598000
C	2.859056000	-0.759710000	1.078444000
N	-0.307655000	1.907031000	0.390186000
C	-0.656855000	2.754798000	1.362546000
C	-0.863614000	4.110730000	1.109457000
C	-0.706070000	4.577656000	-0.196232000
C	-0.339466000	3.684174000	-1.207471000
C	-0.139812000	2.348984000	-0.867875000
N	-1.807192000	-1.066736000	0.413182000
C	-2.314799000	-1.098730000	-0.833821000
C	-3.469912000	-1.819123000	-1.119395000
C	-4.107553000	-2.498091000	-0.076519000
C	-3.572614000	-2.442923000	1.211422000
C	-2.401431000	-1.717409000	1.419606000
C	0.731071000	-1.142487000	-1.937325000
N	-0.158094000	-0.049584000	-1.443195000
C	-1.583724000	-0.236986000	-1.835628000
C	0.346194000	1.296854000	-1.839392000
N	2.557425000	-0.402307000	2.309158000
Cu	0.007413000	-0.214511000	0.549490000
O	0.087369000	-0.382517000	2.297291000
H	4.979157000	-1.180916000	1.296694000
H	5.308028000	-1.819018000	-1.070103000
H	3.350989000	-1.789417000	-2.662619000
H	-0.758905000	2.314485000	2.350679000
H	-1.142897000	4.779413000	1.916665000
H	-0.866073000	5.626195000	-0.428502000
H	-0.206721000	4.021612000	-2.231017000
H	-3.865532000	-1.847138000	-2.129991000
H	-5.011414000	-3.067017000	-0.272115000
H	-4.043569000	-2.960179000	2.040226000
H	-1.894180000	-1.632437000	2.377362000
H	0.921220000	-1.033053000	-3.012085000
H	0.192494000	-2.084465000	-1.781570000
H	-1.648134000	-0.643237000	-2.852263000
H	-2.051610000	0.753231000	-1.847444000
H	0.051237000	1.521137000	-2.871996000
H	1.439627000	1.254436000	-1.807989000
H	1.286301000	-0.360229000	2.497758000
H	3.310010000	-0.442155000	2.987434000

C	-4.310337000	-0.307291000	-0.475242000
C	-4.509503000	-0.635360000	0.852108000
C	-3.413658000	-0.767635000	1.726053000
C	-2.144504000	-0.577672000	1.199804000
N	-1.945072000	-0.235564000	-0.083670000
C	-2.987748000	-0.070158000	-0.946614000
N	0.854497000	1.876837000	-0.391308000
C	1.389226000	2.644521000	-1.352417000
C	1.996444000	3.865332000	-1.067147000
C	2.051792000	4.289376000	0.260908000
C	1.493410000	3.486065000	1.258008000
C	0.892628000	2.284451000	0.891716000
N	1.349127000	-1.584323000	-0.489301000
C	1.865688000	-1.755377000	0.741401000
C	2.663664000	-2.853328000	1.051371000
C	2.941131000	-3.784111000	0.046530000
C	2.408898000	-3.592564000	-1.228984000
C	1.606601000	-2.475852000	-1.456302000
C	-0.874372000	-0.834883000	1.985490000
N	0.250621000	-0.029467000	1.454009000
C	1.569191000	-0.642959000	1.726582000
C	0.183407000	1.384408000	1.882116000
N	-2.675017000	0.360160000	-2.182001000
Cu	-0.011792000	-0.003455000	-0.649869000
O	-0.323309000	-0.054198000	-2.485271000
H	-5.146278000	-0.194910000	-1.157873000
H	-5.517786000	-0.797134000	1.221837000
H	-3.551017000	-1.039759000	2.767026000
H	1.315032000	2.256177000	-2.363309000
H	2.417528000	4.462413000	-1.868854000
H	2.524271000	5.232051000	0.519823000
H	1.519878000	3.789503000	2.300224000
H	3.061784000	-2.977715000	2.053940000
H	3.561862000	-4.648904000	0.260643000
H	2.602264000	-4.295404000	-2.032272000
H	1.147077000	-2.265740000	-2.417759000
H	-1.022641000	-0.651013000	3.058158000
H	-0.599328000	-1.889339000	1.868911000
H	1.634845000	-1.000306000	2.763094000
H	2.325551000	0.140700000	1.604538000
H	0.586144000	1.513992000	2.895874000
H	-0.875445000	1.665061000	1.913041000
H	-1.416186000	0.336724000	-2.509711000
H	-3.409958000	0.242076000	-2.875361000

### <sup>3</sup>TS3'/3<sup>+</sup>

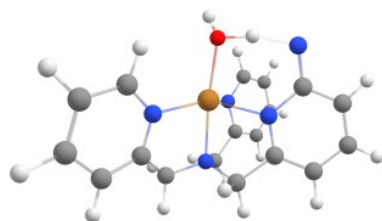


C	3.739935000	1.764130000	0.062924000
C	4.081415000	1.159628000	-1.134673000
C	3.082132000	0.601860000	-1.948461000
C	1.771487000	0.677257000	-1.514036000
N	1.435363000	1.244380000	-0.332545000
C	2.384989000	1.780898000	0.462582000
N	-2.391713000	0.502166000	0.257211000
C	-3.204985000	0.618063000	1.317247000
C	-4.560697000	0.309505000	1.231576000
C	-5.069466000	-0.140700000	0.013062000
C	-4.211647000	-0.267817000	-1.083261000
C	-2.871440000	0.070301000	-0.926303000
N	0.451833000	-1.281766000	0.942265000
C	0.570097000	-2.066373000	-0.140115000
C	1.471844000	-3.126493000	-0.193637000
C	2.266766000	-3.381399000	0.927890000
C	2.135308000	-2.569397000	2.054283000
C	1.214980000	-1.520410000	2.013935000
C	0.599706000	0.222963000	-2.357794000
N	-0.516518000	-0.289941000	-1.525137000
C	-0.399682000	-1.749568000	-1.256828000
C	-1.861922000	0.038967000	-2.055234000
N	2.005801000	2.448914000	1.613426000
Cu	-0.393151000	0.738167000	0.346480000
O	-0.274259000	1.555628000	2.033465000
H	4.484391000	2.223459000	0.703344000
H	5.121040000	1.123667000	-1.446640000
H	3.324551000	0.136057000	-2.897956000
H	-2.727457000	0.961514000	2.229961000
H	-5.196471000	0.415541000	2.103921000
H	-6.120182000	-0.396362000	-0.084651000
H	-4.578001000	-0.621229000	-2.042244000
H	1.550718000	-3.741092000	-1.085504000
H	2.979054000	-4.200983000	0.918228000
H	2.734090000	-2.737683000	2.943352000
H	1.074160000	-0.842226000	2.851482000
H	0.229588000	1.091844000	-2.912519000
H	0.917654000	-0.521943000	-3.097471000
H	-0.133325000	-2.282911000	-2.178499000
H	-1.390700000	-2.100018000	-0.949349000
H	-2.172574000	-0.660198000	-2.842966000
H	-1.810062000	1.036361000	-2.504380000
H	-0.382331000	2.520722000	2.008753000
H	1.965030000	1.848845000	2.442032000

