

Thermally activated delayed fluorescence from Ag(I) complexes: A route to 100% quantum yield at unprecedentedly short decay time.

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Calculated (M06/def2-SVP) gas phase geometry of Ag(phen)(P₂-nCB) **1** in cartesian (XYZ) coordinates

Ground state (S ₀)				Lowest triplet state (T ₁)			
C	0.226392000	-5.335790000	-0.023640000	C	1.382319000	-5.063405000	-1.292308000
C	1.417501000	-6.025269000	0.190078000	C	2.556525000	-5.629888000	-0.806403000
C	2.623750000	-5.328853000	0.249605000	C	3.459229000	-4.851983000	-0.080524000
C	2.641236000	-3.944763000	0.107411000	C	3.192073000	-3.509974000	0.164822000
C	1.446703000	-3.244564000	-0.087807000	C	2.004094000	-2.940157000	-0.309852000
C	0.242701000	-3.950799000	-0.167727000	C	1.105983000	-3.719292000	-1.045870000
C	4.804790000	-0.537995000	-3.254254000	C	4.354504000	0.502519000	-3.515861000
C	5.123000000	-0.674691000	-1.904667000	C	4.858909000	0.416117000	-2.219857000
C	4.126587000	-0.941896000	-0.968481000	C	4.062539000	-0.068926000	-1.184748000
C	2.790827000	-1.055919000	-1.373861000	C	2.740621000	-0.448040000	-1.441755000
C	2.483332000	-0.919202000	-2.733312000	C	2.243230000	-0.369295000	-2.748258000
C	3.482193000	-0.671170000	-3.670496000	C	3.047881000	0.098177000	-3.782780000
C	1.888072000	2.485184000	-0.727050000	C	1.373004000	2.772475000	-0.504376000
C	2.995519000	3.118064000	-0.143812000	C	2.263633000	3.671172000	0.099134000
C	4.010514000	3.634469000	-0.943406000	C	3.047996000	4.504421000	-0.692106000
C	3.937504000	3.525688000	-2.331658000	C	2.950021000	4.450423000	-2.082426000
C	2.842124000	2.901660000	-2.921398000	C	2.060095000	3.566129000	-2.686239000
C	1.826571000	2.383361000	-2.120979000	C	1.274698000	2.727498000	-1.898987000
C	-1.806521000	2.974837000	1.050178000	C	-2.211939000	1.959541000	1.564544000
C	-0.420524000	3.132467000	0.935495000	C	-1.088616000	2.635481000	1.062495000
C	0.165557000	4.328858000	1.358761000	C	-1.142933000	4.021571000	0.877888000
C	-0.621026000	5.338776000	1.907235000	C	-2.302279000	4.722116000	1.205582000
C	-1.997564000	5.165890000	2.035304000	C	-3.411728000	4.045969000	1.704770000
C	-2.591392000	3.981733000	1.603495000	C	-3.363959000	2.663203000	1.887042000
B	2.885040000	-1.202906000	2.495025000	B	3.325443000	-0.753580000	2.458129000
B	2.094058000	-1.140910000	4.059921000	B	2.639832000	-0.935259000	4.066999000
B	1.550308000	0.549113000	4.357976000	B	1.768904000	0.585563000	4.487149000
C	1.196116000	0.798165000	1.671394000	C	1.192318000	0.851160000	1.850899000
C	1.625986000	-0.728547000	1.443058000	C	1.923992000	-0.524575000	1.518797000
B	0.384267000	-0.707997000	3.902491000	B	0.871922000	-0.876906000	4.045145000
B	2.838541000	0.424461000	1.791040000	B	2.889887000	0.855826000	1.855914000
B	1.214031000	-1.729893000	2.669423000	B	1.814832000	-1.642158000	2.699268000
B	3.111396000	0.223195000	3.533028000	B	3.304765000	0.644284000	3.559553000
B	2.053101000	1.493196000	2.953577000	B	1.955732000	1.676268000	3.114770000
B	0.360780000	0.933659000	3.091553000	B	0.439228000	0.741993000	3.319252000
Ag	-0.752739000	-0.234091000	-0.832346000	Ag	-0.685818000	-0.428622000	-0.579447000
P	0.513569000	1.726759000	0.225454000	P	0.316109000	1.654689000	0.468921000

P	1.376924000	-1.423745000	-0.256551000
C	-6.361604000	-0.390024000	-1.119587000
C	-6.268098000	-0.938662000	0.120692000
C	-5.185570000	-0.066574000	-1.870000000
C	-3.902137000	-0.315301000	-1.321471000
N	-2.771622000	-0.023746000	-2.001181000
C	-2.859076000	0.510502000	-3.206343000
C	-4.082846000	0.792879000	-3.833367000
C	-5.247800000	0.501369000	-3.158112000
C	-3.804478000	-0.900272000	0.002510000
C	-4.991782000	-1.208144000	0.710417000
C	-4.853905000	-1.776821000	1.994475000
C	-3.597656000	-2.023198000	2.501139000
C	-2.478888000	-1.690405000	1.715225000
N	-2.585464000	-1.139173000	0.520407000
H	-0.721046000	-5.879578000	-0.081154000
H	1.407983000	-7.113145000	0.304925000
H	3.561045000	-5.868674000	0.411731000
H	3.592222000	-3.406227000	0.158525000
