

Electronic supplementary information

S1. Cartesian coordinates of optimised geometries of cationic Au complexes

N1⁺

Energy (au)

| | | | |
|----|--------------|--------------|--------------|
| Au | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -2.027912000 | 0.000000000 | 0.000000000 |
| N | -2.858970000 | 0.746196000 | 0.746171000 |
| C | -4.179495000 | 0.477472000 | 0.477457000 |
| H | -4.992179000 | 0.976454000 | 0.976422000 |
| C | -4.179495000 | -0.477472000 | -0.477456000 |
| H | -4.992179000 | -0.976454000 | -0.976421000 |
| N | -2.858970000 | -0.746196000 | -0.746171000 |
| C | 2.027912000 | 0.000000000 | 0.000000000 |
| N | 2.858970000 | -0.746195000 | 0.746172000 |
| C | 4.179495000 | -0.477472000 | 0.477456000 |
| H | 4.992179000 | -0.976453000 | 0.976423000 |
| C | 4.179495000 | 0.477472000 | -0.477457000 |
| H | 4.992179000 | 0.976453000 | -0.976424000 |
| N | 2.858970000 | 0.746195000 | -0.746172000 |
| H | 2.533559000 | -1.419394000 | 1.419350000 |
| H | 2.533558000 | 1.419394000 | -1.419351000 |
| H | -2.533558000 | 1.419396000 | 1.419349000 |
| H | -2.533559000 | -1.419396000 | -1.419349000 |

N2⁺

| | | | |
|----|--------------|--------------|--------------|
| Au | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -2.037981000 | 0.000000000 | 0.000000000 |
| N | -2.859547000 | -0.755835000 | -0.755801000 |
| C | -4.174416000 | -0.477412000 | -0.477390000 |
| H | -4.989190000 | -0.975400000 | -0.975356000 |
| C | -4.174416000 | 0.477412000 | 0.477390000 |
| H | -4.989190000 | 0.975400000 | 0.975356000 |
| N | -2.859547000 | 0.755835000 | 0.755801000 |
| C | -2.436877000 | -1.735505000 | -1.735426000 |
| H | -1.349671000 | -1.759565000 | -1.759501000 |
| H | -2.812739000 | -2.722120000 | -1.463010000 |
| H | -2.812757000 | -1.463145000 | -2.722050000 |
| C | -2.436877000 | 1.735505000 | 1.735426000 |
| H | -1.349671000 | 1.759565000 | 1.759501000 |
| H | -2.812758000 | 1.463145000 | 2.722050000 |
| H | -2.812739000 | 2.722121000 | 1.463010000 |
| C | 2.037981000 | 0.000000000 | 0.000000000 |
| N | 2.859547000 | 0.755836000 | -0.755800000 |
| C | 4.174416000 | 0.477412000 | -0.477390000 |
| H | 4.989190000 | 0.975401000 | -0.975355000 |
| C | 4.174416000 | -0.477412000 | 0.477389000 |
| H | 4.989190000 | -0.975401000 | 0.975355000 |
| N | 2.859547000 | -0.755836000 | 0.755800000 |
| C | 2.436877000 | 1.735507000 | -1.735424000 |
| H | 1.349671000 | 1.759567000 | -1.759499000 |
| H | 2.812739000 | 2.722122000 | -1.463007000 |
| H | 2.812757000 | 1.463149000 | -2.722048000 |
| C | 2.436877000 | -1.735507000 | 1.735424000 |
| H | 1.349671000 | -1.759567000 | 1.759500000 |
| H | 2.812758000 | -1.463149000 | 2.722048000 |
| H | 2.812739000 | -2.722122000 | 1.463007000 |

N3⁺

| | | | |
|----|-------------|--------------|--------------|
| Au | 0.000000000 | -0.000001000 | 0.000000000 |
| C | 2.033589000 | 0.000000000 | 0.000000000 |
| N | 2.852351000 | 0.951541000 | -0.487135000 |
| C | 4.167380000 | 0.603273000 | -0.304762000 |
| H | 4.982070000 | 1.233509000 | -0.618945000 |
| C | 4.167381000 | -0.603271000 | 0.304764000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.982071000 | -1.233505000 | 0.618948000 |
| N | 2.852352000 | -0.951541000 | 0.487136000 |
| C | 2.403119000 | 2.215736000 | -1.055392000 |
| H | 1.512033000 | 2.006128000 | -1.649026000 |
| H | 3.180355000 | 2.556502000 | -1.741182000 |
| C | 2.403121000 | -2.215738000 | 1.055390000 |
| H | 1.512034000 | -2.006131000 | 1.649024000 |
| H | 3.180357000 | -2.556506000 | 1.741179000 |
| C | -2.033589000 | 0.000000000 | 0.000000000 |
| N | -2.852352000 | -0.951540000 | -0.487136000 |
| C | -4.167381000 | -0.603269000 | -0.304765000 |
| H | -4.982072000 | -1.233503000 | -0.618950000 |
| C | -4.167380000 | 0.603274000 | 0.304761000 |
| H | -4.982070000 | 1.233511000 | 0.618943000 |
| N | -2.852351000 | 0.951542000 | 0.487135000 |
| C | -2.403121000 | -2.215737000 | -1.055390000 |
| H | -1.512034000 | -2.006131000 | -1.649023000 |
| H | -3.180357000 | -2.556505000 | -1.741179000 |
| C | -2.403118000 | 2.215737000 | 1.055391000 |
| H | -1.512033000 | 2.006128000 | 1.649026000 |
| H | -3.180354000 | 2.556504000 | 1.741181000 |
| C | 2.116442000 | 3.253875000 | 0.010158000 |
| H | 1.785856000 | 4.183708000 | -0.455838000 |
| H | 3.006418000 | 3.467744000 | 0.604763000 |
| H | 1.329293000 | 2.904905000 | 0.681815000 |
| C | 2.116442000 | -3.253874000 | -0.010163000 |
| H | 1.329292000 | -2.904903000 | -0.681818000 |
| H | 1.785860000 | -4.183708000 | 0.455831000 |
| H | 3.006419000 | -3.467738000 | -0.604770000 |
| C | -2.116445000 | -3.253873000 | 0.010163000 |
| H | -1.329298000 | -2.904901000 | 0.681822000 |
| H | -1.785858000 | -4.183707000 | -0.455830000 |
| H | -3.006423000 | -3.467741000 | 0.604767000 |
| C | -2.116438000 | 3.253876000 | -0.010157000 |
| H | -1.785856000 | 4.183708000 | 0.455842000 |
| H | -3.006413000 | 3.467744000 | -0.604765000 |
| H | -1.329287000 | 2.904909000 | -0.681813000 |

N4⁺

| | | | |
|----|--------------|--------------|--------------|
| Au | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -2.037891000 | 0.000000000 | 0.000000000 |
| N | -2.855837000 | -0.757356000 | 0.757355000 |
| C | -4.169972000 | -0.477684000 | 0.477683000 |
| H | -4.990041000 | -0.970471000 | 0.970470000 |
| C | -4.169972000 | 0.477684000 | -0.477683000 |
| H | -4.990041000 | 0.970471000 | -0.970470000 |
| N | -2.855837000 | 0.757356000 | -0.757355000 |
| C | -2.409448000 | -1.745246000 | 1.745246000 |
| H | -1.318179000 | -1.700605000 | 1.700599000 |
| C | -2.409448000 | 1.745246000 | -1.745246000 |
| H | -1.318179000 | 1.700605000 | -1.700599000 |
| C | 2.037891000 | 0.000000000 | 0.000000000 |
| N | 2.855837000 | -0.757357000 | -0.757355000 |
| C | 4.169972000 | -0.477684000 | -0.477683000 |
| H | 4.990041000 | -0.970471000 | -0.970469000 |
| C | 4.169972000 | 0.477684000 | 0.477683000 |
| H | 4.990041000 | 0.970471000 | 0.970469000 |
| N | 2.855837000 | 0.757357000 | 0.757355000 |
| C | 2.409448000 | -1.745249000 | -1.745243000 |
| H | 1.318179000 | -1.700602000 | -1.700601000 |
| C | 2.409448000 | 1.745249000 | 1.745243000 |
| H | 1.318179000 | 1.700602000 | 1.700601000 |
| C | -2.866059000 | -1.348301000 | 3.137459000 |
| C | -2.866068000 | -3.137458000 | 1.348308000 |
| C | -2.866068000 | 3.137458000 | -1.348308000 |
| C | -2.866059000 | 1.348301000 | -3.137459000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.866067000 | -1.348313000 | -3.137456000 |
| C | 2.866059000 | -3.137461000 | -1.348296000 |
| C | 2.866067000 | 1.348313000 | 3.137456000 |
| C | 2.866059000 | 3.137461000 | 1.348296000 |
| H | 2.523348000 | 0.344130000 | 3.392609000 |
| H | 3.955113000 | 1.373514000 | 3.221877000 |
| H | 2.461882000 | 2.047897000 | 3.870592000 |
| H | 3.955105000 | 3.221887000 | 1.373491000 |
| H | 2.461874000 | 3.870600000 | 2.047878000 |
| H | 2.523334000 | 3.392606000 | 0.344113000 |
| H | -3.955114000 | 3.221879000 | -1.373509000 |
| H | -2.523350000 | 3.392609000 | -0.344125000 |
| H | -2.461882000 | 3.870595000 | -2.047891000 |
| H | -2.523333000 | 0.344119000 | -3.392605000 |
| H | -3.955105000 | 1.373495000 | -3.221885000 |
| H | -2.461874000 | 2.047884000 | -3.870596000 |
| H | 2.523348000 | -0.344130000 | -3.392609000 |
| H | 3.955113000 | -1.373514000 | -3.221877000 |
| H | 2.461882000 | -2.047897000 | -3.870592000 |
| H | 2.523334000 | -3.392606000 | -0.344113000 |
| H | 3.955105000 | -3.221887000 | -1.373491000 |
| H | 2.461874000 | -3.870600000 | -2.047878000 |
| H | -2.461882000 | -3.870595000 | 2.047891000 |
| H | -3.955114000 | -3.221879000 | 1.373509000 |
| H | -2.523350000 | -3.392609000 | 0.344125000 |
| H | -2.523333000 | -0.344119000 | 3.392605000 |
| H | -2.461874000 | -2.047884000 | 3.870596000 |
| H | -3.955105000 | -1.373495000 | 3.221885000 |

