

complex1 BP86

30

Energy = -797.6536393511

| | | | |
|----|------------|------------|------------|
| Ag | 15.5185798 | 20.5061175 | 26.1695509 |
| O | 17.3009719 | 20.0960664 | 28.6209598 |
| H | 18.2318238 | 20.3687510 | 28.7012025 |
| H | 17.1057510 | 19.6320723 | 29.4538067 |
| N | 16.4988756 | 18.9784826 | 25.1200563 |
| N | 14.4670797 | 22.0333310 | 27.1608469 |
| C | 17.7399344 | 16.8229144 | 23.7716894 |
| C | 17.8842332 | 17.0122896 | 25.1603460 |
| H | 18.4827159 | 16.3298940 | 25.7627994 |
| C | 17.2639840 | 18.0791583 | 25.7880232 |
| H | 17.3716994 | 18.2512987 | 26.8593300 |
| C | 16.3578081 | 18.8171951 | 23.7842082 |
| H | 15.7451721 | 19.5532181 | 23.2648853 |
| C | 16.9550881 | 17.7739066 | 23.0927704 |
| H | 16.8043541 | 17.6965397 | 22.0155648 |
| C | 13.1170906 | 24.0765589 | 28.5010606 |
| C | 12.6003289 | 23.5377147 | 27.3221293 |
| H | 11.6634804 | 23.8956024 | 26.8968003 |
| C | 13.3006377 | 22.5220379 | 26.6800660 |
| H | 12.9293219 | 22.0781258 | 25.7572617 |
| C | 14.9649352 | 22.5527428 | 28.3071603 |
| H | 15.8987366 | 22.1144649 | 28.6614225 |
| C | 14.3194619 | 23.5731339 | 28.9983601 |
| H | 14.7602293 | 23.9624603 | 29.9154491 |
| H | 12.5901322 | 24.8751887 | 29.0238232 |
| C | 18.3495071 | 15.7199405 | 23.0269147 |
| C | 19.0722507 | 14.7162547 | 23.5482558 |
| H | 18.1768894 | 15.7386747 | 21.9472841 |
| H | 19.4829791 | 13.9353238 | 22.9090259 |
| H | 19.2798340 | 14.6265085 | 24.6157234 |

complex1 GAM-B3LYP

| | | | |
|----|-------------|-------------|-------------|
| Ag | 15.70605900 | 20.33398200 | 26.32424100 |
| O | 17.51779500 | 20.08375200 | 28.23273900 |
| H | 18.41074900 | 20.47567400 | 28.19995900 |
| H | 17.39931400 | 19.54280200 | 29.03609400 |
| N | 16.39792800 | 18.68477600 | 25.13649900 |
| N | 14.73914700 | 22.02937600 | 27.23482700 |
| C | 17.35050700 | 16.49971400 | 23.61725600 |
| C | 17.93384400 | 16.84801800 | 24.85406600 |
| H | 18.76690400 | 16.28589500 | 25.25864600 |
| C | 17.43973800 | 17.92941500 | 25.57498300 |
| H | 17.86933400 | 18.21904400 | 26.52634500 |
| C | 15.82633900 | 18.36229700 | 23.94881400 |
| H | 14.99824600 | 18.97725500 | 23.61836900 |
| C | 16.27214400 | 17.29255300 | 23.17700200 |
| H | 15.78042600 | 17.07724300 | 22.23448600 |
| C | 13.53346900 | 24.23434500 | 28.45955300 |
| C | 13.01006500 | 23.70530500 | 27.27196600 |
| H | 12.13243600 | 24.13439100 | 26.80313500 |
| C | 13.63795700 | 22.60365100 | 26.68782800 |
| H | 13.26090000 | 22.16893400 | 25.77014100 |
| C | 15.24672300 | 22.54008400 | 28.38499900 |
| H | 16.12493900 | 22.04339100 | 28.77919800 |
| C | 14.67066300 | 23.63999200 | 29.02331700 |
| H | 15.10611300 | 24.01886900 | 29.94052300 |
| H | 13.06553700 | 25.09014500 | 28.93449800 |
| C | 17.80660400 | 15.37188400 | 22.78443900 |
| C | 18.81844200 | 14.53431700 | 23.07473100 |
| H | 17.25706400 | 15.22738500 | 21.85638600 |
| H | 19.08406800 | 13.72872200 | 22.39829700 |
| H | 19.41393600 | 14.61320900 | 23.98031900 |