H	-0.691580000	-3.401692000	-0.337883000
H	5.592174000	-0.329396000	-3.984607000
H	6.160779000	-0.576874000	-1.573277000
H	4.392388000	-1.055918000	0.085762000
H	1.438571000	-1.005645000	-3.058339000
H	3.225216000	-0.571655000	-4.729459000
H	3.077651000	3.188455000	0.944926000
H	4.871939000	4.119943000	-0.475870000
H	4.742080000	3.926433000	-2.955281000
H	2.782089000	2.805552000	-4.009652000
H	0.971457000	1.875418000	-2.584375000
H	-2.268923000	2.038334000	0.712340000
H	1.244892000	4.477794000	1.264866000
H	-0.151740000	6.268419000	2.241616000
H	-2.610955000	5.960301000	2.470410000
H	-3.672202000	3.841998000	1.697538000
H	-7.337148000	-0.183872000	-1.570447000
H	-7.167479000	-1.185162000	0.693523000
H	-4.095688000	1.234070000	-4.832190000
H	-3.450092000	-2.461575000	3.490418000
H	2.392737000	-1.861993000	4.974851000
H	1.531397000	1.052269000	5.449530000
H	2.292375000	2.673421000	2.929955000
H	4.177632000	0.482350000	4.021366000
H	3.772705000	-1.927250000	2.121713000
H	-0.429305000	-1.075244000	4.714970000
H	0.946086000	-2.888275000	2.468764000
H	-0.492483000	1.767537000	3.248324000
H	-0.241353000	-0.309814000	2.868122000
H	3.619293000	0.814446000	0.973551000
H	-1.913155000	0.734178000	-3.714966000
H	-1.463102000	-1.888759000	2.086166000
H	-6.226233000	0.704506000	-3.604963000
H	-5.753525000	-2.017011000	2.570283000

P	1.630806000	-1.159635000	-0.166817000
C	-6.093517000	-0.872181000	-0.885298000
C	-5.873022000	-2.079697000	-0.303797000
C	-5.010889000	0.016821000	-1.211162000
C	-3.676363000	-0.416271000	-0.934033000
N	-2.602739000	0.403775000	-1.223632000
C	-2.832938000	1.620882000	-1.747918000
C	-4.093686000	2.101778000	-2.034724000
C	-5.208750000	1.278483000	-1.765085000
C	-3.446122000	-1.672706000	-0.337832000
C	-4.545173000	-2.525204000	0.006596000
C	-4.278459000	-3.735194000	0.639168000
C	-2.954746000	-4.089797000	0.938465000
C	-1.937979000	-3.218911000	0.565676000
N	-2.150456000	-2.064487000	-0.067713000
H	0.672106000	-5.667082000	-1.863943000
H	2.773430000	-6.685307000	-0.994276000
H	4.382916000	-5.295937000	0.300769000
H	3.902066000	-2.907126000	0.738464000
H	0.180135000	-3.272906000	-1.428814000
H	4.986755000	0.880345000	-4.324516000
H	5.887882000	0.721129000	-2.010046000
H	4.473939000	-0.149782000	-0.174977000
H	1.210730000	-0.678629000	-2.958997000
H	2.650868000	0.151265000	-4.800654000
H	2.342707000	3.716477000	1.189736000
H	3.743745000	5.201708000	-0.217335000
H	3.573032000	5.104830000	-2.698821000
H	1.981687000	3.519139000	-3.776119000
H	0.585333000	2.019655000	-2.374610000
H	-2.193899000	0.870690000	1.688056000
H	-0.281225000	4.559901000	0.471811000
H	-2.336215000	5.805841000	1.063601000
H	-4.323458000	4.597764000	1.950305000
H	-4.235463000	2.126215000	2.270950000
H	-7.112424000	-0.540682000	-1.111626000
H	-6.709954000	-2.738822000	-0.050126000
H	-4.210491000	3.102544000	-2.455573000
H	-2.711377000	-5.021845000	1.451782000
H	3.152034000	-1.605673000	4.921917000
H	1.719361000	1.025716000	5.603086000
H	1.922099000	2.878988000	3.125371000
H	4.320374000	1.105550000	4.001322000
H	4.325344000	-1.235548000	1.991208000
H	0.235731000	-1.445981000	4.890096000
H	1.760327000	-2.813114000	2.429865000
H	-0.556551000	1.366653000	3.558517000
H	0.098095000	-0.620286000	3.067987000
H	3.495364000	1.442157000	1.007651000
H	-1.948998000	2.245342000	-1.933752000
H	-0.891621000	-3.468430000	0.789052000
H	-6.226890000	1.619807000	-1.976328000
H	-5.111520000	-4.392949000	0.907832000

Calculated (M06/def2-SVP) gas phase geometry of Ag(idmp)(P₂-nCB) 2 in cartesian (XYZ) coordinates

Ground state (S ₀)				Lowest triplet state (T ₁)			
C	0.420612000	-5.294093000	-0.680839000	C	1.167683000	-5.032412000	-1.635004000
C	1.611781000	-6.011405000	-0.600574000	C	2.293558000	-5.727231000	-1.204504000
C	2.826199000	-5.334525000	-0.497895000	C	3.267775000	-5.077190000	-0.446017000
C	2.852116000	-3.943660000	-0.464144000	C	3.120282000	-3.735552000	-0.113202000
C	1.658374000	-3.218119000	-0.524954000	C	1.981236000	-3.036650000	-0.532053000