N5+

| | | | |
|----|--------------|--------------|--------------|
| 79 | 0.000000000 | 0.000000000 | 0.000001000 |
| 6 | -2.061001000 | 0.000001000 | 0.000155000 |
| 7 | -2.884974000 | 0.962071000 | -0.484682000 |
| 6 | -2.469568000 | 2.271924000 | -1.067644000 |
| 6 | -1.843881000 | 3.108105000 | 0.042674000 |
| 6 | -1.508436000 | 2.037295000 | -2.227081000 |
| 6 | -3.692515000 | 3.004707000 | -1.606303000 |
| 6 | -4.196467000 | 0.601944000 | -0.301232000 |
| 6 | -4.196423000 | -0.601940000 | 0.301858000 |
| 7 | -2.884903000 | -0.962068000 | 0.485114000 |
| 6 | -2.469412000 | -2.271922000 | 1.068013000 |
| 6 | -1.508109000 | -2.037293000 | 2.227310000 |
| 6 | -1.843886000 | -3.108101000 | -0.042397000 |
| 6 | -3.692279000 | -3.004705000 | 1.606850000 |
| 6 | 2.061001000 | -0.000001000 | -0.000154000 |
| 7 | 2.884975000 | 0.962073000 | 0.484673000 |
| 6 | 2.469571000 | 2.271931000 | 1.067624000 |
| 6 | 1.508442000 | 2.037312000 | 2.227065000 |
| 6 | 1.843881000 | 3.108102000 | -0.042700000 |
| 6 | 3.692519000 | 3.004718000 | 1.606274000 |
| 6 | 4.196468000 | 0.601944000 | 0.301221000 |
| 6 | 4.196422000 | -0.601945000 | -0.301858000 |
| 7 | 2.884901000 | -0.962074000 | -0.485107000 |
| 6 | 2.469408000 | -2.271934000 | -1.067994000 |
| 6 | 1.843887000 | -3.108103000 | 0.042426000 |
| 6 | 1.508103000 | -2.037315000 | -2.227289000 |
| 6 | 3.692274000 | -3.004721000 | -1.606828000 |
| 1 | -2.574559000 | 3.305759000 | 0.829741000 |
| 1 | -1.503121000 | 4.063983000 | -0.358936000 |
| 1 | -0.991483000 | 2.598566000 | 0.489479000 |
| 1 | -1.981275000 | 1.430298000 | -3.001707000 |
| 1 | -0.595383000 | 1.531620000 | -1.908614000 |
| 1 | -1.229404000 | 2.997469000 | -2.663983000 |
| 1 | -4.204744000 | 2.431860000 | -2.382075000 |
| 1 | -3.355285000 | 3.939128000 | -2.055689000 |
| 1 | -4.402206000 | 3.263585000 | -0.818442000 |

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|---|--------------|--------------|--------------|
| 1 | -5.027365000 | 1.209383000 | -0.605148000 |
| 1 | -5.027276000 | -1.209380000 | 0.605896000 |
| 1 | -1.980833000 | -1.430293000 | 3.002003000 |
| 1 | -0.595101000 | -1.531622000 | 1.908708000 |
| 1 | -1.229017000 | -2.997467000 | 2.664174000 |
| 1 | -2.574681000 | -3.305758000 | -0.829355000 |
| 1 | -1.503063000 | -4.063978000 | 0.359163000 |
| 1 | -0.991556000 | -2.598559000 | -0.489329000 |
| 1 | -4.402086000 | -3.263582000 | 0.819093000 |
| 1 | -4.204393000 | -2.431860000 | 2.382700000 |
| 1 | -3.354984000 | -3.939128000 | 2.056186000 |
| 1 | 1.981283000 | 1.430322000 | 3.001696000 |
| 1 | 0.595388000 | 1.531634000 | 1.908605000 |
| 1 | 1.229411000 | 2.997490000 | 2.663960000 |
| 1 | 2.574557000 | 3.305749000 | -0.829770000 |
| 1 | 1.503122000 | 4.063984000 | 0.358903000 |
| 1 | 0.991482000 | 2.598559000 | -0.489498000 |
| 1 | 4.402208000 | 3.263592000 | 0.818409000 |
| 1 | 4.204750000 | 2.431878000 | 2.382049000 |
| 1 | 3.355291000 | 3.939143000 | 2.055654000 |
| 1 | 5.027367000 | 1.209387000 | 0.605130000 |
| 1 | 5.027274000 | -1.209387000 | -0.605894000 |
| 1 | 2.574684000 | -3.305753000 | 0.829384000 |
| 1 | 1.503063000 | -4.063983000 | -0.359125000 |
| 1 | 0.991558000 | -2.598558000 | 0.489356000 |
| 1 | 1.980824000 | -1.430322000 | -3.001990000 |
| 1 | 0.595096000 | -1.531640000 | -1.908689000 |
| 1 | 1.229008000 | -2.997493000 | -2.664144000 |
| 1 | 4.204386000 | -2.431883000 | -2.382684000 |
| 1 | 3.354978000 | -3.939148000 | -2.056154000 |
| 1 | 4.402084000 | -3.263591000 | -0.819071000 |

N6+

| | | | |
|----|--------------|--------------|--------------|
| 79 | 0.000000000 | 0.000000000 | 0.000000000 |
| 6 | -0.057499000 | 0.209480000 | -2.022294000 |
| 7 | 0.426650000 | -0.644785000 | -2.944142000 |
| 6 | 1.034037000 | -1.930632000 | -2.637354000 |
| 6 | 0.004075000 | -3.023221000 | -2.417350000 |
| 6 | 0.651526000 | -4.353888000 | -2.071653000 |
| 6 | -0.370236000 | -5.439318000 | -1.781868000 |
| 6 | 0.189415000 | -0.179897000 | -4.213342000 |
| 6 | -0.451601000 | 1.002456000 | -4.078326000 |
| 7 | -0.595847000 | 1.220771000 | -2.731060000 |
| 6 | -1.185419000 | 2.418195000 | -2.146173000 |
| 6 | -0.144920000 | 3.409877000 | -1.655464000 |
| 6 | 0.776838000 | 3.943918000 | -2.738722000 |
| 6 | 1.782026000 | 4.944607000 | -2.194892000 |
| 1 | 1.650071000 | -1.797827000 | -1.745629000 |
| 1 | 1.704064000 | -2.182789000 | -3.461990000 |
| 1 | -0.615191000 | -3.128348000 | -3.314667000 |
| 1 | -0.667735000 | -2.711587000 | -1.609724000 |
| 1 | 1.306575000 | -4.220477000 | -1.202489000 |
| 1 | 1.303080000 | -4.668261000 | -2.894421000 |
| 1 | 0.114438000 | -6.385581000 | -1.534930000 |
| 1 | -1.016213000 | -5.613598000 | -2.645914000 |
| 1 | -1.011546000 | -5.162542000 | -0.940699000 |
| 1 | 0.493850000 | -0.720176000 | -5.093581000 |
| 1 | -0.808180000 | 1.699320000 | -4.817411000 |
| 1 | -1.833146000 | 2.099215000 | -1.327815000 |
| 1 | -1.819821000 | 2.868358000 | -2.912367000 |
| 1 | 0.447077000 | 2.934793000 | -0.864926000 |
| 1 | -0.681083000 | 4.240801000 | -1.184845000 |
| 1 | 0.176432000 | 4.413706000 | -3.526781000 |
| 1 | 1.309610000 | 3.111998000 | -3.211804000 |
| 1 | 2.437004000 | 5.319402000 | -2.983046000 |
| 1 | 2.413996000 | 4.488757000 | -1.427562000 |

| | | | |
|---|--------------|--------------|--------------|
| 1 | 1.279438000 | 5.804199000 | -1.743699000 |
| 6 | 0.057499000 | -0.209480000 | 2.022294000 |
| 7 | -0.426650000 | 0.644785000 | 2.944142000 |
| 6 | -1.034037000 | 1.930632000 | 2.637354000 |
| 6 | -0.004075000 | 3.023221000 | 2.417350000 |
| 6 | -0.651526000 | 4.353888000 | 2.071653000 |
| 6 | 0.370236000 | 5.439318000 | 1.781868000 |
| 6 | -0.189415000 | 0.179897000 | 4.213342000 |
| 6 | 0.451601000 | -1.002456000 | 4.078326000 |
| 7 | 0.595847000 | -1.220771000 | 2.731060000 |
| 6 | 1.185419000 | -2.418195000 | 2.146173000 |
| 6 | 0.144920000 | -3.409877000 | 1.655464000 |
| 6 | -0.776838000 | -3.943918000 | 2.738722000 |
| 6 | -1.782026000 | -4.944607000 | 2.194892000 |
| 1 | -1.650071000 | 1.797827000 | 1.745629000 |
| 1 | -1.704064000 | 2.182789000 | 3.461990000 |
| 1 | 0.615191000 | 3.128348000 | 3.314667000 |
| 1 | 0.667735000 | 2.711587000 | 1.609724000 |
| 1 | -1.306575000 | 4.220477000 | 1.202489000 |
| 1 | -1.303080000 | 4.668261000 | 2.894421000 |
| 1 | -0.114438000 | 6.385581000 | 1.534930000 |
| 1 | 1.016213000 | 5.613598000 | 2.645914000 |
| 1 | 1.011546000 | 5.162542000 | 0.940699000 |
| 1 | -0.493850000 | 0.720176000 | 5.093581000 |
| 1 | 0.808180000 | -1.699320000 | 4.817411000 |
| 1 | 1.833146000 | -2.099215000 | 1.327815000 |
| 1 | 1.819821000 | -2.868358000 | 2.912367000 |
| 1 | -0.447077000 | -2.934793000 | 0.864926000 |
| 1 | 0.681083000 | -4.240801000 | 1.184845000 |
| 1 | -0.176432000 | -4.413706000 | 3.526781000 |
| 1 | -1.309610000 | -3.111998000 | 3.211804000 |
| 1 | -2.437004000 | -5.319402000 | 2.983046000 |
| 1 | -2.413996000 | -4.488757000 | 1.427562000 |
| 1 | -1.279438000 | -5.804199000 | 1.743699000 |