complex1 S1 BP86

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Energy = -797.6319200933

| | | | |
|----|------------|------------|------------|
| Ag | 15.8253016 | 20.4328475 | 26.6565198 |
| O | 17.6027573 | 20.5104942 | 28.1371588 |
| H | 18.3936293 | 20.3304468 | 27.5890771 |
| H | 17.5733519 | 19.7759336 | 28.7805944 |
| N | 16.6773920 | 18.9185389 | 25.5651949 |
| N | 14.8426151 | 22.0345507 | 27.5542505 |
| C | 17.7806801 | 16.8207308 | 23.9398109 |
| C | 17.8515881 | 16.8157387 | 25.3863760 |
| H | 18.3312482 | 15.9915244 | 25.9117170 |
| C | 17.3087767 | 17.8240852 | 26.1252563 |
| H | 17.3388863 | 17.7801984 | 27.2158609 |
| C | 16.5341530 | 18.9179258 | 24.1805521 |
| H | 16.0011355 | 19.7622045 | 23.7417266 |
| C | 17.0474791 | 17.9298623 | 23.3940176 |
| H | 16.9037273 | 17.9984977 | 22.3154724 |
| C | 13.4586878 | 24.1986594 | 28.5978844 |
| C | 12.9438161 | 23.4897687 | 27.5114557 |
| H | 11.9987084 | 23.7639824 | 27.0457209 |
| C | 13.6605208 | 22.4078227 | 27.0148493 |
| H | 13.2903875 | 21.8262043 | 26.1683572 |
| C | 15.3518124 | 22.7185448 | 28.6007785 |
| H | 16.3140084 | 22.3833080 | 28.9833038 |
| C | 14.6782462 | 23.8036666 | 29.1488567 |
| H | 15.1169637 | 24.3308759 | 29.9947149 |
| H | 12.9167291 | 25.0507211 | 29.0082853 |
| C | 18.3634672 | 15.8316973 | 23.1091160 |
| C | 19.0996317 | 14.7432842 | 23.5051796 |
| H | 18.1994650 | 15.9706460 | 22.0358762 |
| H | 19.5034858 | 14.0519853 | 22.7694327 |
| H | 19.3159313 | 14.5241875 | 24.5509158 |

complex1 S1 GAM-B3LYP

| | | | |
|----|-------------|-------------|-------------|
| Ag | 15.69950400 | 20.32000800 | 26.29516300 |
| O | 17.51814400 | 20.09453000 | 28.23980000 |
| H | 18.41671400 | 20.47224600 | 28.19574500 |
| H | 17.40851000 | 19.53547300 | 29.03194300 |
| N | 16.38485600 | 18.68976900 | 25.12593200 |
| N | 14.74779200 | 22.01234900 | 27.22355800 |
| C | 17.30523500 | 16.49799500 | 23.55678300 |
| C | 17.92630000 | 16.84785300 | 24.84050500 |
| H | 18.75970800 | 16.27937300 | 25.23530200 |
| C | 17.43153700 | 17.92612800 | 25.55506800 |
| H | 17.86415200 | 18.21500900 | 26.50600900 |
| C | 15.78048600 | 18.37254800 | 23.90388000 |
| H | 14.95587100 | 19.00270100 | 23.59900000 |
| C | 16.20888100 | 17.31649300 | 23.12861200 |
| H | 15.71045900 | 17.10587100 | 22.18719400 |
| C | 13.55609600 | 24.21444700 | 28.46722200 |
| C | 13.02719800 | 23.69662700 | 27.27701700 |
| H | 12.15059800 | 24.13348900 | 26.81340300 |
| C | 13.64814700 | 22.59613700 | 26.68348300 |
| H | 13.26710900 | 22.16949000 | 25.76361500 |
| C | 15.26093000 | 22.51201700 | 28.37627000 |
| H | 16.13754800 | 22.00648000 | 28.76273500 |
| C | 14.69168500 | 23.61018700 | 29.02377900 |
| H | 15.13122400 | 23.98021500 | 29.94269400 |
| H | 13.09360100 | 25.06911900 | 28.94954700 |
| C | 17.78111000 | 15.40244500 | 22.79076700 |
| C | 18.85637200 | 14.56935100 | 23.17118400 |
| H | 17.28628100 | 15.18667100 | 21.84538300 |
| H | 19.16823300 | 13.74779900 | 22.53332300 |
| H | 19.40310800 | 14.71360000 | 24.09873800 |