**<sup>1</sup>TS3/8<sup>+</sup>****<sup>3</sup>TS3/8<sup>+</sup>**

C	3.791447137	-2.734151568	1.099413712
C	4.430780137	-2.213670568	2.202079712
C	3.707896137	-1.404817568	3.104358712
C	2.373332137	-1.128629568	2.827507712
N	1.703376137	-1.708712568	1.821040712
C	2.378079137	-2.544461568	0.944910712
N	-1.575459863	-0.564063568	1.123955712
C	-2.513842863	-0.662826568	0.173019712
C	-3.837372863	-0.991576568	0.457706712
C	-4.193942863	-1.219657568	1.787074712
C	-3.216862863	-1.117556568	2.778678712
C	-1.912673863	-0.797129568	2.405629712
N	0.953334137	1.827457432	0.921872712
C	0.634173137	2.442540432	2.078633712
C	0.948847137	3.780099432	2.305077712
C	1.601625137	4.499044432	1.301279712
C	1.930849137	3.855156432	0.108351712
C	1.593633137	2.511648432	-0.038580288
C	1.584549137	-0.099790568	3.622158712
N	0.282557137	0.179370432	2.981533712
C	-0.119775863	1.597284432	3.084494712
C	-0.777622863	-0.756673568	3.407221712
N	1.623791137	-3.089103568	0.002601712
Cu	0.554608137	-0.205276568	0.924953712
O	1.111820137	-0.923756568	-0.701285288
H	4.331275137	-3.306986568	0.351425712
H	5.488667137	-2.395677568	2.365383712
H	4.186544137	-0.989485568	3.986362712
H	-2.184016863	-0.475862568	-0.844511288
H	-4.565363863	-1.063871568	-0.343307288
H	-5.216744863	-1.472330568	2.049652712
H	-3.460829863	-1.290067568	3.822742712
H	0.688963137	4.249648432	3.249056712
H	1.856216137	5.543438432	1.453865712
H	2.446249137	4.375983432	-0.691539288
H	1.841435137	1.950502432	-0.933934288
H	1.441718137	-0.422128568	4.663676712
H	2.157658137	0.831822432	3.651906712
H	0.019558137	1.980433432	4.104459712
H	-1.190163863	1.653166432	2.859037712
H	-1.146695863	-0.503701568	4.411199712
H	-0.322555863	-1.751118568	3.455601712
H	0.663074137	-0.693706568	-1.535607288
H	2.217094137	-3.561526568	-0.688006288

C	3.524447000	1.401992000	-0.493071000
C	3.946791000	0.267918000	-1.216707000
C	2.986453000	-0.574748000	-1.814063000
C	1.648916000	-0.272448000	-1.680517000
N	1.246941000	0.864358000	-1.011661000
C	2.170497000	1.688988000	-0.451962000
N	-2.377959000	0.527291000	0.099295000
C	-3.145786000	1.117762000	1.039584000
C	-4.480245000	0.790272000	1.219404000
C	-5.048460000	-0.197284000	0.402283000
C	-4.248604000	-0.826139000	-0.552583000
C	-2.917260000	-0.446358000	-0.690028000
N	0.468998000	-0.554164000	1.405445000
C	0.647025000	-1.759720000	0.821285000
C	1.702687000	-2.602610000	1.157111000
C	2.615417000	-2.187530000	2.128915000
C	2.438290000	-0.935860000	2.727881000
C	1.356788000	-0.155121000	2.333744000
C	0.480269000	-1.027784000	-2.237994000
N	-0.609892000	-1.063137000	-1.211558000
C	-0.405721000	-2.132693000	-0.193232000
C	-1.995530000	-1.033846000	-1.731398000
N	1.639967000	2.880612000	0.058647000
Cu	-0.455718000	0.765692000	-0.181267000
O	0.295000000	2.577976000	0.755985000
H	4.242989000	2.060174000	-0.014356000
H	5.003968000	0.046206000	-1.308379000
H	3.292643000	-1.459644000	-2.363601000
H	-2.654105000	1.862629000	1.657687000
H	-5.060027000	1.290765000	1.987164000
H	-6.090955000	-0.476505000	0.515625000
H	-4.652573000	-1.606880000	-1.189899000
H	1.812534000	-3.563348000	0.662699000
H	3.448731000	-2.824150000	2.409160000
H	3.124071000	-0.572758000	3.486414000
H	1.179008000	0.823976000	2.769509000
H	0.070036000	-0.491072000	-3.104437000
H	0.751379000	-2.041078000	-2.555456000
H	-0.154284000	-3.074540000	-0.696125000
H	-1.364699000	-2.267729000	0.319491000
H	-2.338664000	-2.030114000	-2.039673000
H	-1.990125000	-0.393087000	-2.622689000
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H	2.214701000	3.249966000	0.817091000