N1b⁺

| | | | |
|----|--------------|--------------|--------------|
| Au | 0.000000000 | 0.000000000 | 0.000000000 |
| C | 2.028114000 | 0.000000000 | 0.000000000 |
| N | 2.842643000 | 0.754872000 | 0.755237000 |
| C | 4.175900000 | 0.492700000 | 0.492939000 |
| C | 4.175900000 | -0.492701000 | -0.492938000 |
| N | 2.842643000 | -0.754873000 | -0.755237000 |
| C | -2.028114000 | 0.000000000 | 0.000000000 |
| N | -2.842644000 | 0.755248000 | -0.754861000 |
| C | -4.175900000 | 0.492946000 | -0.492693000 |
| C | -4.175900000 | -0.492945000 | 0.492694000 |
| N | -2.842643000 | -0.755248000 | 0.754861000 |
| H | -2.501453000 | 1.424401000 | -1.423670000 |
| H | -2.501453000 | -1.424400000 | 1.423670000 |
| H | 2.501453000 | 1.423690000 | 1.424380000 |
| H | 2.501453000 | -1.423690000 | -1.424380000 |
| C | 5.354789000 | -1.008695000 | -1.009182000 |
| C | 5.354789000 | 1.008695000 | 1.009184000 |
| C | 6.530890000 | -0.494968000 | -0.495208000 |
| C | 6.530891000 | 0.494968000 | 0.495207000 |
| H | 5.357637000 | -1.774214000 | -1.775076000 |
| H | 7.477299000 | -0.867097000 | -0.867520000 |
| H | 7.477300000 | 0.867098000 | 0.867518000 |
| H | 5.357634000 | 1.774214000 | 1.775077000 |
| C | -5.354789000 | 1.009199000 | -1.008679000 |
| H | -5.357635000 | 1.775104000 | -1.774187000 |
| C | -6.530891000 | 0.495216000 | -0.494959000 |
| H | -7.477300000 | 0.867533000 | -0.867082000 |
| C | -6.530890000 | -0.495216000 | 0.494960000 |
| H | -7.477299000 | -0.867535000 | 0.867082000 |
| C | -5.354789000 | -1.009200000 | 1.008679000 |

H -5.357634000 -1.775105000 1.774186000

N2b⁺

Au 0.000000000 0.000001000 0.000001000
C 2.038396000 0.000001000 0.000000000
N 2.843807000 0.764488000 -0.764143000
C 4.171712000 0.492403000 -0.492182000
C 4.171712000 -0.492403000 0.492181000
N 2.843806000 -0.764487000 0.764143000
C -2.038396000 0.000000000 0.000000000
N -2.843806000 -0.764160000 -0.764470000
C -4.171711000 -0.492192000 -0.492393000
C -4.171712000 0.492192000 0.492391000
N -2.843807000 0.764160000 0.764470000
C 5.351035000 -1.008542000 1.008086000
C 5.351036000 1.008540000 -1.008087000
C 6.528904000 -0.494913000 0.494687000
C 6.528905000 0.494908000 -0.494688000
H 5.355051000 -1.774311000 1.773509000
H 7.475153000 -0.867500000 0.867104000
H 7.475155000 0.867492000 -0.867105000
H 5.355053000 1.774309000 -1.773510000
C -5.351034000 -1.008109000 -1.008520000
H -5.355050000 -1.773548000 -1.774273000
C -6.528903000 -0.494700000 -0.494902000
H -7.475151000 -0.867126000 -0.867479000
C -6.528904000 0.494696000 0.494899000
H -7.475154000 0.867120000 0.867476000
C -5.351036000 1.008107000 1.008518000
H -5.355054000 1.773547000 1.774270000
C -2.412619000 -1.738737000 -1.739445000
H -2.786887000 -1.469417000 -2.728518000
H -1.325180000 -1.759675000 -1.760386000
H -2.786892000 -2.727918000 -1.470531000
C -2.412621000 1.738737000 1.739446000
H -1.325183000 1.759676000 1.760387000
H -2.786896000 2.727918000 1.470534000
H -2.786888000 1.469415000 2.728519000
C 2.412619000 -1.739482000 1.738700000
H 2.786897000 -1.470591000 2.727886000
H 1.325180000 -1.760419000 1.759641000
H 2.786882000 -2.728550000 1.469356000
C 2.412621000 1.739483000 -1.738699000
H 1.325182000 1.760421000 -1.759642000
H 2.786883000 2.728552000 -1.469355000
H 2.786899000 1.470594000 -2.727886000

N3b⁺

Au 0.000000000 0.000000000 0.000000000
C -2.034484000 0.000000000 0.000009000
N -2.836108000 -0.934414000 0.544843000
C -4.165011000 -0.605542000 0.345374000
C -4.165014000 0.605542000 -0.345337000
N -2.836113000 0.934414000 -0.544818000
C -5.346751000 1.240418000 -0.700620000
C -5.346745000 -1.240418000 0.700667000
C -6.524576000 0.609610000 -0.343636000
C -6.524573000 -0.609610000 0.343693000
H -5.354036000 2.185061000 -1.229613000
H -7.470479000 1.069465000 -0.601899000
H -7.470473000 -1.069465000 0.601965000
H -5.354025000 -2.185061000 1.229660000
C -2.374224000 2.159129000 -1.176956000
H -1.408964000 1.940825000 -1.636068000
C -2.374214000 -2.159129000 1.176977000
H -1.408950000 -1.940825000 1.636080000

| | | | |
|---|--------------|--------------|--------------|
| C | -2.263113000 | 3.307300000 | -0.193917000 |
| H | -3.222731000 | 3.517119000 | 0.281938000 |
| H | -1.934082000 | 4.210819000 | -0.710031000 |
| H | -1.537248000 | 3.072141000 | 0.587432000 |
| C | -2.263111000 | -3.307300000 | 0.193937000 |
| H | -1.537253000 | -3.072141000 | -0.587419000 |
| H | -3.222733000 | -3.517119000 | -0.281910000 |
| H | -1.934076000 | -4.210819000 | 0.710048000 |
| H | -3.070257000 | -2.393229000 | 1.984770000 |
| H | -3.070274000 | 2.393229000 | -1.984743000 |
| C | 2.034484000 | 0.000000000 | -0.000009000 |
| N | 2.836108000 | -0.934398000 | -0.544869000 |
| C | 4.165011000 | -0.605532000 | -0.345390000 |
| C | 4.165014000 | 0.605532000 | 0.345354000 |
| N | 2.836113000 | 0.934398000 | 0.544844000 |
| C | 5.346751000 | 1.240399000 | 0.700655000 |
| C | 5.346745000 | -1.240399000 | -0.700702000 |
| C | 6.524576000 | 0.609601000 | 0.343653000 |
| C | 6.524573000 | -0.609601000 | -0.343710000 |
| H | 5.354036000 | 2.185027000 | 1.229674000 |
| H | 7.470479000 | 1.069448000 | 0.601929000 |
| H | 7.470473000 | -1.069448000 | -0.601994000 |
| H | 5.354025000 | -2.185027000 | -1.229721000 |
| C | 2.374224000 | 2.159096000 | 1.177016000 |
| H | 1.408964000 | 1.940779000 | 1.636122000 |
| C | 2.374214000 | -2.159096000 | -1.177037000 |
| H | 1.408950000 | -1.940779000 | -1.636135000 |
| C | 2.263113000 | 3.307295000 | 0.194010000 |
| H | 3.222731000 | 3.517127000 | -0.281840000 |
| H | 1.934082000 | 4.210799000 | 0.710149000 |
| H | 1.537248000 | 3.072157000 | -0.587346000 |
| C | 2.263111000 | -3.307295000 | -0.194030000 |
| H | 1.537253000 | -3.072157000 | 0.587332000 |
| H | 3.222733000 | -3.517127000 | 0.281812000 |
| H | 1.934076000 | -4.210799000 | -0.710166000 |
| H | 3.070257000 | -2.393173000 | -1.984837000 |
| H | 3.070274000 | 2.393173000 | 1.984810000 |

