

Supporting Information for

Tethered Counterion-Directed Catalysis: Merging the Chiral Ion-pairing and Bifunctional Ligand Strategies in Enantioselective Gold(I) Catalysis

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Computational methods

Calculations were carried out with the Gaussian09 package¹ and all structures were fully optimized without any symmetry constraints at the DFT level by means of the M06 functional.² The def2-SVP basis set³ was applied for all atoms and solvent effects are accounted for by continuum solvation method (integral equation formalism version of the polarizable continuum model (IEFPCM) for toluene). Each stationary point has been characterized with frequency analysis and shows the correct number of negative eigenvalues (zero for a local minimum and one for a transition state). All transition states were verified by stepping along the reaction coordinate (intrinsic reaction coordinate calculations) and confirming that they transformed into the corresponding reactants/products. Final energy calculations at the M06 level associated with the def2-TZVPP basis set, including solvation effect, have been achieved on the IEFPCM(toluene)-M06/def2-SVP geometries. To get accurate geometries and energies, the SCF convergence criterion was systematically tightened to 10^{-8} au, and the force minimizations were carried out until the rms force became smaller than (at least) 1×10^{-5} au (“tight” optimization keyword in Gaussian 09). The “UltraFine” grid (99 radial shells and 590 angular points per shell) was used throughout the calculations, as recommended when using Gaussian 09. The Gibbs free energies presented in this article are IEFPCM(toluene)-M06/def2-TZVPP//IEFPCM(toluene)-M06/def2-SVP electronic energies (which include solvation-energy corrections from the IEFPCM method) modified with thermal and entropy corrections from IEFPCM(toluene)-M06/def2-SVP calculations. Due to the well-known errors associated with entropy calculations, we apply a scaling factor of 0.5 to the entropic contributions as recommended in the literature.⁴⁻⁷ Therefore, the calculated ΔG values reported in this study include the ZPE, enthalpic temperature correction, solvation energy, and half the entropy. Note that application of this scheme only slightly modifies the activation barriers and the general profile, but changes the interaction between 2 molecules or the formation of two separate molecules from a single one.

Table S1. Absolute electronic energies and thermal corrections for all molecules.

	E (IEFPCM(toluene)- M06/def2-SVP)	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy	E (IEFPCM(toluene)- M06/def2-TZVPP) ^a
6a	-2579.873720	0.563652	0.457837	-2582.064036
6b	-2579.858139	0.563051	0.458189	-2582.048093
6c	-2579.824963	0.563184	0.456099	-2582.016071
8a	-614.973838	0.231001	0.175881	-615.647943
Ia	-3194.881553	0.796223	0.661093	-3197.736882
TS-I-IIa	-3194.866164	0.794745	0.659083	-3197.721182
IIa	-3194.889867	0.797009	0.663051	-3197.742211
Ib	-3194.876723	0.795906	0.658906	-3197.733102
TS-I-IIb	-3194.859562	0.794646	0.658623	-3197.716113
IIb	-3194.875312	0.796585	0.660517	-3197.730015
II'a	-3558.190359	0.935523	0.783008	-3561.433449
TS-II'-IIIa	-3558.181394	0.935577	0.785308	-3561.424148
IIIa	-3558.206139	0.937570	0.788999	-3561.445807