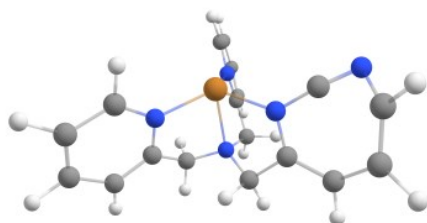
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C	-2.763546760	-1.570764748	2.130419571
C	-2.865087760	-0.568178748	3.074057571
C	-1.847919760	0.397566252	3.126591571
C	-0.754705760	0.319195252	2.246957571
N	-0.581368760	-0.695292748	1.403781571
C	-1.590988760	-1.685575748	1.292696571
N	-1.131939760	0.853760252	-1.076512429
C	-2.074005760	0.182218252	-1.754344429
C	-3.417597760	0.554236252	-1.750328429
C	-3.795813760	1.665606252	-0.998418429
C	-2.817387760	2.365892252	-0.288462429
C	-1.495723760	1.931369252	-0.358029429
N	2.629624240	0.095052252	-0.093138429
C	3.053654240	1.190351252	0.570942571
C	4.369062240	1.311347252	1.011668571
C	5.272266240	0.281327252	0.741258571
C	4.827662240	-0.845327748	0.049839571
C	3.492553240	-0.905595748	-0.340801429
C	0.360285240	1.349360252	2.253247571
N	0.666251240	1.796282252	0.879198571
C	2.043918240	2.308369252	0.738467571
C	-0.367514760	2.690401252	0.317031571
N	-1.461767760	-2.673193748	0.457613571
Cu	0.633393240	-0.150185748	-0.188753429
H	-3.542169760	-2.310815748	1.980308571
H	-3.725241760	-0.495820748	3.732697571
H	-1.894199760	1.207933252	3.848618571
H	-1.734028760	-0.689780748	-2.304132429
H	-4.143317760	-0.021531748	-2.314975429
H	-4.833971760	1.981660252	-0.959855429
H	-3.076521760	3.236417252	0.307393571
H	4.680657240	2.198375252	1.555108571
H	6.303403240	0.356061252	1.072906571
H	5.494625240	-1.670535748	-0.175643429
H	3.076341240	-1.768561748	-0.849357429
H	0.112831240	2.198487252	2.906284571
H	1.263367240	0.873327252	2.650940571
H	2.327551240	2.958687252	1.577788571
H	2.075201240	2.923548252	-0.166477429
H	0.110977240	3.315009252	-0.443672429
H	-0.767414760	3.369478252	1.081864571
O	0.492934240	-2.036522748	-0.998820429
H	0.399177240	-2.291354748	-1.930094429
H	-0.295923760	-2.486253748	-0.381046429

C	-2.751145906	-2.185639371	1.906647070
C	-3.024630906	-1.245852371	2.869346070
C	-2.131929906	-0.165600371	3.096581070
C	-1.004756906	-0.093120371	2.303930070
N	-0.723414906	-0.979215371	1.327478070
C	-1.554052906	-2.059036371	1.114351070
N	-1.600682906	0.870743629	-0.803904930
C	-2.567858906	0.246374629	-1.495200930
C	-3.903317906	0.629588629	-1.424664930
C	-4.248777906	1.691276629	-0.588521930
C	-3.246562906	2.332627629	0.140468070
C	-1.931646906	1.897339629	0.004898070
N	2.237442094	0.114405629	-0.066624930
C	2.673329094	1.124367629	0.715805070
C	3.987198094	1.175928629	1.169575070
C	4.871297094	0.162208629	0.792212070
C	4.411072094	-0.877000371	-0.016300930
C	3.078544094	-0.871539371	-0.419551930
C	0.033477094	0.997653629	2.414357070
N	0.291093094	1.627043629	1.077439070
C	1.655571094	2.205149629	1.004358070
C	-0.775177906	2.586065629	0.693086070
N	-1.202558906	-2.927372371	0.181710070
Cu	0.238794094	0.023211629	-0.276449930
H	-3.405019906	-3.031982371	1.727413070
H	-3.921079906	-1.338698371	3.476262070
H	-2.321408906	0.567215629	3.873739070
H	-2.255576906	-0.591812371	-2.107666930
H	-4.650703906	0.097707629	-2.003390930
H	-5.282508906	2.010298629	-0.497806930
H	-3.481474906	3.155041629	0.808996070
H	4.312052094	1.992832629	1.806510070
H	5.901798094	0.181294629	1.133399070
H	5.064424094	-1.686558371	-0.322937930
H	2.647863094	-1.661638371	-1.025004930
H	-0.254197906	1.769116629	3.138660070
H	0.980081094	0.555860629	2.741313070
H	1.908535094	2.751474629	1.921743070
H	1.672629094	2.925355629	0.179563070
H	-0.341102906	3.303723629	-0.011223930
H	-1.123081906	3.153719629	1.564166070
O	0.196036094	-1.592448371	-1.444323930
H	-0.033488906	-1.574113371	-2.387421930
H	-0.461518906	-2.282075371	-0.915029930