N4b⁺

| | | | |
|----|--------------|--------------|--------------|
| Au | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -2.039748000 | 0.000000000 | 0.000002000 |
| N | -2.836823000 | -0.970461000 | -0.486884000 |
| C | -4.167662000 | -0.624783000 | -0.312809000 |
| C | -4.167662000 | 0.624783000 | 0.312820000 |
| N | -2.836822000 | 0.970461000 | 0.486890000 |
| C | -5.356887000 | 1.270028000 | 0.634261000 |
| C | -5.356889000 | -1.270029000 | -0.634247000 |
| C | -6.535206000 | 0.625515000 | 0.312010000 |
| C | -6.535206000 | -0.625517000 | -0.311993000 |
| H | -5.373815000 | 2.236752000 | 1.116516000 |
| H | -7.479416000 | 1.100304000 | 0.548621000 |
| H | -7.479417000 | -1.100306000 | -0.548601000 |
| H | -5.373818000 | -2.236753000 | -1.116502000 |
| C | -2.329029000 | 2.199301000 | 1.106519000 |
| H | -1.242322000 | 2.084604000 | 1.061223000 |
| C | -2.329031000 | -2.199301000 | -1.106514000 |
| H | -1.242325000 | -2.084603000 | -1.061221000 |
| C | -2.731568000 | 2.287344000 | 2.568452000 |
| H | -3.808594000 | 2.401812000 | 2.694263000 |
| H | -2.250186000 | 3.153724000 | 3.024810000 |
| H | -2.417313000 | 1.394846000 | 3.112235000 |
| C | -2.710368000 | 3.423616000 | 0.292286000 |
| H | -2.378333000 | 3.321162000 | -0.742494000 |
| H | -2.233918000 | 4.306885000 | 0.720770000 |
| H | -3.786986000 | 3.596992000 | 0.287875000 |
| C | -2.731575000 | -2.287344000 | -2.568446000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.250194000 | -3.153723000 | -3.024805000 |
| H | -2.417322000 | -1.394845000 | -3.112230000 |
| H | -3.808601000 | -2.401812000 | -2.694254000 |
| C | -2.710367000 | -3.423615000 | -0.292279000 |
| H | -2.233918000 | -4.306884000 | -0.720765000 |
| H | -3.786986000 | -3.596993000 | -0.287866000 |
| H | -2.378329000 | -3.321161000 | 0.742499000 |
| C | 2.039748000 | 0.000000000 | -0.000003000 |
| N | 2.836823000 | -0.970479000 | 0.486848000 |
| C | 4.167662000 | -0.624795000 | 0.312787000 |
| C | 4.167662000 | 0.624794000 | -0.312797000 |
| N | 2.836822000 | 0.970479000 | -0.486855000 |
| C | 5.356887000 | 1.270051000 | -0.634214000 |
| C | 5.356888000 | -1.270052000 | 0.634202000 |
| C | 6.535206000 | 0.625526000 | -0.311986000 |
| C | 6.535206000 | -0.625528000 | 0.311972000 |
| H | 5.373816000 | 2.236792000 | -1.116434000 |
| H | 7.479416000 | 1.100323000 | -0.548580000 |
| H | 7.479417000 | -1.100326000 | 0.548564000 |
| H | 5.373817000 | -2.236794000 | 1.116422000 |
| C | 2.329029000 | 2.199341000 | -1.106439000 |
| H | 1.242323000 | 2.084642000 | -1.061148000 |
| C | 2.329031000 | -2.199341000 | 1.106433000 |
| H | 1.242324000 | -2.084642000 | 1.061144000 |
| C | 2.731569000 | 2.287437000 | -2.568369000 |
| H | 3.808595000 | 2.401909000 | -2.694176000 |
| H | 2.250188000 | 3.153834000 | -3.024695000 |
| H | 2.417314000 | 1.394959000 | -3.112184000 |
| C | 2.710368000 | 3.423626000 | -0.292161000 |
| H | 2.378333000 | 3.321135000 | 0.742614000 |
| H | 2.233918000 | 4.306911000 | -0.720613000 |
| H | 3.786987000 | 3.597003000 | -0.287744000 |
| C | 2.731573000 | -2.287437000 | 2.568363000 |
| H | 2.250192000 | -3.153834000 | 3.024689000 |
| H | 2.417319000 | -1.394959000 | 3.112178000 |
| H | 3.808599000 | -2.401910000 | 2.694167000 |
| C | 2.710367000 | -3.423626000 | 0.292155000 |
| H | 2.233918000 | -4.306911000 | 0.720608000 |
| H | 3.786986000 | -3.597003000 | 0.287736000 |
| H | 2.378330000 | -3.321135000 | -0.742620000 |

N5b⁺

| | | | |
|----|--------------|--------------|--------------|
| 79 | 0.000000000 | -0.000015000 | 0.365581000 |
| 6 | -2.030263000 | -0.293171000 | 0.226758000 |
| 7 | -2.967212000 | 0.553338000 | 0.720252000 |
| 6 | -4.156456000 | 0.399076000 | 0.012873000 |
| 6 | -3.945410000 | -0.637917000 | -0.895094000 |
| 7 | -2.636529000 | -1.072694000 | -0.702176000 |
| 6 | 2.030261000 | 0.293153000 | 0.226763000 |
| 7 | 2.967216000 | -0.553369000 | 0.720220000 |
| 6 | 4.156462000 | -0.399063000 | 0.012852000 |
| 6 | 3.945408000 | 0.637969000 | -0.895068000 |
| 7 | 2.636522000 | 1.072723000 | -0.702135000 |
| 6 | -4.938209000 | -1.003740000 | -1.802845000 |
| 6 | -5.365196000 | 1.093143000 | 0.035042000 |
| 6 | -6.134781000 | -0.317849000 | -1.768913000 |
| 6 | -6.346037000 | 0.718801000 | -0.860036000 |
| 1 | -4.791438000 | -1.779916000 | -2.537485000 |
| 1 | -6.915245000 | -0.581857000 | -2.471813000 |
| 1 | -7.288972000 | 1.251483000 | -0.864106000 |
| 1 | -5.544537000 | 1.918974000 | 0.705508000 |
| 6 | 5.365209000 | -1.093117000 | 0.034994000 |
| 1 | 5.544557000 | -1.918977000 | 0.705423000 |
| 6 | 6.346051000 | -0.718722000 | -0.860062000 |
| 1 | 7.288991000 | -1.251393000 | -0.864151000 |
| 6 | 6.134787000 | 0.317967000 | -1.768892000 |

| | | | |
|---|--------------|--------------|--------------|
| 1 | 6.915251000 | 0.582017000 | -2.471777000 |
| 6 | 4.938207000 | 1.003845000 | -1.802798000 |
| 1 | 4.791431000 | 1.780054000 | -2.537403000 |
| 6 | -2.840992000 | 1.489710000 | 1.880540000 |
| 6 | -2.912554000 | 2.923198000 | 1.361770000 |
| 6 | -3.957199000 | 1.165605000 | 2.878053000 |
| 6 | -1.536276000 | 1.314947000 | 2.643074000 |
| 1 | -2.076891000 | 3.117855000 | 0.685925000 |
| 1 | -2.843822000 | 3.619342000 | 2.199302000 |
| 1 | -3.835716000 | 3.133733000 | 0.824441000 |
| 1 | -3.837354000 | 0.147865000 | 3.255268000 |
| 1 | -4.958754000 | 1.253323000 | 2.468239000 |
| 1 | -3.884131000 | 1.850930000 | 3.723465000 |
| 1 | -1.382062000 | 0.281879000 | 2.958136000 |
| 1 | -1.597511000 | 1.934132000 | 3.539978000 |
| 1 | -0.666405000 | 1.649757000 | 2.075592000 |
| 6 | -2.079365000 | -2.267561000 | -1.410457000 |
| 6 | -3.023775000 | -3.448725000 | -1.166344000 |
| 6 | -1.926955000 | -1.930069000 | -2.890959000 |
| 6 | -0.723560000 | -2.700770000 | -0.872721000 |
| 1 | -3.062556000 | -3.681677000 | -0.100169000 |
| 1 | -2.636647000 | -4.323478000 | -1.690438000 |
| 1 | -4.040835000 | -3.283167000 | -1.508054000 |
| 1 | -1.214617000 | -1.111220000 | -3.014492000 |
| 1 | -2.865077000 | -1.633305000 | -3.356841000 |
| 1 | -1.544135000 | -2.799748000 | -3.427520000 |
| 1 | 0.071342000 | -1.992746000 | -1.111161000 |
| 1 | -0.472553000 | -3.649298000 | -1.351386000 |
| 1 | -0.746367000 | -2.864174000 | 0.205925000 |
| 6 | 2.841004000 | -1.489798000 | 1.880464000 |
| 6 | 2.912582000 | -2.923260000 | 1.361627000 |
| 6 | 3.957204000 | -1.165727000 | 2.877995000 |
| 6 | 1.536283000 | -1.315084000 | 2.643003000 |
| 1 | 2.076920000 | -3.117896000 | 0.685775000 |
| 1 | 2.843860000 | -3.619444000 | 2.199126000 |
| 1 | 3.835746000 | -3.133759000 | 0.824286000 |
| 1 | 3.837351000 | -0.148004000 | 3.255253000 |
| 1 | 4.958761000 | -1.253421000 | 2.468182000 |
| 1 | 3.884137000 | -1.851089000 | 3.723378000 |
| 1 | 1.382059000 | -0.282034000 | 2.958116000 |
| 1 | 1.597522000 | -1.934314000 | 3.539876000 |
| 1 | 0.666417000 | -1.649874000 | 2.075501000 |
| 6 | 2.079349000 | 2.267615000 | -1.410369000 |
| 6 | 3.023742000 | 3.448780000 | -1.166195000 |
| 6 | 1.926956000 | 1.930184000 | -2.890887000 |
| 6 | 0.723533000 | 2.700785000 | -0.872629000 |
| 1 | 3.062493000 | 3.681699000 | -0.100012000 |
| 1 | 2.636618000 | 4.323546000 | -1.690271000 |
| 1 | 4.040812000 | 3.283243000 | -1.507884000 |
| 1 | 1.214634000 | 1.111326000 | -3.014460000 |
| 1 | 2.865086000 | 1.633458000 | -3.356777000 |
| 1 | 1.544122000 | 2.799879000 | -3.427412000 |
| 1 | -0.071359000 | 1.992764000 | -1.111111000 |
| 1 | 0.472523000 | 3.649333000 | -1.351255000 |
| 1 | 0.746326000 | 2.864142000 | 0.206025000 |