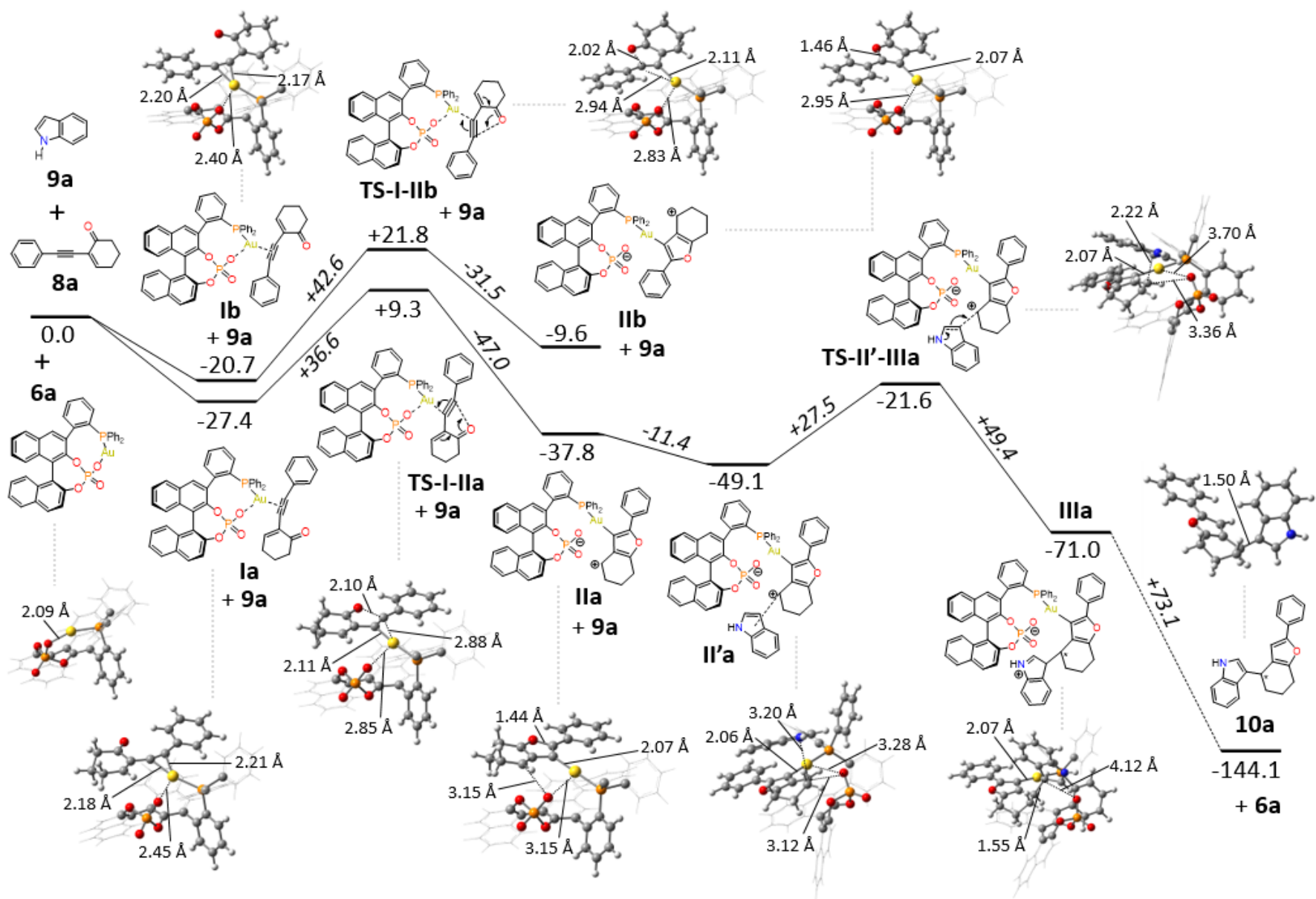
9a	-363.281615	0.136580	0.099133	-363.675534
10a	-978.341694	0.372484	0.305026	-979.395817
14	-2581.082261	0.585818	0.476289	

^a Energies computed at the IEFPCM(toluene)-M06/def2-SVP geometries.

Comment: The main steps of the postulated reaction mechanism have been modelled in order to confirm the relevance of the mechanistic hypothesis and to estimate the influence of the tethered phosphate group (Figure S1). Coordination of the alkyne **8a** to the catalyst **6a** led to several conformers of intermediate **I**. Two of them, **1a** and **1b**, are represented in Figure S1. Both display in-plane coordination of the alkyne unit. In **1a** the enone moiety is close to the phosphate group, while in **1b**, the two groups are remote. **1a** is favored by 6.7 kJ.mol⁻¹ with respect to **1b**. Starting from **1a**, the exoergonic cycloisomerization step leads to the carbocationic intermediate **IIa** which features an electrostatic pairing between the carbocation and the phosphate group. The absence of this electrostatic interaction, as modeled in path b, leads to a higher energy barrier (42.6 vs 36.6 kJ.mol⁻¹) and ends up to an endergonic process. The interaction of **IIa** with indole **9a** leads to **II'a** with a further 11.3 kJ.mol⁻¹ energy gain. Then, addition of indole to the carbocation through its C3-carbon goes across a 27.5 kJ.mol⁻¹ activation barrier. It results in **IIIa** that lies at -71.0 kJ.mol⁻¹ on the free energy surface.