<sup>1</sup>TS5/6<sup>+</sup>

<sup>3</sup>TS5/6<sup>+</sup>

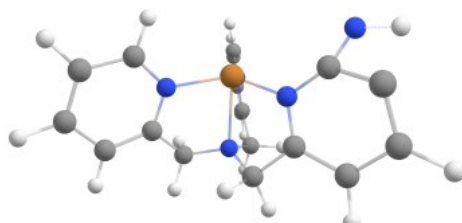


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C	-1.329142077	-0.977026254	1.990471326
N	-1.079019077	-0.666419254	0.676369326
C	-2.212011077	-0.411051254	0.085946326
N	1.193009923	1.925656746	0.574574326
C	1.594743923	2.829332746	-0.338523674
C	1.986788923	4.121275746	-0.001288674
C	1.974077923	4.491211746	1.343043326
C	1.561862923	3.556484746	2.293080326
C	1.166627923	2.285548746	1.878974326
N	2.298572923	-1.462975254	0.472731326
C	2.751865923	-1.582571254	1.742634326
C	3.639478923	-2.592216254	2.108582326
C	4.088857923	-3.494290254	1.142802326
C	3.627086923	-3.362266254	-0.165797674
C	2.731151923	-2.336143254	-0.454230674
C	-0.104913077	-1.077982254	2.884337326
N	0.919733923	-0.105154254	2.511993326
C	2.297447923	-0.533634254	2.747859326
C	0.619820923	1.277538746	2.879681326
N	-3.256446077	0.217963746	-0.138990674
Cu	0.867758923	-0.042773254	0.259174326
H	-4.159581077	-1.760714254	-0.575299674
H	-4.342542077	-2.450010254	1.839214326
H	-2.692774077	-1.638677254	3.484666326
H	1.599713923	2.494206746	-1.370712674
H	2.299150923	4.812190746	-0.777039674
H	2.281780923	5.486673746	1.648143326
H	1.540641923	3.809463746	3.348903326
H	3.975406923	-2.667274254	3.138482326
H	4.781815923	-4.286209254	1.410031326
H	3.945432923	-4.039854254	-0.950859674
H	2.338936923	-2.200593254	-1.457143674
H	-0.411629077	-0.995385254	3.938347326
H	0.327572923	-2.077340254	2.752925326
H	2.936932923	0.349757746	2.630131326
H	2.455696923	-0.906585254	3.771760326
H	-0.472232077	1.381025746	2.894497326
H	0.973667923	1.529789746	3.891173326

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C	-2.987652000	-2.210819000	1.250965000
C	-2.044646000	-1.420211000	1.888348000
C	-0.767218000	-1.143745000	1.353804000
N	-0.479458000	-1.501788000	0.031962000
C	-1.363085000	-2.209416000	-0.540773000
N	-1.214443000	1.231962000	-0.923248000
C	-2.170619000	1.096150000	-1.862315000
C	-3.501131000	1.430403000	-1.632786000
C	-3.856951000	1.921352000	-0.377055000
C	-2.868007000	2.063362000	0.596246000
C	-1.553432000	1.712971000	0.297133000
N	2.474716000	0.105088000	-0.701074000
C	2.930402000	0.495675000	0.514836000
C	4.225288000	0.197545000	0.931508000
C	5.078526000	-0.505443000	0.079480000
C	4.607056000	-0.895929000	-1.172893000
C	3.299174000	-0.573421000	-1.521514000
C	0.279117000	-0.314139000	2.033983000
N	0.602352000	0.900250000	1.260004000
C	1.996086000	1.331371000	1.382658000
C	-0.432044000	1.935032000	1.306341000
N	-2.261244000	-2.701451000	-1.282140000
Cu	0.550613000	0.363462000	-0.949031000
H	-2.625753000	-4.170045000	0.254292000
H	-3.980852000	-2.338889000	1.676589000
H	-2.299790000	-0.958992000	2.839367000
H	-1.846848000	0.706634000	-2.821592000
H	-4.234451000	1.301224000	-2.421391000
H	-4.886512000	2.186746000	-0.157076000
H	-3.111213000	2.441526000	1.584639000
H	4.559368000	0.515594000	1.914459000
H	6.090442000	-0.745657000	0.390941000
H	5.232525000	-1.443266000	-1.869794000
H	2.887330000	-0.859601000	-2.483394000
H	-0.045544000	-0.061459000	3.054651000
H	1.203948000	-0.897690000	2.118045000
H	2.059950000	2.369785000	1.039052000
H	2.355602000	1.316733000	2.422236000
H	-0.868133000	2.035172000	2.311505000
H	0.038891000	2.895602000	1.068778000

<sup>1</sup>TS5/9<sup>+</sup>

<sup>3</sup>TS5/9<sup>+</sup>



C	-4.14550000	1.325097000	-0.766920000
C	-4.316274000	1.624823000	0.627525000
C	-3.372888000	1.074681000	1.472681000
C	-2.134556000	0.535499000	0.966899000
N	-1.778865000	0.636300000	-0.306837000
C	-2.778970000	1.149855000	-1.092152000
N	1.676070000	1.254481000	-0.559475000
C	2.542134000	1.644828000	-1.511639000
C	3.709126000	2.348277000	-1.226382000
C	3.995801000	2.651189000	0.103722000
C	3.100079000	2.245337000	1.094173000
C	1.943621000	1.557957000	0.731523000
N	0.378602000	-1.962501000	-0.623208000
C	0.679292000	-2.364164000	0.632865000
C	0.735486000	-3.714249000	0.974064000
C	0.494813000	-4.679639000	-0.005043000
C	0.196163000	-4.262010000	-1.300947000
C	0.144027000	-2.895208000	-1.562773000
C	-1.165782000	-0.148084000	1.920040000
N	0.217264000	-0.073587000	1.466183000
C	1.015361000	-1.284349000	1.651518000
C	0.899064000	1.183693000	1.773361000
N	-2.834763000	2.047932000	-2.039217000
Cu	0.071030000	0.059577000	-0.799901000
H	-4.124727000	1.977571000	-1.987627000
H	-5.232980000	2.060941000	1.013378000
H	-3.551265000	1.012858000	2.542989000
H	2.282171000	1.379512000	-2.531304000
H	4.373920000	2.642636000	-2.031397000
H	4.900301000	3.190371000	0.367979000
H	3.292137000	2.463478000	2.140422000
H	0.968368000	-4.003816000	1.994459000
H	0.536049000	-5.735978000	0.242371000
H	-0.000100000	-4.973918000	-2.095574000
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H	-1.299114000	0.256220000	2.935477000
H	-1.458433000	-1.205309000	1.967184000
H	2.066314000	-1.004311000	1.512074000
H	0.930224000	-1.694264000	2.669620000
H	0.138119000	1.973723000	1.781111000
H	1.360315000	1.177212000	2.773315000