C	0.445283000	-3.902133000	-0.648850000	C	1.011379000	-3.687937000	-1.300509000
C	4.942215000	-0.152278000	-3.430132000	C	4.618183000	0.404935000	-3.515042000
C	5.300856000	-0.457648000	-2.118845000	C	5.115447000	0.178816000	-2.233287000
C	4.331800000	-0.836285000	-1.192348000	C	4.280680000	-0.307397000	-1.229597000
C	2.983279000	-0.893138000	-1.566188000	C	2.929244000	-0.546291000	-1.501663000
C	2.635022000	-0.586179000	-2.887514000	C	2.438377000	-0.328003000	-2.794582000
C	3.606375000	-0.227251000	-3.817677000	C	3.279920000	0.139765000	-3.799321000
C	2.152694000	2.543864000	-0.440890000	C	1.835492000	2.710938000	-0.337872000
C	3.278907000	3.093598000	0.188936000	C	2.805877000	3.487839000	0.310233000
C	4.279356000	3.699688000	-0.564706000	C	3.651840000	4.302108000	-0.436005000
C	4.173349000	3.764166000	-1.953607000	C	3.536989000	4.349742000	-1.825275000
C	3.059527000	3.223591000	-2.589329000	C	2.568732000	3.587003000	-2.472729000
C	2.058473000	2.615633000	-1.834929000	C	1.721251000	2.767830000	-1.730797000
C	-1.489671000	2.832826000	1.479693000	C	-1.788367000	2.066565000	1.722404000
C	-0.104655000	2.990289000	1.353376000	C	-0.615393000	2.677210000	1.251621000
C	0.506220000	4.114636000	1.916190000	C	-0.551478000	4.072246000	1.162371000
C	-0.254437000	5.051434000	2.611322000	C	-1.643226000	4.845012000	1.553455000
C	-1.629945000	4.877064000	2.748560000	C	-2.802759000	4.233226000	2.020860000
C	-2.248601000	3.766049000	2.179246000	C	-2.872757000	2.842213000	2.107897000
B	3.193954000	-1.532132000	2.250716000	B	3.504129000	-1.161523000	2.355910000
B	2.448614000	-1.664918000	3.833656000	B	2.818611000	-1.392263000	3.958077000
B	1.931562000	-0.022921000	4.360519000	B	2.083904000	0.164921000	4.489833000
C	1.503671000	0.569524000	1.739276000	C	1.510695000	0.655278000	1.885128000
C	1.910336000	-0.918626000	1.305824000	C	2.119782000	-0.752421000	1.452534000
B	0.739808000	-1.203510000	3.783909000	B	1.061926000	-1.183480000	3.963606000
B	3.144642000	0.172016000	1.761632000	B	3.202186000	0.515346000	1.866917000
B	1.522858000	-2.065480000	2.406372000	B	1.925491000	-1.933476000	2.557659000
B	3.465013000	-0.251814000	3.454880000	B	3.611675000	0.155872000	3.547260000
B	2.404103000	1.088961000	3.073690000	B	2.352236000	1.325692000	3.190314000
B	0.710469000	0.528081000	3.188949000	B	0.763246000	0.511734000	3.353334000
Ag	-0.530905000	-0.125782000	-0.817465000	Ag	-0.482741000	-0.298119000	-0.602680000
P	0.793144000	1.679779000	0.441848000	P	0.694212000	1.623254000	0.572734000
P	1.600759000	-1.390126000	-0.459199000	P	1.763092000	-1.243510000	-0.269575000
C	-6.141028000	-0.076815000	-0.963570000	C	-5.906548000	-0.249904000	-0.751321000
C	-6.031687000	-0.767652000	0.204422000	C	-5.785711000	-1.507363000	-0.239464000
C	-4.984177000	0.298724000	-1.716802000	C	-4.763936000	0.562210000	-1.066701000
C	-3.700017000	-0.056112000	-1.233035000	C	-3.471573000	-0.008929000	-0.855403000
N	-2.569184000	0.271352000	-1.898520000	N	-2.328150000	0.712529000	-1.135352000
C	-2.667536000	0.943045000	-3.029696000	C	-2.456468000	1.978965000	-1.588737000
C	-3.892481000	1.334764000	-3.585777000	C	-3.670413000	2.583066000	-1.807146000
C	-5.074080000	1.020607000	-2.939488000	C	-3.346814000	-1.315405000	-0.332229000
C	-3.585510000	-0.794588000	0.012585000	C	-4.506157000	-2.091858000	0.005325000
C	-4.756142000	-1.148260000	0.726894000	C	-4.337329000	-3.367973000	0.569386000
C	-4.611016000	-1.870575000	1.945941000	C	-5.508188000	-4.219975000	0.942284000
C	-3.329653000	-2.197906000	2.347621000	H	-6.151473000	-4.433639000	0.072118000
C	-2.229372000	-1.811979000	1.565818000	H	-6.146532000	-3.727808000	1.695353000
N	-2.354119000	-1.124652000	0.447234000	H	-5.181286000	-5.182510000	1.361072000
H	-0.533692000	-5.821166000	-0.771227000	C	-3.030906000	-3.824539000	0.788844000
H	1.595628000	-7.105019000	-0.624172000	C	-1.950182000	-3.022192000	0.426629000
H	3.763369000	-5.895449000	-0.440143000	N	-2.080902000	-1.826573000	-0.129569000
H	3.809603000	-3.420914000	-0.380513000	H	0.402136000	-5.535362000	-2.232188000