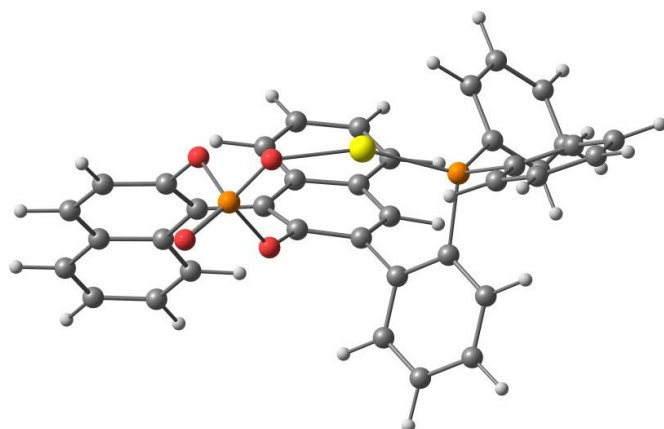
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Cartesian coordinates of the optimized geometries

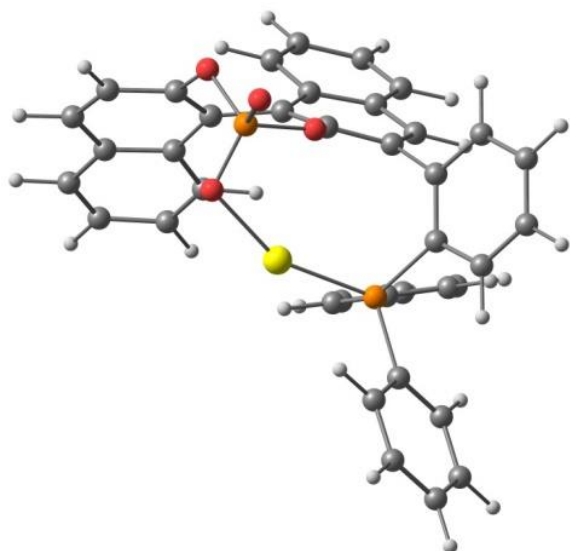
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Structure **6b**