N6b+

| | | | |
|----|--------------|--------------|--------------|
| 79 | 0.000007000 | -0.000003000 | 0.000009000 |
| 6 | -2.023146000 | 0.195723000 | -0.071983000 |
| 7 | -2.742236000 | 1.219500000 | 0.424861000 |
| 6 | -2.174791000 | 2.398800000 | 1.053331000 |
| 6 | -1.811934000 | 3.477685000 | 0.049292000 |
| 6 | -1.228984000 | 4.709269000 | 0.721862000 |
| 6 | -0.767611000 | 5.754882000 | -0.278089000 |
| 6 | -4.088103000 | 1.033781000 | 0.168166000 |
| 6 | -4.190239000 | -0.182854000 | -0.506203000 |

| | | | |
|---|--------------|--------------|--------------|
| 7 | -2.897533000 | -0.659594000 | -0.636303000 |
| 6 | -2.526713000 | -1.927249000 | -1.247778000 |
| 6 | -2.263283000 | -3.025052000 | -0.231378000 |
| 6 | -3.456176000 | -3.384014000 | 0.638552000 |
| 6 | -3.127148000 | -4.481635000 | 1.635552000 |
| 1 | -1.291469000 | 2.079950000 | 1.610456000 |
| 1 | -2.898919000 | 2.766764000 | 1.783602000 |
| 1 | -2.698655000 | 3.750961000 | -0.532554000 |
| 1 | -1.089407000 | 3.060920000 | -0.661613000 |
| 1 | -0.387234000 | 4.408820000 | 1.357092000 |
| 1 | -1.974744000 | 5.144085000 | 1.396559000 |
| 1 | -0.356765000 | 6.632169000 | 0.224794000 |
| 1 | -1.595310000 | 6.090813000 | -0.907679000 |
| 1 | 0.007114000 | 5.353982000 | -0.937444000 |
| 1 | -1.640847000 | -1.748285000 | -1.859940000 |
| 1 | -3.335087000 | -2.208175000 | -1.925120000 |
| 1 | -1.421881000 | -2.719690000 | 0.401720000 |
| 1 | -1.930027000 | -3.910757000 | -0.782877000 |
| 1 | -4.288630000 | -3.701456000 | 0.000087000 |
| 1 | -3.803913000 | -2.494275000 | 1.173961000 |
| 1 | -3.991544000 | -4.731146000 | 2.253000000 |
| 1 | -2.318904000 | -4.174384000 | 2.305167000 |
| 1 | -2.807357000 | -5.394871000 | 1.126575000 |
| 6 | 2.023159000 | -0.195732000 | 0.071995000 |
| 7 | 2.742249000 | -1.219477000 | -0.424918000 |
| 6 | 2.174800000 | -2.398732000 | -1.053468000 |
| 6 | 1.811915000 | -3.477672000 | -0.049497000 |
| 6 | 1.228924000 | -4.709194000 | -0.722143000 |
| 6 | 0.767534000 | -5.754862000 | 0.277743000 |
| 6 | 4.088116000 | -1.033776000 | -0.168209000 |
| 6 | 4.190252000 | 0.182812000 | 0.506243000 |
| 7 | 2.897547000 | 0.659545000 | 0.636374000 |
| 6 | 2.526728000 | 1.927160000 | 1.247933000 |
| 6 | 2.263287000 | 3.025026000 | 0.231604000 |
| 6 | 3.456170000 | 3.384038000 | -0.638320000 |
| 6 | 3.127131000 | 4.481716000 | -1.635253000 |
| 1 | 1.291490000 | -2.079839000 | -1.610587000 |
| 1 | 2.898934000 | -2.766662000 | -1.783751000 |
| 1 | 2.698629000 | -3.751012000 | 0.532328000 |
| 1 | 1.089402000 | -3.060930000 | 0.661436000 |
| 1 | 0.387173000 | -4.408679000 | -1.357343000 |
| 1 | 1.974662000 | -5.143986000 | -1.396880000 |
| 1 | 0.356650000 | -6.632101000 | -0.225194000 |
| 1 | 1.595233000 | -6.090864000 | 0.907295000 |
| 1 | -0.007166000 | -5.353983000 | 0.937140000 |
| 1 | 1.640867000 | 1.748155000 | 1.860091000 |
| 1 | 3.335107000 | 2.208045000 | 1.925286000 |
| 1 | 1.421876000 | 2.719706000 | -0.401502000 |
| 1 | 1.930042000 | 3.910698000 | 0.783163000 |
| 1 | 4.288631000 | 3.701442000 | 0.000154000 |
| 1 | 3.803899000 | 2.494330000 | -1.173784000 |
| 1 | 3.991522000 | 4.731266000 | -2.252692000 |
| 1 | 2.318884000 | 4.174500000 | -2.304881000 |
| 1 | 2.807340000 | 5.394921000 | -1.126221000 |
| 6 | 5.206635000 | -1.801209000 | -0.461508000 |
| 1 | 5.131171000 | -2.749993000 | -0.977548000 |
| 6 | 6.430433000 | -1.299612000 | -0.058557000 |
| 1 | 7.329756000 | -1.865935000 | -0.266868000 |
| 6 | 6.534670000 | -0.076029000 | 0.612888000 |
| 1 | 7.513080000 | 0.281475000 | 0.909255000 |
| 6 | 5.419855000 | 0.687262000 | 0.906701000 |
| 1 | 5.511260000 | 1.635075000 | 1.421059000 |
| 6 | -5.419842000 | -0.687333000 | -0.906624000 |
| 1 | -5.511247000 | -1.635181000 | -1.420916000 |
| 6 | -6.534657000 | 0.075978000 | -0.612861000 |
| 1 | -7.513067000 | -0.281547000 | -0.909203000 |

| | | | |
|---|--------------|-------------|-------------|
| 6 | -6.430420000 | 1.299608000 | 0.058498000 |
| 1 | -7.329743000 | 1.865944000 | 0.266771000 |
| 6 | -5.206621000 | 1.801233000 | 0.461413000 |
| 1 | -5.131157000 | 2.750053000 | 0.977386000 |

S2. Cartesian coordinates of optimised geometries of neutral Au complexes

N1⁰

| | | | |
|----|--------------|--------------|--------------|
| Au | 0.000000000 | 0.000000000 | 0.585870000 |
| C | 0.000000000 | 0.000000000 | -1.391982000 |
| N | 0.000000000 | 1.055579000 | -2.229647000 |
| C | 0.000000000 | 0.674671000 | -3.551826000 |
| H | 0.000001000 | 1.378958000 | -4.365231000 |
| C | 0.000000000 | -0.674671000 | -3.551826000 |
| H | -0.000001000 | -1.378958000 | -4.365231000 |
| N | 0.000000000 | -1.055579000 | -2.229647000 |
| H | 0.000000000 | 2.002482000 | -1.892706000 |
| H | 0.000000000 | -2.002482000 | -1.892706000 |
| Cl | 0.000000000 | 0.000000000 | 2.848296000 |

N2⁰

| | | | |
|----|--------------|--------------|--------------|
| Au | -0.774497000 | 0.000000000 | 0.000000000 |
| C | 1.215883000 | 0.000000000 | 0.000000000 |
| N | 2.043370000 | 1.068993000 | -0.000002000 |
| C | 3.359696000 | 0.674677000 | -0.000001000 |
| H | 4.174150000 | 1.378931000 | -0.000001000 |
| C | 3.359696000 | -0.674677000 | 0.000001000 |
| H | 4.174150000 | -1.378931000 | 0.000001000 |
| N | 2.043370000 | -1.068993000 | 0.000002000 |
| C | 1.610929000 | 2.448708000 | 0.000001000 |
| H | 0.522896000 | 2.466201000 | -0.000023000 |
| H | 1.980251000 | 2.958166000 | 0.891258000 |
| H | 1.980291000 | 2.958180000 | -0.891231000 |
| C | 1.610929000 | -2.448708000 | -0.000001000 |
| H | 0.522896000 | -2.466201000 | 0.000023000 |
| H | 1.980291000 | -2.958180000 | 0.891231000 |
| H | 1.980251000 | -2.958166000 | -0.891258000 |
| Cl | -3.039996000 | 0.000000000 | 0.000000000 |