complex2 BP86

33

Energy = -874.1366045697

| | | | |
|----|------------|------------|------------|
| Ag | 15.6519058 | 20.4206959 | 26.1529753 |
| O | 17.6918034 | 20.1961176 | 28.1431895 |
| H | 18.6213641 | 20.5229485 | 28.0466831 |
| H | 17.6671162 | 19.7564052 | 29.0098497 |
| O | 20.3070929 | 21.1106534 | 27.9316079 |
| H | 21.0707023 | 20.6383710 | 27.5609644 |
| H | 20.6137887 | 22.0152664 | 28.1079268 |
| N | 16.4257555 | 18.8177165 | 25.0326229 |
| N | 14.7192081 | 22.0154440 | 27.1696945 |
| C | 17.3978175 | 16.5661295 | 23.6252346 |
| C | 17.8334149 | 16.8711681 | 24.9296106 |
| H | 18.5667545 | 16.2464249 | 25.4381790 |
| C | 17.3370085 | 17.9828694 | 25.5897549 |
| H | 17.6647789 | 18.2494741 | 26.5949894 |
| C | 16.0064861 | 18.5471100 | 23.7760546 |
| H | 15.2801072 | 19.2355060 | 23.3450303 |
| C | 16.4663670 | 17.4544065 | 23.0563298 |
| H | 16.0908975 | 17.2873241 | 22.0462842 |
| C | 13.5147423 | 24.1103352 | 28.5668903 |
| C | 12.8944097 | 23.5539322 | 27.4476874 |
| H | 11.9303140 | 23.9167749 | 27.0932247 |
| C | 13.5246541 | 22.5122372 | 26.7751831 |
| H | 13.0714643 | 22.0523554 | 25.8979872 |
| C | 15.3198645 | 22.5546960 | 28.2554243 |
| H | 16.2761409 | 22.1085158 | 28.5344314 |
| C | 14.7481618 | 23.6007180 | 28.9731950 |
| H | 15.2686082 | 24.0045816 | 29.8408632 |
| H | 13.0430129 | 24.9272985 | 29.1136123 |
| C | 17.8562367 | 15.4048267 | 22.8602928 |
| C | 18.6259467 | 14.4075442 | 23.3228764 |
| H | 17.5097930 | 15.3651298 | 21.8238594 |
| H | 18.9098088 | 13.5761432 | 22.6785906 |
| H | 18.9920559 | 14.3702515 | 24.3501913 |