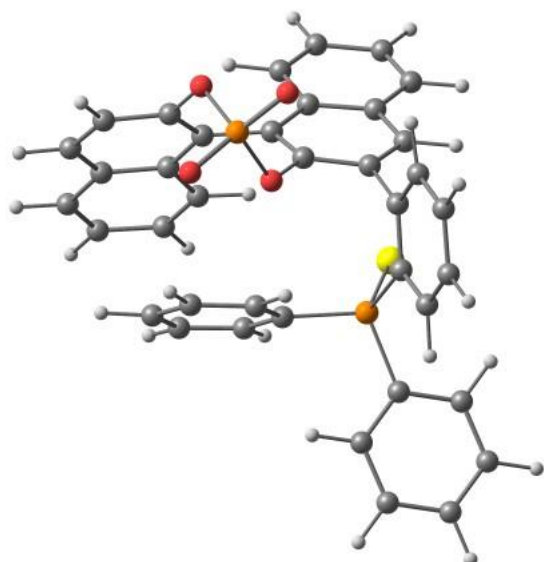


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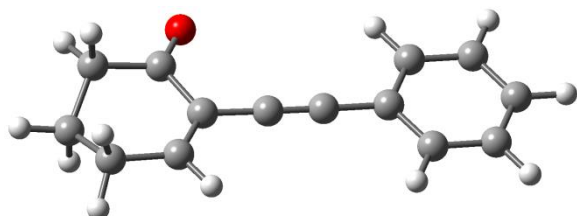
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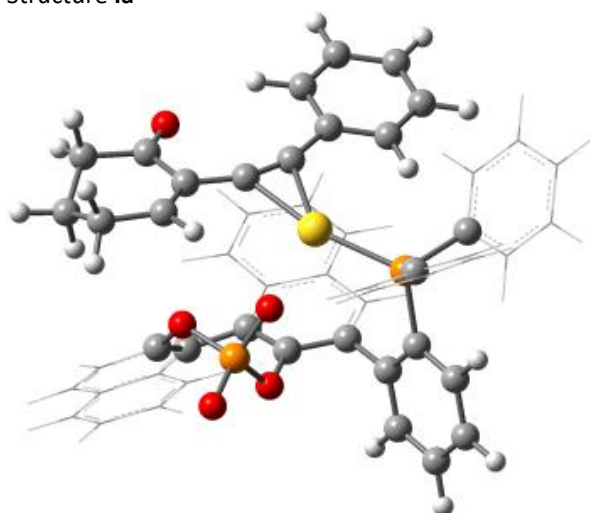
Structure **8a**



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H	-5.085219000	-2.126136000	0.013423000
H	-4.837631000	2.177475000	0.052047000
H	-6.206898000	0.096964000	0.048640000
C	1.746568000	-0.268619000	-0.054874000
C	2.446188000	-1.429780000	-0.098975000
H	1.883502000	-2.369565000	-0.151528000
C	2.457463000	1.048831000	-0.058512000
O	1.856251000	2.097826000	0.011729000
C	3.956715000	0.984937000	-0.215341000
H	4.375457000	1.934689000	0.151166000
H	4.155414000	0.953531000	-1.305765000
C	3.932036000	-1.505896000	-0.087390000
H	4.280334000	-1.699361000	-1.123908000
H	4.252945000	-2.392340000	0.486129000
C	4.565312000	-0.235118000	0.452169000
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Structure Ia

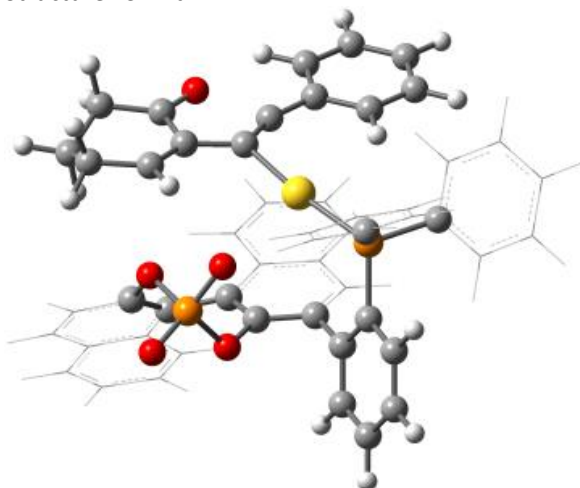


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C	4.657473000	-0.181969000	2.779018000
C	5.776365000	-1.482996000	1.045603000
C	4.544901000	-2.423840000	-0.813938000
C	5.842026000	-0.081344000	3.470967000
H	3.751027000	0.259784000	3.200238000
C	6.984933000	-1.350289000	1.775538000
C	5.726421000	-2.255001000	-0.143159000
C	7.025685000	-0.658031000	2.961308000
H	5.863853000	0.444836000	4.429739000
H	7.886392000	-1.826472000	1.375491000
H	6.643358000	-2.736026000	-0.498381000
H	7.962955000	-0.566667000	3.517323000
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C	1.978037000	1.044479000	1.502637000
C	0.982389000	-1.163998000	1.418756000
C	2.986006000	1.978564000	1.146763000
C	0.784442000	1.542159000	2.108713000
C	-0.217126000	-0.675618000	2.014941000