H	-0.489104000	-3.330953000	-0.712596000	H	2.416480000	-6.783199000	-1.461616000

H	5.708289000	0.142969000	-4.153253000	H	4.153601000	-5.621976000	-0.108048000
H	6.349106000	-0.405877000	-1.810787000	H	3.885665000	-3.233740000	0.485924000
H	4.629086000	-1.082445000	-0.169544000	H	0.123755000	-3.140113000	-1.639970000
H	1.579881000	-0.626515000	-3.187137000	H	5.280072000	0.783031000	-4.299507000
H	3.317561000	0.004769000	-4.847307000	H	6.168124000	0.374139000	-2.010643000
H	3.387241000	3.027979000	1.275641000	H	4.685449000	-0.498831000	-0.232177000
H	5.155445000	4.118734000	-0.061469000	H	1.381631000	-0.526869000	-3.017916000
H	4.966548000	4.234750000	-2.542063000	H	2.887154000	0.302812000	-4.807136000
H	2.973470000	3.262889000	-3.679393000	H	2.898522000	3.453076000	1.400159000
H	1.188922000	2.173393000	-2.337123000	H	4.409419000	4.904129000	0.073267000
H	-1.971704000	1.953919000	1.032482000	H	4.208454000	4.988337000	-2.406388000
H	1.585079000	4.263605000	1.817265000	H	2.476585000	3.619902000	-3.562057000
H	0.234447000	5.924137000	3.053716000	H	0.968899000	2.155095000	-2.241624000
H	-2.222918000	5.613445000	3.298891000	H	-1.863353000	0.974391000	1.770301000
H	-3.328820000	3.625911000	2.279784000	H	0.349876000	4.561718000	0.781352000
H	-7.131087000	0.198499000	-1.335404000	H	-1.584865000	5.934875000	1.485744000
H	-6.935795000	-1.038279000	0.755894000	H	-3.661615000	4.842695000	2.315838000
H	-3.906092000	1.889163000	-4.528249000	H	-3.784551000	2.355877000	2.464924000
H	-3.157602000	-2.751720000	3.274724000	H	-6.904416000	0.164099000	-0.922090000
H	2.765805000	-2.498848000	4.640177000	H	-6.687211000	-2.080236000	-0.004014000
H	1.949287000	0.336925000	5.507486000	H	-3.701669000	3.613561000	-2.172472000
H	2.655733000	2.260674000	3.194259000	H	-2.849151000	-4.803221000	1.240335000
H	4.547487000	-0.064517000	3.940565000	H	3.278568000	-2.159594000	4.759683000
H	4.063160000	-2.209029000	1.762431000	H	2.080838000	0.531757000	5.633128000
H	-0.054021000	-1.665431000	4.567104000	H	2.421326000	2.523493000	3.281506000
H	1.237112000	-3.186903000	2.068367000	H	4.666449000	0.499081000	4.004662000
H	-0.129768000	1.340558000	3.475725000	H	4.455885000	-1.693598000	1.844739000
H	0.090218000	-0.674065000	2.826543000	H	0.386111000	-1.752049000	4.777830000
H	3.905826000	0.658770000	0.978185000	H	1.770521000	-3.075432000	2.212745000
C	-6.394777000	1.426537000	-3.504606000	H	-0.173307000	1.200917000	3.648111000
C	-5.800483000	-2.262131000	2.759214000	H	0.304919000	-0.795973000	3.016791000
H	-1.727864000	1.195047000	-3.537139000	H	3.849937000	1.101449000	1.050270000
H	-1.210426000	-2.084084000	1.876381000	H	-1.523888000	2.528821000	-1.769760000
H	-6.948128000	2.077584000	-2.807536000	H	-0.924496000	-3.377931000	0.597559000
H	-7.036204000	0.551080000	-3.699771000	C	-6.203334000	2.520208000	-1.784684000
H	-6.272706000	1.972649000	-4.450271000	C	-4.874843000	1.876345000	-1.552609000
H	-6.487397000	-2.907846000	2.187009000	H	-6.808018000	2.579001000	-0.861523000
H	-6.380463000	-1.379410000	3.076155000	H	-6.813681000	1.969040000	-2.522856000
H	-5.499590000	-2.808430000	3.663720000	H	-6.083485000	3.546672000	-2.162295000

Calculated (M06/def2-SVP) gas phase geometry of Ag(dmp)(P₂-nCB) **3** in cartesian (XYZ) coordinates

Ground state (S ₀)				Lowest triplet state (T ₁)			
C	-1.360040000	4.974685000	-0.915915000	C	2.719396000	-3.788403000	-2.877645000
C	-0.498303000	6.051573000	-0.724723000	C	3.951094000	-4.291278000	-2.467546000
C	0.777011000	5.837691000	-0.203293000	C	4.636210000	-3.682400000	-1.417527000
C	1.197648000	4.550137000	0.114018000	C	4.096646000	-2.574085000	-0.771078000
C	0.345403000	3.460957000	-0.094521000	C	2.853757000	-2.066148000	-1.173388000
C	-0.940949000	3.685724000	-0.594835000	C	2.173554000	-2.681739000	-2.232147000
C	2.796800000	1.894242000	4.460415000	C	4.290160000	2.995655000	-2.470842000
C	3.550692000	2.300004000	3.360466000	C	4.997069000	1.835632000	-2.157998000
C	3.003179000	2.276701000	2.080395000	C	4.344312000	0.744647000	-1.591025000