C	-4.148811000	1.075879000	-0.892991000
C	-4.566643000	0.793439000	0.456928000
C	-3.584118000	0.376818000	1.304002000
C	-2.217025000	0.201438000	0.844630000
N	-1.833446000	0.397938000	-0.393420000
C	-2.775794000	0.852060000	-1.330767000
N	1.510871000	1.447726000	-0.538981000
C	2.350887000	1.950193000	-1.461185000
C	3.403718000	2.802185000	-1.138687000
C	3.600644000	3.139996000	0.199360000
C	2.732371000	2.618079000	1.159354000
C	1.690887000	1.783301000	0.759063000
N	0.663172000	-1.914347000	-0.640532000
C	0.979300000	-2.272776000	0.624942000
C	1.209332000	-3.602996000	0.971485000
C	1.130913000	-4.591268000	-0.011111000
C	0.815121000	-4.216822000	-1.316150000
C	0.584667000	-2.869610000	-1.583379000
C	-1.192485000	-0.336828000	1.839193000
N	0.181808000	-0.069761000	1.438431000
C	1.133415000	-1.158263000	1.650122000
C	0.670835000	1.269001000	1.764587000
N	-3.128903000	2.231519000	-1.267743000
Cu	0.081449000	0.042945000	-0.825809000
H	-4.276805000	2.131092000	-1.668709000
H	-5.607564000	0.853659000	0.757668000
H	-3.811386000	0.132573000	2.338193000
H	2.164921000	1.652733000	-2.488271000
H	4.051908000	3.182186000	-1.921117000
H	4.415867000	3.794206000	0.492858000
H	2.856967000	2.858550000	2.210929000
H	1.449941000	-3.858916000	1.999077000
H	1.308926000	-5.632349000	0.240431000
H	0.740483000	-4.948084000	-2.113973000
H	0.324721000	-2.533510000	-2.582342000
H	-1.419854000	0.054041000	2.843676000
H	-1.333600000	-1.424061000	1.892363000
H	2.139376000	-0.735804000	1.540353000
H	1.076462000	-1.578195000	2.666308000
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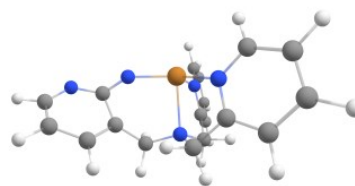


<sup>1</sup>TS6/

7'+



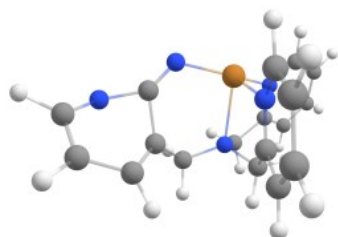
<sup>1</sup>TS6/7'+



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C	1.762665775	-1.322503631	2.539409412
N	3.931066775	-1.019606631	0.980983412
C	2.688074775	-0.795830631	1.244211412
N	-2.112808225	-0.882085631	1.236684412
C	-3.101756225	-0.981192631	0.328993412
C	-4.374433225	-1.445989631	0.647273412
C	-4.638843225	-1.812693631	1.966100412
C	-3.616673225	-1.709252631	2.910399412
C	-2.361336225	-1.251294631	2.515022412
N	-0.051801225	2.019522369	1.431778412
C	-0.172545225	2.297965369	2.750628412
C	0.153157775	3.551782369	3.264072412
C	0.600178775	4.552136369	2.399361412
C	0.714481775	4.263919369	1.040222412
C	0.381653775	2.984916369	0.601859412
C	1.134523775	-0.418877631	3.577923412
N	-0.264199225	-0.125272631	3.241180412
C	-0.731530225	1.200921369	3.644623412
C	-1.197744225	-1.220949631	3.495476412
N	1.451183775	-0.897906631	1.086351412
Cu	-0.357204225	0.057694369	0.983844412
H	5.181723775	-2.670433631	0.953238412
H	3.716548775	-4.135526631	2.277261412
H	2.064615775	-3.070966631	3.747889412
H	-2.853670225	-0.674732631	-0.681993588
H	-5.135487225	-1.509939631	-0.123034588
H	-5.621937225	-2.170179631	2.256728412
H	-3.787478225	-1.984930631	3.946734412
H	0.055471775	3.740198369	4.329005412
H	0.858342775	5.534799369	2.782062412
H	1.060116775	5.007127369	0.329652412
H	0.463456775	2.712802369	-0.445779588
H	1.239156775	-0.873331631	4.575206412
H	1.674983775	0.533203369	3.604791412
H	-0.503968225	1.426685369	4.697906412
H	-1.824096225	1.206606369	3.547845412
H	-1.583183225	-1.214057631	4.527106412
H	-0.639927225	-2.157210631	3.371816412

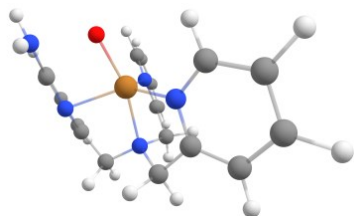
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C	-2.833818000	-0.369338000	-0.625281000
N	1.424648000	1.561779000	-0.673968000
C	2.330327000	2.031662000	-1.549358000
C	3.274611000	2.997728000	-1.211334000
C	3.286200000	3.490181000	0.092841000
C	2.347828000	3.003547000	1.004651000
C	1.425125000	2.046585000	0.588429000
N	1.037388000	-1.833591000	-0.452004000
C	1.201690000	-2.017863000	0.876626000
C	1.558717000	-3.257744000	1.403829000
C	1.767828000	-4.334103000	0.540391000
C	1.606625000	-4.137840000	-0.830383000
C	1.235253000	-2.873460000	-1.280466000
C	-1.355034000	-0.279356000	1.561978000
N	0.030449000	0.130809000	1.279950000
C	1.047093000	-0.799474000	1.775580000
C	0.328687000	1.543787000	1.513383000
N	-1.720651000	-0.077610000	-1.148819000
Cu	0.167101000	-0.021714000	-0.945589000
H	-5.956371000	0.333836000	-0.815386000
H	-5.128243000	2.309636000	0.470802000
H	-2.981966000	2.102527000	1.698470000
H	2.288209000	1.614443000	-2.550488000
H	3.982960000	3.346240000	-1.955284000
H	4.012599000	4.237355000	0.397482000
H	2.328342000	3.363435000	2.028987000
H	1.672052000	-3.376110000	2.477348000
H	2.046057000	-5.307466000	0.932762000
H	1.754604000	-4.944477000	-1.540424000
H	1.083958000	-2.677107000	-2.337353000
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H	2.004094000	-0.264449000	1.784454000
H	0.589567000	1.756657000	2.561567000
H	-0.580401000	2.112010000	1.287010000