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C	0.677366000	2.924950000	2.405703000
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H	3.622199000	4.020235000	1.114138000
H	-0.238755000	3.285068000	2.886268000
H	-1.184912000	1.039280000	2.868874000
H	1.582896000	4.865022000	2.293874000
O	2.241568000	-1.937662000	-1.087563000
O	1.013113000	-2.471687000	1.050663000
P	0.952655000	-2.861811000	-0.570526000
O	1.220459000	-4.308130000	-0.700462000
O	-0.240338000	-2.172431000	-1.207957000
C	-1.304159000	-1.640197000	2.338411000
C	-2.516565000	-1.741891000	1.630975000
C	-1.094805000	-2.493366000	3.430746000
C	-3.486843000	-2.666456000	2.045409000
C	-2.061269000	-3.405390000	3.834272000
C	-3.268287000	-3.488711000	3.142901000
H	-4.428196000	-2.749173000	1.492056000
H	-4.035999000	-4.203855000	3.450126000
H	-1.869569000	-4.057893000	4.690504000
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H	4.466385000	-3.045456000	-1.710378000
P	-2.875772000	-0.712234000	0.158855000
Au	-0.918827000	0.170563000	-0.965565000
C	-3.984064000	0.614040000	0.758350000
C	-4.221557000	0.832705000	2.118298000
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H	-6.051232000	-4.142429000	-3.127456000
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C	-1.693714000	3.522018000	0.105744000
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H	1.052303000	4.503652000	-1.659733000
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C	2.812937000	1.913154000	-2.941025000
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H	4.827414000	2.067398000	-3.586696000
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Structure TS-I-IIa

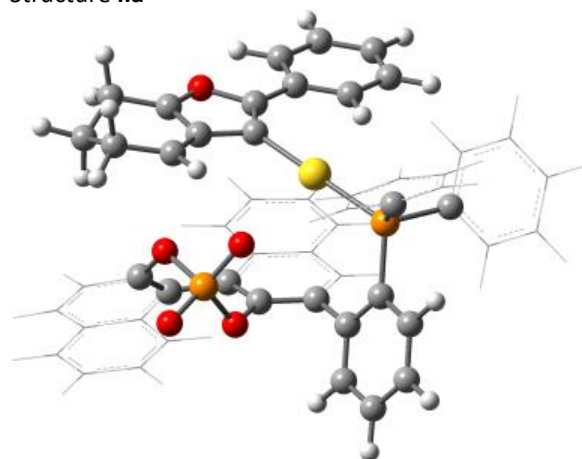


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C	-4.558993000	-2.518918000	0.966528000
C	-5.845558000	-0.363749000	-3.417972000
H	-3.753871000	-0.017818000	-3.159753000
C	-6.994204000	-1.551135000	-1.668542000
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H	-5.863788000	0.116281000	-4.400812000
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H	-6.657277000	-2.843910000	0.660119000
H	-7.967876000	-0.845949000	-3.446127000
C	-2.104522000	-0.548643000	-1.163048000
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C	-0.993050000	-1.372725000	-1.302920000
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C	0.213345000	-0.917879000	-1.912608000

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H	-3.631078000	3.829548000	-1.340128000
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O	-1.351979000	-4.439070000	0.894454000
O	0.221785000	-2.354986000	1.362214000
C	1.303905000	-1.896473000	-2.164178000
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C	3.524243000	-2.830049000	-1.837287000
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H	4.487765000	-2.821396000	-1.316185000
H	4.056941000	-4.523569000	-3.056907000
H	1.838103000	-4.585446000	-4.208267000
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H	-1.775474000	5.071583000	1.356529000
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C	-1.551931000	0.925825000	2.583473000
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H	-4.585678000	2.307047000	3.327069000
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Structure IIa