N3⁰

| | | | |
|----|--------------|--------------|--------------|
| Au | -0.895318000 | 0.000000000 | 0.000000000 |
| C | 1.093356000 | 0.000001000 | -0.000001000 |
| N | 1.917533000 | -1.020465000 | 0.318451000 |
| C | 3.233966000 | -0.645967000 | 0.197119000 |
| H | 4.047887000 | -1.321615000 | 0.397754000 |
| C | 3.233965000 | 0.645971000 | -0.197119000 |
| H | 4.047885000 | 1.321620000 | -0.397754000 |
| N | 1.917532000 | 1.020467000 | -0.318452000 |
| C | 1.463713000 | -2.360248000 | 0.657658000 |
| H | 0.558399000 | -2.251366000 | 1.256286000 |
| H | 2.231301000 | -2.812575000 | 1.289096000 |
| C | 1.463711000 | 2.360250000 | -0.657657000 |
| H | 0.558399000 | 2.251371000 | -1.256287000 |
| H | 2.231301000 | 2.812581000 | -1.289090000 |
| C | 1.192967000 | -3.200846000 | -0.573533000 |
| H | 0.861311000 | -4.198028000 | -0.278409000 |
| H | 2.090232000 | -3.303600000 | -1.187850000 |
| H | 0.406643000 | -2.742226000 | -1.175761000 |
| C | 1.192960000 | 3.200844000 | 0.573534000 |
| H | 0.406639000 | 2.742218000 | 1.175761000 |
| H | 0.861297000 | 4.198024000 | 0.278410000 |
| H | 2.090224000 | 3.303606000 | 1.187853000 |
| Cl | -3.162037000 | -0.000001000 | 0.000000000 |

N4⁰

| | | | |
|----|-------------|-------------|-------------|
| Au | 1.142905000 | 0.000000000 | 0.000000000 |
|----|-------------|-------------|-------------|

| | | | |
|----|--------------|--------------|--------------|
| C | -0.849156000 | 0.000000000 | 0.000000000 |
| N | -1.672581000 | -1.070923000 | 0.000000000 |
| C | -2.988532000 | -0.674996000 | 0.000000000 |
| H | -3.807865000 | -1.372670000 | 0.000000000 |
| C | -2.988532000 | 0.674996000 | 0.000000000 |
| H | -3.807865000 | 1.372670000 | 0.000000000 |
| N | -1.672581000 | 1.070923000 | 0.000000000 |
| C | -1.218703000 | -2.461855000 | 0.000000000 |
| H | -0.128427000 | -2.388811000 | 0.000000000 |
| C | -1.218703000 | 2.461855000 | 0.000000000 |
| H | -0.128427000 | 2.388811000 | 0.000000000 |
| C | -1.668772000 | -3.169021000 | 1.265661000 |
| C | -1.668771000 | -3.169021000 | -1.265661000 |
| C | -1.668772000 | 3.169021000 | -1.265661000 |
| C | -1.668771000 | 3.169021000 | 1.265661000 |
| H | -1.320506000 | 2.636592000 | -2.152215000 |
| H | -2.758183000 | 3.249112000 | -1.313238000 |
| H | -1.258762000 | 4.180063000 | -1.288506000 |
| H | -2.758182000 | 3.249112000 | 1.313239000 |
| H | -1.258761000 | 4.180063000 | 1.288506000 |
| H | -1.320505000 | 2.636592000 | 2.152215000 |
| H | -1.320506000 | -2.636592000 | 2.152215000 |
| H | -2.758183000 | -3.249112000 | 1.313238000 |
| H | -1.258762000 | -4.180063000 | 1.288506000 |
| H | -1.320505000 | -2.636592000 | -2.152215000 |
| H | -2.758182000 | -3.249112000 | -1.313238000 |
| H | -1.258761000 | -4.180063000 | -1.288506000 |
| Cl | 3.410664000 | 0.000000000 | 0.000000000 |

N5°

| | | | |
|----|--------------|--------------|--------------|
| Au | -1.137663000 | 0.000009000 | 0.000000000 |
| C | 0.868647000 | -0.000007000 | 0.000001000 |
| N | 1.691902000 | 1.078445000 | -0.000001000 |
| C | 1.256521000 | 2.505325000 | 0.000001000 |
| C | 0.444636000 | 2.784470000 | 1.260363000 |
| C | 0.444634000 | 2.784472000 | -1.260359000 |
| C | 2.485296000 | 3.406944000 | 0.000000000 |
| C | 3.005453000 | 0.673324000 | -0.000003000 |
| C | 3.005443000 | -0.673372000 | -0.000003000 |
| N | 1.691885000 | -1.078472000 | 0.000000000 |
| C | 1.256481000 | -2.505344000 | 0.000000000 |
| C | 0.444589000 | -2.784476000 | 1.260361000 |
| C | 0.444591000 | -2.784478000 | -1.260361000 |
| C | 2.485242000 | -3.406983000 | 0.000003000 |
| H | 1.034279000 | 2.567359000 | 2.153970000 |
| H | -0.465437000 | 2.184086000 | 1.289578000 |
| H | 0.159194000 | 3.837993000 | 1.280586000 |
| H | 1.034275000 | 2.567363000 | -2.153968000 |
| H | 0.159194000 | 3.837996000 | -1.280581000 |
| H | -0.465440000 | 2.184090000 | -1.289574000 |
| H | 3.100640000 | 3.264147000 | -0.891153000 |
| H | 3.100647000 | 3.264139000 | 0.891148000 |
| H | 2.143947000 | 4.442464000 | 0.000007000 |
| H | 3.836703000 | 1.352102000 | -0.000005000 |
| H | 3.836680000 | -1.352163000 | -0.000005000 |
| H | 1.034234000 | -2.567377000 | 2.153970000 |
| H | 0.159130000 | -3.837994000 | 1.280583000 |
| H | -0.465474000 | -2.184077000 | 1.289576000 |
| H | 1.034238000 | -2.567378000 | -2.153969000 |
| H | -0.465472000 | -2.184080000 | -1.289577000 |
| H | 0.159133000 | -3.837995000 | -1.280583000 |
| H | 3.100590000 | -3.264196000 | -0.891148000 |
| H | 2.143876000 | -4.442498000 | 0.000007000 |
| H | 3.100592000 | -3.264188000 | 0.891152000 |
| Cl | -3.407992000 | 0.000025000 | -0.000001000 |

N6^o

| | | | |
|----|--------------|--------------|--------------|
| 79 | 1.224196000 | -0.000010000 | -0.276586000 |
| 6 | -0.633009000 | 0.000000000 | -0.994172000 |
| 7 | -1.413874000 | -1.069854000 | -1.261966000 |
| 6 | -1.020827000 | -2.454124000 | -1.060099000 |
| 6 | -1.605748000 | -3.050276000 | 0.210430000 |
| 6 | -1.151121000 | -2.356234000 | 1.483966000 |
| 6 | -1.721322000 | -3.006250000 | 2.732273000 |
| 6 | -2.662728000 | -0.675064000 | -1.677915000 |
| 6 | -2.662720000 | 0.675090000 | -1.677915000 |
| 7 | -1.413861000 | 1.069864000 | -1.261965000 |
| 6 | -1.020794000 | 2.454132000 | -1.060112000 |
| 6 | -1.605708000 | 3.050299000 | 0.210413000 |
| 6 | -1.151055000 | 2.356280000 | 1.483953000 |
| 6 | -1.721251000 | 3.006302000 | 2.732258000 |
| 1 | 0.069757000 | -2.465750000 | -1.024369000 |
| 1 | -1.336245000 | -3.023197000 | -1.938038000 |
| 1 | -1.313637000 | -4.105735000 | 0.240126000 |
| 1 | -2.701029000 | -3.038013000 | 0.149952000 |
| 1 | -1.444691000 | -1.301948000 | 1.451316000 |
| 1 | -0.056739000 | -2.354791000 | 1.524987000 |
| 1 | -1.385101000 | -2.491691000 | 3.634528000 |
| 1 | -1.410196000 | -4.051663000 | 2.811124000 |
| 1 | -2.815182000 | -2.986750000 | 2.724942000 |
| 1 | -3.430282000 | -1.379547000 | -1.949735000 |
| 1 | -3.430264000 | 1.379583000 | -1.949737000 |
| 1 | 0.069791000 | 2.465740000 | -1.024379000 |
| 1 | -1.336198000 | 3.023199000 | -1.938059000 |
| 1 | -2.700989000 | 3.038015000 | 0.149949000 |
| 1 | -1.313615000 | 4.105764000 | 0.240092000 |
| 1 | -0.056672000 | 2.354852000 | 1.524962000 |
| 1 | -1.444614000 | 1.301991000 | 1.451317000 |
| 1 | -1.410147000 | 4.051724000 | 2.811087000 |
| 1 | -1.385004000 | 2.491765000 | 3.634516000 |
| 1 | -2.815111000 | 2.986777000 | 2.724945000 |
| 17 | 3.321559000 | -0.000033000 | 0.586461000 |

N1b^o

| | | | |
|----|--------------|--------------|--------------|
| Au | -1.481148000 | 0.000000000 | 0.000000000 |
| C | 0.492073000 | -0.000002000 | -0.000001000 |
| N | 1.315649000 | 1.068504000 | -0.000001000 |
| C | 2.646669000 | 0.697923000 | -0.000002000 |
| C | 2.646668000 | -0.697930000 | 0.000000000 |
| N | 1.315647000 | -1.068509000 | 0.000000000 |
| C | 3.826573000 | -1.423250000 | 0.000000000 |
| C | 3.826575000 | 1.423243000 | -0.000002000 |
| C | 5.007087000 | -0.698679000 | 0.000001000 |
| C | 5.007074000 | 0.698694000 | 0.000002000 |
| H | 3.827982000 | -2.506328000 | 0.000000000 |
| H | 5.952388000 | -1.227505000 | -0.000007000 |
| H | 5.952368000 | 1.227530000 | 0.000012000 |
| H | 3.827982000 | 2.506321000 | 0.000004000 |
| Cl | -3.742001000 | 0.000003000 | 0.000001000 |
| H | 0.964305000 | -2.010084000 | 0.000000000 |
| H | 0.964308000 | 2.010080000 | -0.000003000 |