# <sup>1</sup>TS7/10<sup>+</sup>



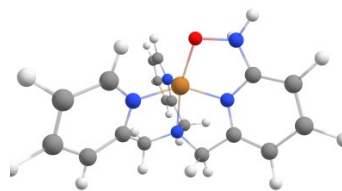
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C	-2.061236000	-1.172344000	0.560559000
N	-2.879001000	-2.416951000	-0.827348000
C	-1.823161000	-1.465076000	-0.938985000
N	-0.375983000	1.576496000	-0.472410000
C	-1.068303000	2.406271000	-1.266432000
C	-1.964183000	3.350221000	-0.767753000
C	-2.152957000	3.423647000	0.612012000
C	-1.446281000	2.548067000	1.437747000
C	-0.567065000	1.634294000	0.858961000
N	2.531657000	-0.222078000	-0.565131000
C	2.782275000	-0.716375000	0.668681000
C	4.064756000	-0.701614000	1.211782000
C	5.119653000	-0.181573000	0.460066000
C	4.857090000	0.319984000	-0.814223000
C	3.548482000	0.284851000	-1.286081000
C	-0.847387000	-1.483276000	1.417421000
N	0.341117000	-0.671601000	1.125236000
C	1.618093000	-1.343549000	1.416826000
C	0.269403000	0.688069000	1.696148000
N	-0.876890000	-1.203123000	-1.657224000
Cu	0.599048000	-0.235692000	-1.067412000
H	-4.896768000	-2.477520000	-1.280463000
H	-5.429018000	-0.656967000	0.514339000
H	-3.294896000	-0.015795000	1.874479000
H	-0.895125000	2.303261000	-2.333498000
H	-2.497499000	4.005741000	-1.447980000
H	-2.843849000	4.144423000	1.038887000
H	-1.576781000	2.570192000	2.515792000
H	4.233874000	-1.096165000	2.209031000
H	6.126592000	-0.165201000	0.865586000
H	5.644598000	0.735411000	-1.433631000
H	3.293140000	0.669495000	-2.268102000
H	-1.145139000	-1.362126000	2.467873000
H	-0.591261000	-2.536883000	1.273378000
H	1.838740000	-1.358146000	2.494733000
H	1.523350000	-2.385629000	1.091539000
H	-0.106809000	0.661018000	2.729041000
H	1.289966000	1.083519000	1.736365000

# <sup>1</sup>TS2/11<sup>+</sup>



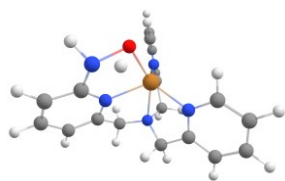
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C	2.877013252	-1.640121584	1.986589009
N	2.469136252	-2.737519584	1.321456009
C	3.339212252	-3.378721584	0.522949009
N	-1.192497748	-1.630181584	-0.036689991
C	-2.008183748	-1.954030584	-1.055309991
C	-3.357757748	-1.612939584	-1.048455991
C	-3.866048748	-0.908313584	0.042717009
C	-3.012898748	-0.575897584	1.097393009
C	-1.677198748	-0.961774584	1.033911009
N	2.017125252	-0.312002584	-0.738835991
C	2.011575252	0.759726416	0.069477009
C	2.941737252	1.787249416	-0.061945991
C	3.903550252	1.688229416	-1.071394991
C	3.908510252	0.567455416	-1.901974991
C	2.943658252	-0.419193584	-1.695616991
C	1.732405252	-0.933006584	2.677717009
N	0.678734252	-0.584478584	1.670379009
C	0.894254252	0.766088416	1.088738009
C	-0.704781748	-0.733059584	2.174882009
N	2.796975252	-4.379549584	-0.235937991
Cu	0.747257252	-1.929433584	0.000692009
O	1.200052252	-3.245719584	-1.101831991
H	5.360391252	-3.494095584	-0.271759991
H	6.125233252	-1.522863584	1.047261009
H	4.479453252	-0.288940584	2.487104009
H	-1.549915748	-2.497008584	-1.874336991
H	-3.988871748	-1.892766584	-1.884964991
H	-4.912035748	-0.619090584	0.074457009
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H	2.919182252	2.641868416	0.607750009
H	4.641999252	2.473918416	-1.200932991
H	4.643633252	0.455531416	-2.692178991
H	2.893993252	-1.327266584	-2.290331991
H	1.284386252	-1.614319584	3.405157009
H	2.069546252	-0.037180584	3.211797009
H	1.079968252	1.503986416	1.880632009
H	-0.033718748	1.054909416	0.582318009
H	-1.017678748	0.126754416	2.783466009
H	-0.726022748	-1.616482584	2.821787009
H	3.357576252	-4.875017584	-0.916641991
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# <sup>3</sup>TS2/11<sup>+</sup>



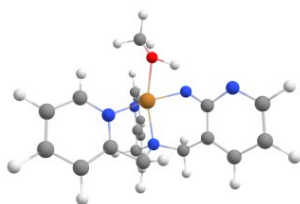
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C	-3.336183443	1.167285375	0.399536316
C	-2.030639443	0.933313375	0.050649316
N	-1.532841443	1.314026375	-1.160226684
C	-2.406269443	1.781832375	-2.120405684
N	1.868576557	1.090064375	-1.766009684
C	2.752429557	1.319690375	-2.747169684
C	4.013058557	1.862517375	-2.505644684
C	4.363764557	2.166692375	-1.189767684
C	3.445350557	1.921076375	-0.167034684
C	2.200216557	1.387191375	-0.495694684
N	0.121034557	-1.834851625	-1.853345684
C	0.486318557	-2.319988625	-0.648424684
C	0.482355557	-3.687300625	-0.385693684
C	0.102807557	-4.569631625	-1.399834684
C	-0.272291443	-4.058399625	-2.642520684
C	-0.257233443	-2.678300625	-2.826704684
C	-1.066146443	0.063446375	0.846109316
N	0.268809557	0.000639375	0.185793316
C	0.953568557	-1.296309625	0.368658316
C	1.121433557	1.153238375	0.542942316
N	-1.746901443	1.797398375	-3.388107684
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H	-5.274680443	1.883440375	-0.342278684
H	-3.710388443	0.868716375	1.373768316
H	2.426658557	1.056353375	-3.749776684
H	4.699730557	2.034704375	-3.327713684
H	5.339641557	2.583971375	-0.960435684
H	3.690099557	2.141910375	0.867683316
H	0.769586557	-4.054821625	0.594777316
H	0.093341557	-5.639928625	-1.217472684
H	-0.580455443	-4.710640625	-3.452523684
H	-0.559683443	-2.214243625	-3.760605684
H	-0.965418443	0.388165375	1.890693316
H	-1.461431443	-0.957494625	0.861404316
H	0.828393557	-1.675388625	1.391465316
H	2.025624557	-1.127444625	0.216544316
H	1.563131557	1.024197375	1.541056316
H	0.469650557	2.032249375	0.580355316
H	-2.399095443	1.876687375	-4.172093684
H	-1.040470443	2.536671375	-3.464025684