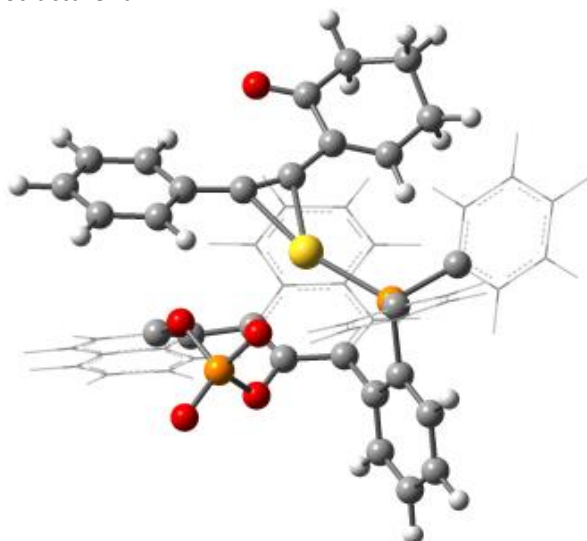


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C	5.809852000	-0.510286000	3.462180000
H	3.717201000	-0.163475000	3.203856000
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C	5.745553000	-2.328428000	-0.345746000
C	7.003350000	-1.024261000	2.909603000
H	5.818339000	-0.081323000	4.468408000
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H	6.667929000	-2.773442000	-0.732642000
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C	0.986813000	-1.473635000	1.267782000
C	2.918640000	1.730988000	1.334926000
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P	1.041555000	-3.055276000	-0.839618000
O	1.536152000	-4.437477000	-1.025109000
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C	-1.329585000	-2.057155000	2.046296000
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C	-3.569732000	-2.918822000	1.669598000
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H	-1.874553000	-4.927169000	3.823792000
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H	4.500961000	-2.987530000	-1.985126000
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Au	-1.131244000	0.480011000	-0.825949000
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H	-5.400441000	3.634113000	0.490540000
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C	-4.045727000	-1.464804000	-1.012912000
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C	1.205859000	5.157825000	-0.824582000
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C	-1.287020000	5.149443000	0.411366000
H	-1.437146000	3.094546000	-0.231362000

C	-0.506746000	6.306246000	0.436617000
H	1.360639000	7.203993000	-0.173858000
H	-2.268250000	5.138192000	0.895543000
H	-0.871604000	7.207757000	0.937111000
C	1.490753000	0.859520000	-2.449293000
C	1.572792000	-0.382653000	-3.041733000
C	2.493439000	1.816133000	-2.706870000
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Structure **1b**

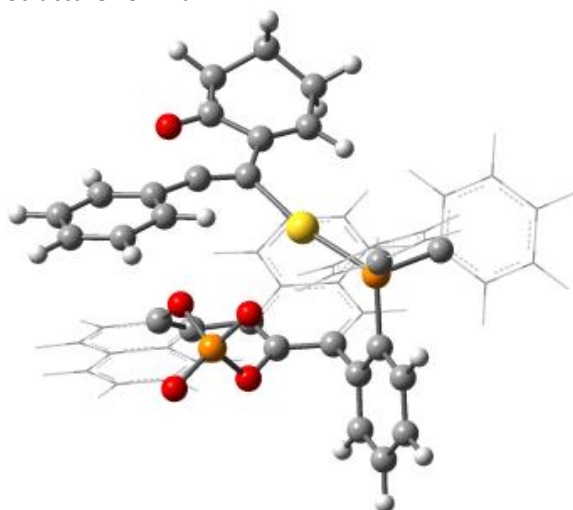


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C	-4.405530000	-2.319651000	0.865201000
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H	-3.769910000	0.246151000	-3.252790000
C	-6.966570000	-1.193546000	-1.583158000
C	-5.621459000	-2.107635000	0.273103000
C	-7.057441000	-0.523976000	-2.779241000
H	-5.951443000	0.497844000	-4.346326000
H	-7.858669000	-1.621734000	-1.113769000
H	-6.533501000	-2.531188000	0.705787000
H	-8.025186000	-0.403819000	-3.274305000
C	-2.026130000	-0.362908000	-1.355221000
C	-1.900492000	1.041438000	-1.617457000
C	-0.922057000	-1.178234000	-1.577377000
C	-2.893874000	1.983500000	-1.239196000
C	-0.720379000	1.534086000	-2.252620000