N2b^o

| | | | |
|----|--------------|--------------|--------------|
| Au | 1.556771000 | 0.000000000 | -0.000002000 |
| C | -0.428621000 | 0.000001000 | -0.000001000 |
| N | -1.242627000 | 1.081653000 | -0.000001000 |
| C | -2.568026000 | 0.697130000 | 0.000000000 |
| C | -2.568026000 | -0.697129000 | -0.000001000 |
| N | -1.242627000 | -1.081652000 | -0.000001000 |
| C | -3.747878000 | -1.423213000 | -0.000001000 |
| C | -3.747878000 | 1.423215000 | 0.000001000 |
| C | -4.929651000 | -0.698470000 | 0.000001000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -4.929657000 | 0.698464000 | 0.000005000 |
| H | -3.749309000 | -2.506089000 | -0.000006000 |
| H | -5.875021000 | -1.227347000 | 0.000005000 |
| H | -5.875034000 | 1.227335000 | 0.000009000 |
| H | -3.749306000 | 2.506091000 | -0.000002000 |
| C | -0.803613000 | -2.455827000 | 0.000001000 |
| H | -1.172832000 | -2.968075000 | -0.890693000 |
| H | 0.284395000 | -2.470228000 | -0.000009000 |
| H | -1.172816000 | -2.968068000 | 0.890706000 |
| C | -0.803617000 | 2.455830000 | -0.000001000 |
| H | 0.284392000 | 2.470232000 | -0.000006000 |
| H | -1.172833000 | 2.968074000 | -0.890699000 |
| H | -1.172824000 | 2.968073000 | 0.890701000 |
| Cl | 3.820288000 | 0.000000000 | 0.000007000 |

N3b⁰

| | | | |
|----|--------------|--------------|--------------|
| Au | -1.608633000 | -0.000001000 | -0.000001000 |
| C | 0.375694000 | 0.000002000 | -0.000008000 |
| N | 1.185745000 | -1.044161000 | -0.284576000 |
| C | 2.512184000 | -0.675250000 | -0.176301000 |
| C | 2.512184000 | 0.675250000 | 0.176291000 |
| N | 1.185746000 | 1.044164000 | 0.284560000 |
| C | 3.694323000 | 1.377780000 | 0.352313000 |
| C | 3.694323000 | -1.377783000 | -0.352310000 |
| C | 4.875817000 | 0.677009000 | 0.172443000 |
| C | 4.875817000 | -0.677017000 | -0.172427000 |
| H | 3.698753000 | 2.427983000 | 0.616109000 |
| H | 5.820904000 | 1.190344000 | 0.301940000 |
| H | 5.820901000 | -1.190352000 | -0.301915000 |
| H | 3.698752000 | -2.427986000 | -0.616108000 |
| C | 0.721568000 | 2.388668000 | 0.575301000 |
| H | -0.253344000 | 2.292462000 | 1.054493000 |
| C | 0.721565000 | -2.388667000 | -0.575305000 |
| H | -0.253349000 | -2.292465000 | -1.054493000 |
| Cl | -3.873251000 | 0.000000000 | 0.000009000 |
| C | 0.625380000 | 3.242600000 | -0.673261000 |
| H | 1.590813000 | 3.318923000 | -1.178156000 |
| H | 0.292926000 | 4.249180000 | -0.413217000 |
| H | -0.097828000 | 2.811375000 | -1.367851000 |
| C | 0.625381000 | -3.242585000 | 0.673267000 |
| H | -0.097834000 | -2.811357000 | 1.367848000 |
| H | 1.590814000 | -3.318893000 | 1.178165000 |
| H | 0.292937000 | -4.249172000 | 0.413234000 |
| H | 1.408485000 | -2.822746000 | -1.305571000 |
| H | 1.408492000 | 2.822741000 | 1.305566000 |

N4b⁰

| | | | |
|----|--------------|--------------|--------------|
| Au | 1.730245000 | -0.000002000 | 0.000001000 |
| C | -0.260255000 | -0.000002000 | 0.000007000 |
| N | -1.065528000 | 1.086382000 | 0.000007000 |
| C | -2.394106000 | 0.699409000 | 0.000004000 |
| C | -2.394109000 | -0.699407000 | 0.000004000 |
| N | -1.065531000 | -1.086383000 | 0.000006000 |
| C | -3.583455000 | -1.417430000 | -0.000002000 |
| C | -3.583450000 | 1.417437000 | -0.000007000 |
| C | -4.765183000 | -0.697920000 | -0.000010000 |
| C | -4.765180000 | 0.697932000 | -0.000013000 |
| H | -3.597672000 | -2.497989000 | -0.000004000 |
| H | -5.708621000 | -1.230303000 | -0.000014000 |
| H | -5.708618000 | 1.230320000 | -0.000024000 |
| H | -3.597662000 | 2.497996000 | -0.000014000 |
| C | -0.554577000 | -2.459033000 | 0.000005000 |
| H | 0.530740000 | -2.329975000 | 0.000010000 |
| C | -0.554571000 | 2.459031000 | 0.000008000 |
| H | 0.530746000 | 2.329970000 | 0.000017000 |
| Cl | 3.995757000 | 0.000002000 | -0.000008000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.943368000 | -3.191537000 | -1.272620000 |
| H | -2.020665000 | -3.347146000 | -1.349833000 |
| H | -0.461490000 | -4.170611000 | -1.287697000 |
| H | -0.612468000 | -2.635369000 | -2.151365000 |
| C | -0.943379000 | -3.191541000 | 1.272623000 |
| H | -0.612480000 | -2.635381000 | 2.151374000 |
| H | -0.461509000 | -4.170620000 | 1.287698000 |
| H | -2.020678000 | -3.347143000 | 1.349830000 |
| C | -0.943375000 | 3.191544000 | 1.272622000 |
| H | -0.461487000 | 4.170613000 | 1.287703000 |
| H | -0.612498000 | 2.635377000 | 2.151377000 |
| H | -2.020673000 | 3.347167000 | 1.349816000 |
| C | -0.943354000 | 3.191533000 | -1.272620000 |
| H | -0.461471000 | 4.170605000 | -1.287700000 |
| H | -2.020651000 | 3.347148000 | -1.349836000 |
| H | -0.612456000 | 2.635360000 | -2.151363000 |

N5b⁰

| | | | |
|----|--------------|--------------|--------------|
| 79 | 1.660907000 | 0.000000000 | -0.000015000 |
| 6 | -0.356473000 | 0.000000000 | 0.000024000 |
| 7 | -1.155036000 | 1.098471000 | 0.000017000 |
| 6 | -2.491169000 | 0.702539000 | -0.000015000 |
| 6 | -2.491168000 | -0.702540000 | -0.000014000 |
| 7 | -1.155037000 | -1.098471000 | 0.000018000 |
| 6 | -3.698668000 | 1.403437000 | -0.000057000 |
| 1 | -3.742341000 | 2.476215000 | -0.000065000 |
| 6 | -4.882218000 | 0.694964000 | -0.000093000 |
| 1 | -5.819787000 | 1.237718000 | -0.000126000 |
| 6 | -4.882218000 | -0.694965000 | -0.000091000 |
| 1 | -5.819786000 | -1.237718000 | -0.000122000 |
| 6 | -3.698668000 | -1.403437000 | -0.000053000 |
| 1 | -3.742341000 | -2.476216000 | -0.000059000 |
| 6 | -0.590577000 | 2.496037000 | 0.000054000 |
| 6 | 0.235535000 | 2.699524000 | 1.268133000 |
| 6 | 0.235518000 | 2.699599000 | -1.268023000 |
| 6 | -1.673406000 | 3.567903000 | 0.000099000 |
| 1 | -0.385882000 | 2.549656000 | 2.154163000 |
| 1 | 0.619590000 | 3.721274000 | 1.284449000 |
| 1 | 1.086519000 | 2.020396000 | 1.320641000 |
| 1 | -0.385907000 | 2.549775000 | -2.154054000 |
| 1 | 1.086506000 | 2.020478000 | -1.320575000 |
| 1 | 0.619567000 | 3.721352000 | -1.284289000 |
| 1 | -2.295150000 | 3.533579000 | -0.894703000 |
| 1 | -1.161735000 | 4.530950000 | 0.000168000 |
| 1 | -2.295187000 | 3.533466000 | 0.894871000 |
| 6 | -0.590577000 | -2.496037000 | 0.000053000 |
| 6 | 0.235516000 | -2.699598000 | -1.268025000 |
| 6 | 0.235538000 | -2.699524000 | 1.268130000 |
| 6 | -1.673406000 | -3.567901000 | 0.000100000 |
| 1 | -0.385910000 | -2.549778000 | -2.154055000 |
| 1 | 0.619568000 | -3.721350000 | -1.284289000 |
| 1 | 1.086501000 | -2.020474000 | -1.320578000 |
| 1 | -0.385877000 | -2.549664000 | 2.154162000 |
| 1 | 1.086519000 | -2.020392000 | 1.320638000 |
| 1 | 0.619597000 | -3.721272000 | 1.284440000 |
| 1 | -2.295186000 | -3.533465000 | 0.894873000 |
| 1 | -1.161737000 | -4.530950000 | 0.000167000 |
| 1 | -2.295153000 | -3.533576000 | -0.894701000 |
| 17 | 3.930890000 | 0.000000000 | -0.000079000 |