### $^3\text{TS11/8}^+$



C	-4.542851803	2.198094952	-1.576608125
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C	-4.019798803	1.263785952	0.584946875
C	-2.871676803	0.698492952	0.031461875
N	-2.550196803	0.893657952	-1.258936125
C	-3.357615803	1.617000952	-2.025582125
N	0.949295197	0.876693952	-1.736797125
C	1.844500197	1.158477952	-2.700808125
C	3.130408197	1.618382952	-2.430062125
C	3.509924197	1.785257952	-1.098600125
C	2.585551197	1.490347952	-0.095863125
C	1.310633197	1.046843952	-0.446066125
N	-0.946227803	-2.063788048	-1.909208125
C	-0.628446803	-2.586258048	-0.704318125
C	-0.807335803	-3.940419048	-0.424899125
C	-1.310690803	-4.784629048	-1.415917125
C	-1.629730803	-4.242833048	-2.660415125
C	-1.435378803	-2.878277048	-2.860468125
C	-1.967613803	-0.230861048	0.832805875
N	-0.623999803	-0.321112048	0.290591875
C	-0.016434803	-1.645312048	0.322541875
C	0.256035197	0.790380952	0.619962875
N	-2.925833803	1.815996952	-3.373764125
Cu	-0.842564803	-0.035822048	-2.086801125
O	-1.870584803	0.849545952	-3.894642125
H	-5.176552803	2.777993952	-2.240531125
H	-5.773656803	2.455379952	0.170561875
H	-4.252841803	1.110274952	1.634166875
H	1.506471197	1.002529952	-3.720902125
H	3.813678197	1.830810952	-3.245626125
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H	2.847604197	1.602872952	0.952092875
H	-0.551533803	-4.326652048	0.557428875
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H	-1.981528803	0.070760952	1.893226875
H	-2.414420803	-1.231855048	0.790773875
H	-0.059575803	-2.110503048	1.320910875
H	1.045681197	-1.523650048	0.078212875
H	0.750053197	0.665336952	1.598181875
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H	-3.670467803	1.875511952	-4.066126125
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# <sup>1</sup>TS12/13<sup>+</sup>



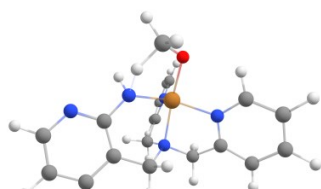
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N	-4.488676243	-1.561251787	0.303329509
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Cu	-0.896640243	-0.658554787	-0.311135491
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C	0.965630757	3.278197213	-0.371089491
C	0.597434757	1.996024213	0.027466509
N	0.856941757	-2.053468787	-0.878324491
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C	2.073372757	-4.118442787	-0.714515491
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C	1.354428757	-3.312532787	-2.861451491
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C	0.125126757	-1.089078787	-2.968959491
N	-1.171071243	-0.700030787	-2.344613491
C	-1.517252243	0.702257213	-2.681720491
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H	0.796335757	4.737387213	-1.954700491
H	1.582430757	3.891792213	0.276489509
H	0.908402757	1.582780213	0.981265509
H	1.497605757	-2.828308787	0.923427509
H	2.566684757	-4.847929787	-0.080936491
H	2.448838757	-5.152880787	-2.573591491
H	1.279151757	-3.409623787	-3.940347491
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H	0.779489757	-0.212328787	-2.950789491
H	-1.468541243	0.872455213	-3.765789491
H	-2.555599243	0.865574213	-2.369609491
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H	-2.456911243	-1.557394787	-3.812469491
O	-1.255620243	-0.545482787	1.627984509
H	-1.956972243	-1.353873787	1.296391509
C	-0.278476243	-1.067030787	2.533321509
H	-0.160294243	-2.149435787	2.398784509
H	0.682678757	-0.568183787	2.369317509
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# <sup>1</sup>TS12/13<sup>+</sup>

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C	0.350988000	3.661196000	-1.461144000
C	1.092783000	4.587915000	-0.724958000
C	1.662290000	4.196337000	0.487754000
C	1.478507000	2.883159000	0.915600000
N	1.896398000	-1.252752000	0.046662000
C	2.679494000	-2.064284000	0.775437000
C	3.501148000	-3.028416000	0.195591000
C	3.496402000	-3.160897000	-1.192962000
C	2.676926000	-2.321766000	-1.951254000
C	1.894275000	-1.373625000	-1.296746000
C	1.045797000	-0.369032000	-2.044427000
N	-0.198545000	-0.037419000	-1.310469000
C	-0.664410000	1.327800000	-1.633988000
C	-1.239406000	-1.077014000	-1.542406000
H	-3.772838000	-1.188303000	-2.513977000
H	-5.901326000	-1.098818000	-1.197534000
H	-5.779371000	-0.808577000	1.285352000
H	-0.110760000	3.937829000	-2.404229000
H	1.220744000	5.601405000	-1.092874000
H	2.237564000	4.889975000	1.091497000
H	1.886624000	2.519760000	1.853564000
H	2.636571000	-1.930703000	1.850744000
H	4.120445000	-3.661000000	0.822352000
H	4.115962000	-3.907909000	-1.679639000
H	2.646058000	-2.400949000	-3.033609000
H	0.816911000	-0.726062000	-3.057649000
H	1.623370000	0.555967000	-2.147819000
H	-0.699344000	1.488134000	-2.720898000
H	-1.688708000	1.421866000	-1.258029000
H	-0.779234000	-2.032760000	-1.264428000
H	-1.465357000	-1.126109000	-2.617953000
O	0.281709000	0.176360000	2.724695000
H	-0.872021000	-0.191684000	2.410867000
C	0.964787000	-0.628572000	3.667573000
H	0.791929000	-1.702863000	3.494715000
H	2.043254000	-0.426824000	3.622954000
H	0.616283000	-0.383517000	4.678824000