C	0.277055000	-0.683516000	-2.169348000
C	-2.758370000	3.320192000	-1.536329000
H	-3.776110000	1.633717000	-0.695819000
C	-0.621463000	2.912015000	-2.573046000
C	0.343388000	0.642300000	-2.531346000
C	-1.623801000	3.789623000	-2.235988000
H	-3.536566000	4.024407000	-1.227408000
H	0.280517000	3.260113000	-3.090480000
H	1.242643000	1.029413000	-3.025629000
H	-1.540199000	4.850212000	-2.495055000
O	-2.064535000	-1.963340000	0.944670000
O	-0.963490000	-2.495097000	-1.254383000
P	-0.880187000	-2.961438000	0.349429000
O	-1.239497000	-4.391152000	0.422980000
O	0.385089000	-2.384956000	0.963649000
C	1.390502000	-1.624209000	-2.463180000
C	2.583733000	-1.667873000	-1.717703000
C	1.245054000	-2.493630000	-3.551040000
C	3.604882000	-2.551083000	-2.096169000
C	2.261174000	-3.367982000	-3.916756000
C	3.451175000	-3.390745000	-3.192502000
H	4.532006000	-2.591107000	-1.515087000
H	4.257268000	-4.074368000	-3.472016000
H	2.121913000	-4.037599000	-4.769880000
H	0.305632000	-2.474250000	-4.112327000
H	-4.292460000	-2.916210000	1.774172000
P	2.820993000	-0.635954000	-0.220717000
Au	0.787607000	-0.018422000	0.981066000
C	3.784642000	0.821326000	-0.763885000
C	4.047560000	1.092062000	-2.109325000
C	4.198556000	1.737014000	0.215143000
C	4.705973000	2.268760000	-2.471557000
H	3.739245000	0.380567000	-2.883313000
C	4.877495000	2.895161000	-0.146903000
H	3.979228000	1.540771000	1.272284000
C	5.124915000	3.167253000	-1.494247000
H	4.902060000	2.475349000	-3.527460000
H	5.207285000	3.596052000	0.625549000
H	5.649437000	4.083215000	-1.780862000
C	3.983242000	-1.601780000	0.812161000
C	5.359789000	-1.348704000	0.836245000
C	3.453030000	-2.656402000	1.568817000
C	6.199499000	-2.140663000	1.617018000
H	5.784579000	-0.533618000	0.241007000
C	4.302151000	-3.445118000	2.341118000
H	2.374560000	-2.858528000	1.536783000
C	5.672011000	-3.188046000	2.369526000
H	7.274245000	-1.938139000	1.633331000
H	3.885985000	-4.268872000	2.927751000
H	6.333411000	-3.808310000	2.981322000
C	-0.813619000	1.022491000	2.082259000
C	-0.162111000	1.880719000	1.432681000
C	-1.814475000	0.427106000	2.921893000
C	-3.005342000	1.141275000	3.143999000
C	-1.629976000	-0.825794000	3.524556000
C	-3.994691000	0.597452000	3.954909000
H	-3.121244000	2.125646000	2.682164000

C	-2.621832000	-1.355449000	4.340001000
H	-0.713771000	-1.388737000	3.321914000
C	-3.804884000	-0.647896000	4.554380000
H	-4.921436000	1.152807000	4.124436000
H	-2.474549000	-2.333883000	4.805331000
H	-4.585747000	-1.071166000	5.193025000
C	0.184685000	3.192013000	0.966606000
C	1.198998000	3.463975000	0.110929000
C	-0.731390000	4.282447000	1.429671000
O	-1.680869000	4.061210000	2.149681000
C	-0.446498000	5.658144000	0.881482000
H	-0.893601000	6.392783000	1.568553000
H	-1.016717000	5.727592000	-0.067453000
C	1.576545000	4.835955000	-0.316275000
H	1.196145000	4.992103000	-1.347978000
H	2.675493000	4.896760000	-0.408682000
C	1.027753000	5.900767000	0.617077000
H	1.188000000	6.907112000	0.199188000
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H	1.778374000	2.626018000	-0.296667000