C	1.686451000	1.839319000	1.883112000	C	2.971782000	0.810216000	-1.322960000
C	0.934789000	1.453088000	2.998582000	C	2.267998000	1.972731000	-1.655538000
C	1.481018000	1.476851000	4.279204000	C	2.921146000	3.062362000	-2.222591000
C	2.156103000	-2.137022000	1.188506000	C	-0.168375000	2.893124000	0.748084000
C	3.540163000	-2.085534000	1.386131000	C	0.781608000	3.816383000	1.204295000
C	4.100177000	-2.593937000	2.557509000	C	0.743374000	5.130558000	0.744528000
C	3.294673000	-3.169633000	3.536465000	C	-0.229509000	5.534199000	-0.168076000
C	1.917905000	-3.252925000	3.335490000	C	-1.182849000	4.620692000	-0.618276000
C	1.357506000	-2.737845000	2.171178000	C	-1.152693000	3.306710000	-0.166985000
C	-0.150907000	-3.324703000	-1.883920000	C	-2.028183000	-0.589610000	2.273196000
C	1.078877000	-3.048401000	-1.279679000	C	-1.739161000	0.749126000	1.963697000
C	2.144357000	-3.937801000	-1.453505000	C	-2.712940000	1.733443000	2.188912000
C	1.987541000	-5.067565000	-2.249940000	C	-3.953997000	1.377683000	2.706234000
C	0.765536000	-5.324328000	-2.870884000	C	-4.235244000	0.046035000	3.003889000
C	-0.306285000	-4.455484000	-2.682927000	C	-3.265282000	-0.934745000	2.798243000
B	3.406658000	2.131579000	-1.466243000	B	3.869868000	-0.277699000	1.980365000
B	3.535890000	1.900591000	-3.195602000	B	3.669737000	-1.001074000	3.562258000
B	3.743665000	0.139937000	-3.518044000	B	2.463338000	-0.028158000	4.481080000
C	2.210662000	-0.341847000	-1.314800000	C	1.236617000	0.471098000	2.107484000
C	2.001543000	1.236609000	-1.083005000	C	2.304916000	-0.424437000	1.326334000
B	2.195053000	0.943040000	-3.828006000	B	2.033007000	-1.612938000	3.815491000
B	3.506940000	0.544882000	-0.685084000	B	2.793420000	1.123137000	1.872366000
B	1.957708000	2.110591000	-2.465500000	B	2.835848000	-1.698832000	2.187732000
B	4.522673000	0.901777000	-2.094170000	B	3.633445000	0.778778000	3.388830000
B	3.749292000	-0.665191000	-1.947999000	B	1.952225000	1.284450000	3.422970000
B	2.263306000	-0.653854000	-2.940976000	B	0.930672000	-0.172152000	3.603352000
Ag	-0.866140000	-0.180524000	0.224926000	Ag	-0.295469000	-0.403818000	-0.985495000
P	1.233806000	-1.519916000	-0.281664000	P	-0.166320000	1.130796000	1.165670000
P	0.823915000	1.729531000	0.259240000	P	2.074303000	-0.559614000	-0.499249000
C	-6.489538000	-0.460689000	0.693424000	C	-5.710000000	-0.667081000	-0.989170000
C	-6.446456000	-0.145143000	-0.628067000	C	-5.522518000	-1.835130000	-0.319119000
C	-5.283062000	-0.632987000	1.440947000	C	-4.607425000	0.057309000	-1.557704000
C	-4.019950000	-0.474706000	0.820522000	C	-3.283748000	-0.444423000	-1.365195000
N	-2.861653000	-0.626046000	1.504046000	N	-2.194180000	0.238293000	-1.876966000
C	-2.887240000	-0.945447000	2.789929000	C	-2.394742000	1.307373000	-2.689333000
C	-4.108668000	-1.124170000	3.481686000	C	-3.657852000	1.824510000	-2.916964000
C	-5.294867000	-0.965146000	2.811757000	C	-4.780944000	1.217328000	-2.311047000
C	-3.975346000	-0.144710000	-0.591366000	C	-3.085880000	-1.660091000	-0.667647000
C	-5.193735000	0.016983000	-1.296486000	C	-4.211255000	-2.379600000	-0.146489000
C	-5.108078000	0.338389000	-2.666521000	C	-3.972995000	-3.577170000	0.523279000
C	-3.877509000	0.477428000	-3.261322000	C	-2.665916000	-4.038482000	0.689363000
C	-2.706839000	0.295327000	-2.489529000	C	-1.606814000	-3.277480000	0.172399000
N	-2.780134000	-0.004875000	-1.197636000	N	-1.808067000	-2.135508000	-0.484985000
H	-2.365662000	5.138609000	-1.313985000	H	2.175352000	-4.259723000	-3.700619000
H	-0.823148000	7.065208000	-0.977126000	H	4.380641000	-5.163767000	-2.967982000
H	1.453750000	6.682491000	-0.046639000	H	5.603432000	-4.075215000	-1.092250000
H	2.202743000	4.392402000	0.515844000	H	4.642771000	-2.109896000	0.054069000
H	-1.619938000	2.835210000	-0.734319000	H	1.197655000	-2.295217000	-2.553765000
H	3.236925000	1.906774000	5.461821000	H	4.809536000	3.848735000	-2.916560000

H	4.582482000	2.636086000	3.497910000	H	6.070535000	1.777225000	-2.358018000
H	3.612285000	2.589292000	1.228211000	H	4.911601000	-0.160979000	-1.357992000