# <sup>1</sup>TS13/14<sup>+</sup>

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C	-1.882571286	-1.285324735	-3.651204275
C	-3.031612286	-1.520392735	-4.411532275
C	-4.291844286	-1.467864735	-3.818609275
C	-4.367511286	-1.130019735	-2.463257275
N	-3.291316286	-0.872745735	-1.719425275
C	-2.075026286	-0.981198735	-2.280901275
N	-0.981271286	-0.769069735	-1.425621275
Cu	0.839726714	-0.315428735	-1.959545275
N	0.848933714	1.882395265	-2.251406275
C	0.304142714	2.265750265	-3.420453275
C	0.311510714	3.597015265	-3.835886275
C	0.886090714	4.559934265	-3.003701275
C	1.443092714	4.160267265	-1.788201275
C	1.406240714	2.807106265	-1.455230275
N	2.548468714	-1.055728735	-2.731204275
C	3.479941714	-1.712623735	-2.023172275
C	4.547418714	-2.362322735	-2.638102275
C	4.629346714	-2.345178735	-4.031124275
C	3.651109714	-1.667645735	-4.762281275
C	2.626331714	-1.020392735	-4.076208275
C	1.590431714	-0.168088735	-4.772247275
N	0.310278714	-0.117123735	-4.033512275
C	-0.364911286	1.176590265	-4.241114275
C	-0.527633286	-1.317198735	-4.317598275
H	-2.936914286	-1.741119735	-5.471720275
H	-5.192605286	-1.657272735	-4.392737275
H	-5.327507286	-1.048893735	-1.959690275
H	-0.125902286	3.874022265	-4.790642275
H	0.901970714	5.603599265	-3.302900275
H	1.901351714	4.875689265	-1.113601275
H	1.832901714	2.439823265	-0.525915275
H	3.328370714	-1.707728735	-0.948194275
H	5.287331714	-2.877275735	-2.034879275
H	5.439915714	-2.854645735	-4.543316275
H	3.683788714	-1.638187735	-5.847114275
H	1.434562714	-0.505866735	-5.806606275
H	1.980579714	0.854524265	-4.823918275
H	-0.389935286	1.455364265	-5.304537275
H	-1.403580286	1.073198265	-3.914545275
H	0.056810714	-2.183053735	-3.983552275
H	-0.673136286	-1.424656735	-5.403040275
O	1.306366714	-1.044881735	-0.158690275
C	-1.312262286	-0.129418735	-0.693493275
H	0.424949714	-1.850930735	0.400603725
H	-0.574337286	-1.735779735	-0.389128275
H	0.649363714	-2.929279735	0.347595725
H	0.000701714	-1.514582735	1.359749725

C	-2.395106000	-1.083015000	-0.807586000
C	-3.528004000	-1.411769000	-1.557986000
C	-4.800718000	-1.313986000	-0.998967000
C	-4.900803000	-0.843140000	0.313378000
N	-3.839689000	-0.518203000	1.052992000
C	-2.610287000	-0.654259000	0.526300000
N	-1.543770000	-0.309410000	1.360787000
Cu	0.407043000	-0.124405000	0.813457000
N	0.614081000	2.038974000	0.412009000
C	0.007112000	2.399345000	-0.733676000
C	0.029086000	3.714497000	-1.196298000
C	0.684686000	4.684328000	-0.434784000
C	1.304093000	4.308217000	0.758067000
C	1.247469000	2.969369000	1.141459000
N	2.040869000	-1.052635000	0.068371000
C	2.930158000	-1.748343000	0.797212000
C	3.944967000	-2.489891000	0.198643000
C	4.022211000	-2.517654000	-1.195021000
C	3.092445000	-1.794416000	-1.945574000
C	2.115855000	-1.061546000	-1.276479000
C	1.128645000	-0.162118000	-1.980892000
N	-0.131019000	-0.015028000	-1.212530000
C	-0.748015000	1.304541000	-1.464565000
C	-1.037743000	-1.173242000	-1.468256000
H	-3.411232000	-1.735151000	-2.589712000
H	-5.688389000	-1.571055000	-1.566826000
H	-5.870099000	-0.717655000	0.789755000
H	-0.459993000	3.974756000	-2.130371000
H	0.713152000	5.716533000	-0.770517000
H	1.823149000	5.031449000	1.377963000
H	1.714826000	2.618750000	2.057359000
H	2.799757000	-1.690443000	1.872658000
H	4.650182000	-3.037411000	0.814466000
H	4.794134000	-3.096508000	-1.692903000
H	3.126057000	-1.796143000	-3.030668000
H	0.924846000	-0.517185000	-3.000010000
H	1.581046000	0.831881000	-2.067929000
H	-0.799360000	1.517649000	-2.541356000
H	-1.775686000	1.269832000	-1.093511000
H	-0.491317000	-2.064760000	-1.137143000
H	-1.187587000	-1.278312000	-2.552600000
O	0.764107000	-0.584127000	2.662182000
H	-1.882650000	0.349203000	2.066391000
C	-0.028867000	-1.619905000	2.962009000
H	-1.132519000	-1.235634000	2.283647000
H	0.131703000	-2.557763000	2.397965000
H	-0.203543000	-1.779211000	4.032332000