N6b⁰

| | | | |
|----|--------------|--------------|--------------|
| 79 | 1.636080000 | 0.000002000 | -0.565119000 |
| 6 | -0.348893000 | 0.000000000 | -0.641965000 |
| 7 | -1.160029000 | -1.083009000 | -0.647487000 |
| 6 | -0.708304000 | -2.460349000 | -0.583784000 |
| 6 | -0.840278000 | -3.060805000 | 0.807758000 |

| | | | |
|----|--------------|--------------|--------------|
| 6 | 0.005129000 | -2.364174000 | 1.861576000 |
| 6 | -0.123662000 | -3.013833000 | 3.228070000 |
| 6 | -2.486179000 | -0.697619000 | -0.647182000 |
| 6 | -2.486181000 | 0.697613000 | -0.647182000 |
| 7 | -1.160031000 | 1.083007000 | -0.647487000 |
| 6 | -0.708309000 | 2.460348000 | -0.583784000 |
| 6 | -0.840288000 | 3.060804000 | 0.807757000 |
| 6 | 0.005109000 | 2.364169000 | 1.861580000 |
| 6 | -0.123680000 | 3.013834000 | 3.228071000 |
| 1 | 0.334246000 | -2.462903000 | -0.906310000 |
| 1 | -1.285984000 | -3.034773000 | -1.312924000 |
| 1 | -0.548218000 | -4.114322000 | 0.737302000 |
| 1 | -1.892830000 | -3.053597000 | 1.113914000 |
| 1 | -0.286381000 | -1.310746000 | 1.927410000 |
| 1 | 1.052883000 | -2.360377000 | 1.542687000 |
| 1 | 0.488375000 | -2.497911000 | 3.970456000 |
| 1 | 0.198128000 | -4.058646000 | 3.200879000 |
| 1 | -1.159766000 | -2.995967000 | 3.578729000 |
| 1 | 0.334242000 | 2.462903000 | -0.906308000 |
| 1 | -1.285988000 | 3.034770000 | -1.312926000 |
| 1 | -1.892841000 | 3.053602000 | 1.113907000 |
| 1 | -0.548223000 | 4.114319000 | 0.737302000 |
| 1 | 1.052865000 | 2.360361000 | 1.542695000 |
| 1 | -0.286411000 | 1.310744000 | 1.927417000 |
| 1 | 0.198124000 | 4.058642000 | 3.200878000 |
| 1 | 0.488346000 | 2.497905000 | 3.970462000 |
| 1 | -1.159786000 | 2.995983000 | 3.578726000 |
| 17 | 3.898118000 | 0.000005000 | -0.431051000 |
| 6 | -3.668165000 | -1.422148000 | -0.663658000 |
| 1 | -3.671263000 | -2.504839000 | -0.664427000 |
| 6 | -4.849628000 | -0.698672000 | -0.678396000 |
| 1 | -5.794686000 | -1.228063000 | -0.689582000 |
| 6 | -4.849629000 | 0.698661000 | -0.678397000 |
| 1 | -5.794689000 | 1.228049000 | -0.689586000 |
| 6 | -3.668168000 | 1.422140000 | -0.663659000 |
| 1 | -3.671268000 | 2.504831000 | -0.664431000 |

S3. Potential energy surface scans

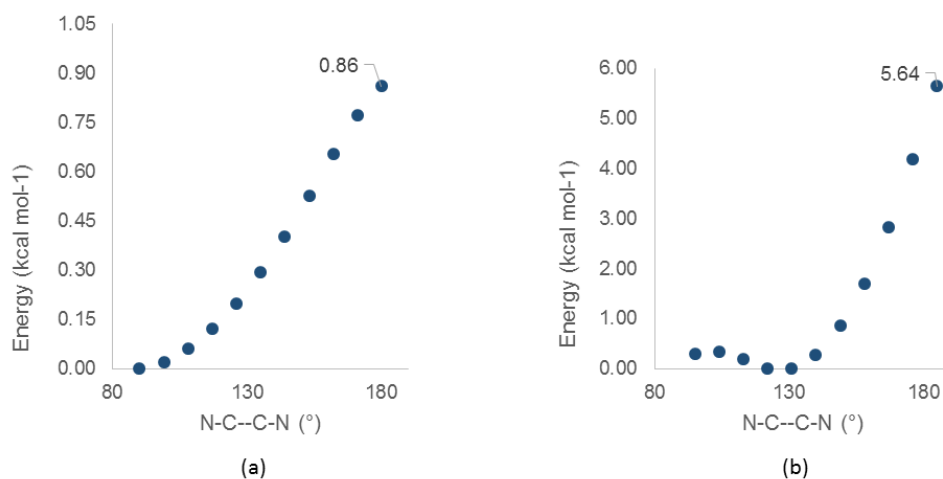


Figure S1. Potential energy surface scans around the N-C...(Au)...C-N torsion angle in (a) N₂⁺ and (b) N₅⁺.

S4. Bond Dissociation Energies

Table S1. BDEs (kcal/mol) at the PBE0-D3/def2-TZVP level of theory.

| | ΔE (kcal mol ⁻¹) | | ΔE (kcal mol ⁻¹) | | ΔE (kcal mol ⁻¹) | | ΔE (kcal mol ⁻¹) |
|-----------------|--------------------------------------|------------------|--------------------------------------|-----------------|--------------------------------------|------------------|--------------------------------------|
| N1 ⁺ | 91.8 | N1b ⁺ | 90.1 | N1 ⁰ | 79.3 | N1b ⁰ | 78.9 |
| N2 ⁺ | 92.5 | N2b ⁺ | 90.6 | N2 ⁰ | 81.9 | N2b ⁰ | 81.2 |
| N3 ⁺ | 94.1 | N3b ⁺ | 91.9 | N3 ⁰ | 83.9 | N3b ⁰ | 82.8 |
| N4 ⁺ | 93.5 | N4b ⁺ | 91.5 | N4 ⁰ | 83.9 | N4b ⁰ | 82.8 |
| N5 ⁺ | 90.5 | N5b ⁺ | 79.1 | N5 ⁰ | 81.0 | N5b ⁰ | 69.4 |
| N6 ⁺ | 95.5 | N6b ⁺ | 93.1 | N6 ⁰ | 85.1 | N6b ⁰ | 84.3 |

S5. Energy Decomposition Analysis

Table S2. Energy Decomposition Analysis results (kcal/mol) at the PBE0-D3/ZORA-TZP level of theory.

| Complex | ΔE (kcal/mol) | | | | | | |
|------------------|-----------------------|---------|-------|--------|---------|------------|-------------|
| | Total EDA energy | Coulomb | Pauli | Steric | Orbital | Dispersion | Preparation |
| N1 ⁺ | -92.3 | -198.7 | 171.6 | -27.1 | -63.2 | -2.0 | 1.9 |
| N2 ⁺ | -93.9 | -200.8 | 175.4 | -25.4 | -65.1 | -3.4 | 2.4 |
| N3 ⁺ | -95.9 | -202.8 | 178.8 | -23.9 | -66.0 | -6.0 | 2.6 |
| N4 ⁺ | -95.0 | -202.7 | 178.8 | -23.9 | -66.4 | -4.6 | 2.6 |
| N5 ⁺ | -95.9 | -198.7 | 183.8 | -14.9 | -70.5 | -10.5 | 5.2 |
| N6 ⁺ | -98.7 | -203.5 | 181.5 | -22.0 | -67.4 | -9.3 | 4.5 |
| N1b ⁺ | -90.8 | -195.3 | 171.5 | -23.8 | -64.9 | -2.2 | 2.0 |
| N2b ⁺ | -92.1 | -197.0 | 174.9 | -22.0 | -66.6 | -3.6 | 2.4 |
| N3b ⁺ | -93.9 | -199.3 | 178.2 | -21.1 | -67.2 | -5.6 | 2.5 |
| N4b ⁺ | -93.2 | -199.9 | 180.1 | -19.8 | -68.1 | -5.3 | 2.7 |
| N5b ⁺ | -88.2 | -187.8 | 179.8 | -8.1 | -70.9 | -9.2 | 9.6 |
| N6b ⁺ | -97.6 | -200.3 | 181.1 | -19.2 | -68.6 | -9.8 | 5.2 |
| N1 ⁰ | -78.3 | -217.1 | 204.9 | -12.2 | -64.2 | -1.9 | 0.8 |
| N2 ⁰ | -81.4 | -218.9 | 205.3 | -13.6 | -64.9 | -3.0 | 1.0 |
| N3 ⁰ | -83.9 | -221.1 | 206.8 | -14.3 | -65.5 | -4.1 | 1.4 |
| N4 ⁰ | -83.5 | -220.9 | 207.0 | -14.0 | -65.8 | -3.7 | 1.1 |
| N5 ⁰ | -83.2 | -221.4 | 211.4 | -9.9 | -67.8 | -5.5 | 3.1 |
| N6 ⁰ | -84.9 | -220.2 | 206.7 | -13.5 | -66.2 | -5.2 | 1.1 |
| N1b ⁰ | -77.8 | -217.4 | 207.4 | -10.1 | -65.7 | -2.1 | 0.8 |
| N2b ⁰ | -80.6 | -219.0 | 207.7 | -11.3 | -66.3 | -3.1 | 0.9 |
| N3b ⁰ | -82.5 | -220.9 | 209.1 | -11.8 | -66.7 | -4.0 | 1.3 |
| N4b ⁰ | -82.4 | -221.2 | 209.8 | -11.5 | -67.1 | -3.9 | 1.1 |
| N5b ⁰ | -78.5 | -218.9 | 215.3 | -3.5 | -69.5 | -5.5 | 10.1 |
| N6b ⁰ | -83.9 | -220.4 | 209.3 | -11.1 | -67.4 | -5.4 | 0.8 |