H	-0.103000000	1.132118000	2.851844000	H	1.193644000	2.032809000	-1.454725000
H	0.877501000	1.166025000	5.137798000	H	2.352943000	3.964105000	-2.470776000
H	4.189296000	-1.652437000	0.622826000	H	1.545796000	3.514645000	1.922640000
H	5.183210000	-2.540297000	2.700999000	H	1.485105000	5.846469000	1.108858000
H	3.741296000	-3.562365000	4.454558000	H	-0.247142000	6.566789000	-0.528160000
H	1.277254000	-3.719994000	4.090164000	H	-1.952955000	4.922831000	-1.334849000
H	0.274794000	-2.810440000	2.008390000	H	-1.900604000	2.593356000	-0.535564000
H	-0.995210000	-2.641619000	-1.724786000	H	-1.283676000	-1.371699000	2.097387000
H	3.107552000	-3.738623000	-0.973137000	H	-2.499870000	2.783648000	1.973486000
H	2.828414000	-5.752577000	-2.390996000	H	-4.705780000	2.151596000	2.882574000
H	0.647415000	-6.211897000	-3.499313000	H	-5.215127000	-0.229920000	3.403312000
H	-1.270215000	-4.660402000	-3.157687000	H	-3.475616000	-1.982045000	3.031198000
H	-7.444651000	-0.589131000	1.211779000	H	-6.716614000	-0.259332000	-1.130705000
H	-7.366078000	-0.011214000	-1.205941000	H	-6.372778000	-2.386613000	0.096571000
C	-1.604245000	-1.124669000	3.530444000	C	-1.187657000	1.908410000	-3.332161000
H	-4.086920000	-1.385931000	4.543340000	H	-3.774326000	2.684194000	-3.582786000
H	-6.254672000	-1.094235000	3.322101000	H	-5.788164000	1.617558000	-2.462459000
H	-6.029919000	0.472377000	-3.241635000	H	-4.822064000	-4.144997000	0.919514000
H	-3.785711000	0.724917000	-4.321772000	H	-2.455505000	-4.975887000	1.210166000
C	-1.355653000	0.436573000	-3.097616000	C	-0.191509000	-3.721287000	0.361230000
H	-0.734192000	-0.985644000	2.872589000	H	-0.554142000	2.435944000	-2.595762000
H	-1.547122000	-2.132876000	3.974803000	H	-1.464261000	2.636364000	-4.108888000
H	-1.529436000	-0.406973000	4.365170000	H	-0.558949000	1.126237000	-3.793167000
H	-0.792544000	1.261145000	-2.623093000	H	0.306370000	-3.879078000	-0.610651000
H	-0.763736000	-0.482362000	-2.940746000	H	0.399556000	-2.951328000	0.893124000
H	4.015962000	2.723772000	-3.929040000	H	4.557811000	-1.573752000	4.133506000
H	4.410528000	-0.289573000	-4.421218000	H	2.519992000	0.143270000	5.667966000
H	4.292762000	-1.703442000	-1.671185000	H	1.521398000	2.358623000	3.745564000
H	5.712593000	1.015695000	-1.976391000	H	4.503075000	1.506159000	3.780306000
H	3.742249000	3.083002000	-0.808364000	H	4.831695000	-0.246574000	1.256414000
H	1.814862000	1.071677000	-4.964024000	H	1.832080000	-2.527531000	4.567635000
H	1.286543000	3.108537000	-2.550832000	H	3.112822000	-2.740354000	1.656607000
H	1.866640000	-1.694968000	-3.397146000	H	-0.137019000	-0.031104000	4.130967000
H	1.297449000	0.362817000	-3.157170000	H	1.036765000	-1.492165000	3.045126000
H	3.861647000	0.405427000	0.447292000	H	2.980051000	2.025182000	1.107152000
H	-1.396798000	0.637961000	-4.176780000	H	-0.123700000	-4.653712000	0.938620000

Calculated (M06/def2-SVP) gas phase geometry of Ag(dbp)(P₂-nCB) **4** in cartesian (XYZ) coordinates

Ground state (S ₀)				Lowest triplet state (T ₁)			
C	3.945691000	-0.529290000	-3.418584000	C	-4.095339000	0.295025000	3.240927000
C	4.569360000	0.528537000	-4.074314000	C	-5.015785000	1.337947000	3.256062000
C	4.118933000	1.834299000	-3.875183000	C	-4.837841000	2.440323000	2.418129000
C	3.058179000	2.085153000	-3.012286000	C	-3.740574000	2.503864000	1.567489000
C	2.443731000	1.028374000	-2.330883000	C	-2.824325000	1.444510000	1.532919000
C	2.882422000	-0.278209000	-2.552425000	C	-3.002529000	0.344422000	2.376018000
C	-1.530719000	4.053628000	-3.847199000	C	0.873590000	4.894662000	2.817159000
C	-0.956681000	4.614984000	-2.711183000	C	0.278636000	5.214234000	1.599630000
C	-0.167268000	3.843387000	-1.856245000	C	-0.374800000	4.236300000	0.851354000
C	0.042889000	2.487555000	-2.123105000	C	-0.421893000	2.917336000	1.315738000
C	-0.542672000	1.931000000	-3.272140000	C	0.170446000	2.605880000	2.548529000
C	-1.314280000	2.704708000	-4.131527000	C	0.809306000	3.587456000	3.297224000