complex2 GAM-B3LYP

| | | | |
|----|-------------|-------------|-------------|
| Ag | 15.84074300 | 20.35038100 | 26.32784600 |
| O | 17.59751700 | 20.11269800 | 28.09941800 |
| H | 18.49237700 | 20.56723500 | 28.05269900 |
| H | 17.51341400 | 19.53784500 | 28.87992400 |
| O | 19.91258400 | 21.28870200 | 27.97619500 |
| H | 20.64767100 | 20.98207500 | 27.41720400 |
| H | 20.11905900 | 22.13331500 | 28.41313700 |
| N | 16.47030100 | 18.68591800 | 25.09972100 |
| N | 14.83122600 | 22.04469000 | 27.22849800 |
| C | 17.35307900 | 16.45524200 | 23.60670100 |
| C | 17.96971900 | 16.81894000 | 24.82246500 |
| H | 18.80150800 | 16.25014300 | 25.22064200 |
| C | 17.50945100 | 17.92372000 | 25.53138800 |
| H | 17.96110500 | 18.23051600 | 26.46757800 |
| C | 15.86819500 | 18.35013200 | 23.93225300 |
| H | 15.04269100 | 18.97233100 | 23.60900700 |
| C | 16.27979300 | 17.25748800 | 23.17213900 |
| H | 15.76416600 | 17.03088100 | 22.24508800 |
| C | 13.58693400 | 24.19696200 | 28.50595000 |
| C | 13.10760600 | 23.72559700 | 27.27619700 |
| H | 12.24928800 | 24.17950900 | 26.79499200 |
| C | 13.75414000 | 22.64782300 | 26.66712900 |
| H | 13.41133800 | 22.25517400 | 25.71758900 |
| C | 15.29756700 | 22.49992000 | 28.41828200 |
| H | 16.15963000 | 21.97833600 | 28.81767700 |
| C | 14.70030700 | 23.57229500 | 29.08444700 |
| H | 15.09965600 | 23.90552300 | 30.03531100 |
| H | 13.10269300 | 25.03143800 | 29.00221200 |
| C | 17.77071400 | 15.30085400 | 22.78907700 |
| C | 18.76040300 | 14.43922700 | 23.08471900 |
| H | 17.20802100 | 15.15577400 | 21.86889700 |
| H | 18.99642100 | 13.61466300 | 22.42024000 |
| H | 19.36427300 | 14.51538400 | 23.98496800 |

complex2 S1 BP86

33

Energy = -874.1082996554

| | | | |
|----|------------|------------|------------|
| Ag | 15.8209402 | 20.4269603 | 26.6808473 |
| O | 17.5291360 | 20.5477450 | 28.1393231 |
| H | 18.3664035 | 20.3205342 | 27.5625002 |
| H | 17.4597076 | 19.8364797 | 28.8039949 |
| O | 19.4763194 | 19.9951211 | 26.5771970 |
| H | 19.2767762 | 19.1798725 | 26.0695757 |
| H | 20.4245886 | 19.9795831 | 26.7920965 |
| N | 16.6772408 | 18.9001161 | 25.5585537 |
| N | 14.8458512 | 22.0495268 | 27.5638453 |
| C | 17.7843104 | 16.8044700 | 23.9177614 |
| C | 17.8687387 | 16.8029886 | 25.3643933 |
| H | 18.3489134 | 15.9779676 | 25.8893546 |
| C | 17.3128507 | 17.8058440 | 26.1089879 |
| H | 17.3481474 | 17.7576244 | 27.1985660 |
| C | 16.5142200 | 18.8863149 | 24.1783021 |
| H | 15.9692505 | 19.7237184 | 23.7423361 |
| C | 17.0267620 | 17.9024876 | 23.3828094 |
| H | 16.8658975 | 17.9703500 | 22.3061520 |
| C | 13.4470143 | 24.2081065 | 28.6001550 |
| C | 12.9447660 | 23.5027093 | 27.5055017 |
| H | 12.0033843 | 23.7760351 | 27.0312367 |
| C | 13.6691315 | 22.4240295 | 27.0140488 |
| H | 13.3088345 | 21.8453712 | 26.1605819 |
| C | 15.3437260 | 22.7316372 | 28.6160072 |
| H | 16.3045736 | 22.3931244 | 29.0012574 |
| C | 14.6621307 | 23.8147389 | 29.1612916 |
| H | 15.0907790 | 24.3395429 | 30.0137851 |
| H | 12.8973492 | 25.0563238 | 29.0083412 |
| C | 18.3728384 | 15.8188441 | 23.0854623 |
| C | 19.1103319 | 14.7317188 | 23.4823740 |
| H | 18.2105292 | 15.9577787 | 22.0121500 |
| H | 19.5160709 | 14.0371101 | 22.7505454 |
| H | 19.3150515 | 14.5095503 | 24.5296338 |