C	-1.981627000	1.571152000	2.021438000	C	2.410590000	1.247907000	-1.683927000
C	-2.110621000	2.912389000	2.398506000	C	2.606825000	2.535205000	-2.198734000
C	-3.374964000	3.482444000	2.550393000	C	3.884241000	3.092525000	-2.208365000
C	-4.524004000	2.723432000	2.347445000	C	4.971653000	2.376134000	-1.715857000
C	-4.407061000	1.381229000	1.987547000	C	4.783715000	1.089243000	-1.210537000
C	-3.147428000	0.815848000	1.816287000	C	3.512209000	0.529960000	-1.183993000
C	-0.015520000	-1.659285000	3.363745000	C	0.474521000	-2.310736000	-2.396283000
C	-0.377657000	-0.309919000	3.394129000	C	1.152376000	-1.116983000	-2.663613000
C	-0.688436000	0.289399000	4.619393000	C	2.019090000	-1.036368000	-3.761266000
C	-0.600617000	-0.444891000	5.797620000	C	2.185106000	-2.141226000	-4.590071000
C	-0.211018000	-1.783715000	5.763493000	C	1.505744000	-3.329091000	-4.322107000
C	0.075184000	-2.393182000	4.544706000	C	0.653910000	-3.414813000	-3.222913000
B	2.587502000	3.516730000	0.417764000	B	-2.503799000	3.155048000	-1.864876000
B	3.880019000	3.256705000	1.571980000	B	-3.426265000	2.483141000	-3.195068000
B	3.150662000	2.826814000	3.159859000	B	-2.277773000	1.766506000	-4.381266000
C	1.109195000	1.643199000	1.795933000	C	-0.656086000	1.171693000	-2.284424000
C	1.818397000	1.991323000	0.382104000	C	-1.716535000	1.768921000	-1.251938000
B	3.910685000	1.586465000	2.150943000	B	-3.238694000	0.730186000	-3.311584000
B	1.045805000	3.237264000	1.249562000	B	-0.787747000	2.858662000	-2.186531000
B	3.456049000	1.986670000	0.450025000	B	-3.270431000	1.574783000	-1.708170000
B	2.374288000	4.051842000	2.099330000	B	-1.863010000	3.285812000	-3.520420000
B	1.406567000	2.856293000	2.937476000	B	-0.654456000	2.029167000	-3.745520000
B	2.278702000	1.294489000	2.915291000	B	-1.452940000	0.436279000	-3.540829000
Ag	-0.207841000	-0.696804000	-0.360398000	Ag	0.086499000	-0.462499000	0.711302000
P	-0.419381000	0.611572000	1.810470000	P	0.831374000	0.345393000	-1.634784000
P	1.065369000	1.293852000	-1.154435000	P	-1.311315000	1.524505000	0.514271000
C	-2.771207000	-5.579323000	-1.405552000	C	2.376774000	-5.324165000	1.698478000
C	-1.604525000	-6.108487000	-0.947402000	C	1.190631000	-5.827420000	1.261383000
C	-2.943707000	-4.162243000	-1.497737000	C	2.599038000	-3.910048000	1.801928000
C	-1.892340000	-3.291802000	-1.122223000	C	1.539444000	-3.018886000	1.447006000
N	-2.020411000	-1.954257000	-1.193245000	N	1.731777000	-1.654608000	1.506046000
C	-3.147125000	-1.393325000	-1.615217000	C	2.906469000	-1.145227000	1.969582000
C	-4.248118000	-2.191954000	-1.998333000	C	3.955975000	-1.966837000	2.331338000
C	-4.140002000	-3.563206000	-1.942733000	C	3.810353000	-3.369458000	2.232400000
C	-0.649237000	-3.855323000	-0.631293000	C	0.291621000	-3.540754000	1.031046000
C	-0.523787000	-5.261285000	-0.545013000	C	0.114856000	-4.959106000	0.904934000
C	0.693770000	-5.766188000	-0.040403000	C	-1.101556000	-5.429176000	0.411839000
C	1.688486000	-4.899346000	0.342699000	C	-2.102124000	-4.531384000	0.050403000
C	1.486049000	-3.503399000	0.220901000	C	-1.881611000	-3.152962000	0.228706000
N	0.346310000	-3.023077000	-0.258169000	N	-0.738577000	-2.676190000	0.716407000
H	4.281237000	-1.557766000	-3.587576000	H	-4.227008000	-0.568902000	3.899240000
H	5.404990000	0.336043000	-4.753527000	H	-5.878273000	1.296769000	3.927543000
H	4.604111000	2.665662000	-4.394425000	H	-5.559425000	3.261720000	2.431573000
H	2.715732000	3.112410000	-2.849640000	H	-3.601473000	3.373637000	0.917295000
H	2.380023000	-1.108364000	-2.039247000	H	-2.282933000	-0.484424000	2.359003000
H	-2.141026000	4.666703000	-4.516792000	H	1.382143000	5.668558000	3.399059000

H	-1.109655000	5.674383000	-2.485874000	H	0.312229000	6.241326000	1.225613000
H	0.297440000	4.311405000	-0.987872000	H	-0.858311000	4.510460000	-0.087948000
H	-0.373457000	0.870377000	-3.501992000	H	0.120485000	1.578904000	2.933900000
H	-1.749604000	2.253031000	-5.028350000	H	1.261959000	3.327912000	4.259077000
H	-1.223004000	3.517750000	2.589101000	H	1.771188000	3.097120000	-2.616585000
H	-3.456687000	4.533189000	2.843238000	H	4.027620000	4.095106000	-2.620398000
H	-5.512313000	3.175348000	2.474176000	H	5.972247000	2.817714000	-1.731984000
H	-5.303714000	0.770958000	1.837956000	H	5.635022000	0.513246000	-0.835421000
H	-3.061384000	-0.240938000	1.528327000	H	3.375730000	-0.481929000	-0.780382000
H	0.195414000	-2.137675000	2.399874000	H	-0.200745000	-2.376659000	-1.538454000
H	-0.985781000	1.342512000	4.653447000	H	2.549734000	-0.104409000	-3.981203000
H	-0.832993000	0.033538000	6.753324000	H	2.849417000	-2.072100000	-5.455871000
H	-0.138839000	-2.356025000	6.692975000	H	1.644240000	-4.195075000	-4.975568000
H	0.365459000	-3.447587000	4.511176000	H	0.121891000	-4.344393000	-3.001866000
H	-3.600834000	-6.225917000	-1.707803000	H	3.198780000	-5.992293000	1.976371000
H	-1.471034000	-7.192090000	-0.871955000	H	1.038239000	-6.908127000	1.170204000
H	2.634382000	-5.270839000	0.746538000	H	-3.052574000	-4.876822000	-0.364967000
H	4.933666000	3.832796000	1.510739000	H	-4.474812000	2.945402000	-3.554747000
H	3.631164000	3.150551000	4.212984000	H	-2.467152000	1.775797000	-5.566793000
H	0.577045000	3.077614000	3.781014000	H	0.377391000	2.111858000	-4.359135000
H	2.300074000	5.216438000	2.383918000	H	-1.761014000	4.346945000	-4.070728000
H	2.558521000	4.242981000	-0.542960000	H	-2.758433000	4.089264000	-1.149592000
H	4.940518000	1.083416000	2.520845000	H	-4.110836000	0.049883000	-3.781854000
H	4.127233000	1.667050000	-0.495700000	H	-4.139643000	1.422769000	-0.893791000
H	2.082214000	0.517095000	3.812160000	H	-0.976571000	-0.500117000	-4.122452000
H	3.070344000	0.666857000	1.911961000	H	-2.458990000	-0.019810000	-2.644532000
H	0.005253000	3.708541000	0.894457000	H	0.085909000	3.508612000	-1.698011000
C	-3.168138000	0.102327000	-1.686112000	C	2.962175000	0.348044000	2.100780000
C	2.561799000	-2.544633000	0.630788000	C	-2.958340000	-2.187947000	-0.177290000
H	-4.978118000	-4.202953000	-2.237875000	H	4.633618000	-4.038770000	2.500318000
H	0.827043000	-6.849362000	0.047099000	H	-1.249398000	-6.508887000	0.300748000
H	-2.636475000	0.406487000	-2.610397000	H	2.312569000	0.643735000	2.951762000
H	-2.523766000	0.481487000	-0.868354000	H	2.465327000	0.791713000	1.213551000
C	-4.511436000	0.801783000	-1.622801000	C	4.326012000	0.988975000	2.261898000
H	2.746860000	-2.646624000	1.718930000	H	-3.167996000	-2.325019000	-1.257493000
H	2.186918000	-1.512709000	0.485418000	H	-2.579706000	-1.153388000	-0.070724000
C	3.879032000	-2.720108000	-0.118177000	C	-4.259420000	-2.345350000	0.600678000
H	-5.093753000	0.419172000	-0.760034000	H	5.013042000	0.593628000	1.488632000
H	-5.117959000	0.577727000	-2.522626000	H	4.776631000	0.704412000	3.232364000
C	-4.339145000	2.306635000	-1.487917000	C	4.269001000	2.503414000	2.151497000
H	3.684778000	-2.730132000	-1.209657000	H	-4.045283000	-2.278825000	1.686385000
H	4.321312000	-3.709846000	0.111069000	H	-4.665555000	-3.363761000	0.446604000
C	4.873318000	-1.621661000	0.214916000	C	-5.309724000	-1.315883000	0.223798000
H	-3.720128000	2.678090000	-2.327781000	H	3.600521000	2.903224000	2.937854000
H	-3.746177000	2.512916000	-0.575501000	H	3.781266000	2.776020000	1.192886000
C	-5.656507000	3.051142000	-1.424862000	C	5.634398000	3.153955000	2.242371000
H	5.035424000	-1.599370000	1.309131000	H	-5.481688000	-1.351013000	-0.868969000
H	4.423441000	-0.639459000	-0.028604000	H	-4.908600000	-0.303573000	0.418745000
C	6.193823000	-1.774501000	-0.510168000	C	-6.613818000	-1.508984000	0.970922000
H	-6.265163000	2.708171000	-0.569839000	H	6.298465000	2.795971000	1.436195000
H	-6.257144000	2.892313000	-2.337086000	H	6.130610000	2.915494000	3.198634000
H	-5.509998000	4.136136000	-1.309290000	H	5.579147000	4.250752000	2.162126000
H	6.053008000	-1.735164000	-1.604343000	H	-6.458310000	-1.449722000	2.062658000
H	6.680165000	-2.736974000	-0.273677000	H	-7.058859000	-2.496626000	0.759958000
H	6.896402000	-0.970939000	-0.242581000	H	-7.359636000	-0.744640000	0.702449000
H	-5.171653000	-1.716940000	-2.337701000	H	4.886223000	-1.532784000	2.704319000