Structure **TS-I-IIb**

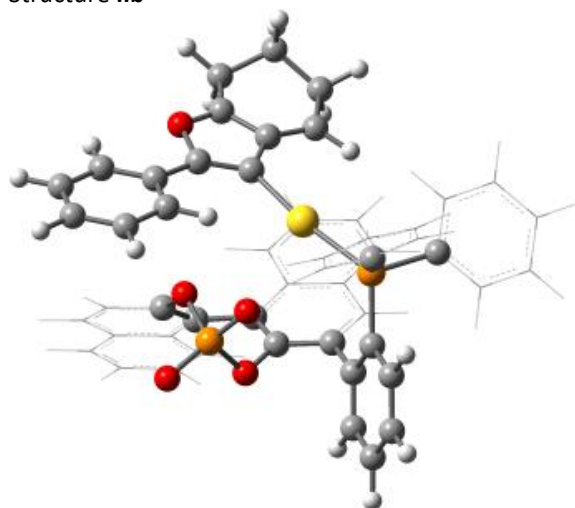


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C	-4.377173000	0.220493000	-3.177423000
C	-5.445345000	-1.266913000	-1.563765000
C	-4.162570000	-2.371661000	0.168606000
C	-5.576172000	0.375155000	-3.833773000
H	-3.481888000	0.713504000	-3.566073000
C	-6.669070000	-1.076774000	-2.254621000
C	-5.359590000	-2.153513000	-0.459176000
C	-6.741966000	-0.268305000	-3.363372000
H	-5.623950000	0.995219000	-4.733899000
H	-7.557041000	-1.603963000	-1.889305000
H	-6.263600000	-2.680385000	-0.136484000
H	-7.691178000	-0.135621000	-3.890347000
C	-1.779170000	-0.087564000	-1.690728000
C	-1.652526000	1.337469000	-1.754659000
C	-0.656047000	-0.869170000	-1.943384000
C	-2.693661000	2.217184000	-1.352497000

C	-0.420710000	1.916198000	-2.190148000
C	0.578700000	-0.294333000	-2.364852000
C	-2.544040000	3.582915000	-1.430826000
H	-3.627751000	1.790968000	-0.975003000
C	-0.295210000	3.327411000	-2.261028000
C	0.669221000	1.070648000	-2.511453000
C	-1.337765000	4.149167000	-1.902605000
H	-3.367967000	4.236937000	-1.125884000
H	0.656269000	3.746660000	-2.607477000
H	1.608891000	1.523292000	-2.850528000
H	-1.233858000	5.236486000	-1.974814000
O	-1.852447000	-1.897942000	0.416611000
O	-0.710335000	-2.210429000	-1.794864000
P	-0.654542000	-2.869570000	-0.239384000
O	-1.117305000	-4.271554000	-0.349476000
O	0.608152000	-2.414362000	0.435271000
C	1.731584000	-1.190475000	-2.626314000
C	2.859091000	-1.224435000	-1.785907000
C	1.689762000	-2.044667000	-3.733651000
C	3.920639000	-2.089825000	-2.082918000
C	2.749363000	-2.894708000	-4.026109000
C	3.872492000	-2.913863000	-3.201926000
H	4.794753000	-2.126010000	-1.423948000
H	4.708709000	-3.583480000	-3.420805000
H	2.694834000	-3.552484000	-4.897901000
H	0.796954000	-2.036931000	-4.366259000
H	-4.048870000	-3.075099000	0.998390000
P	2.947563000	-0.171248000	-0.289260000
Au	0.950246000	0.360680000	0.874970000
C	3.830663000	1.342489000	-0.825994000
C	4.611387000	1.382527000	-1.986265000
C	3.715958000	2.493800000	-0.036861000
C	5.263911000	2.559236000	-2.351115000
H	4.705812000	0.491903000	-2.616621000
C	4.376008000	3.665097000	-0.398714000
H	3.101221000	2.465447000	0.871676000
C	5.147672000	3.700039000	-1.559717000
H	5.867074000	2.583319000	-3.263065000
H	4.283715000	4.557744000	0.226529000
H	5.659361000	4.622094000	-1.849906000
C	4.114334000	-1.046417000	0.811523000
C	5.409915000	-0.587560000	1.064964000
C	3.646858000	-2.218171000	1.426332000
C	6.239901000	-1.299299000	1.931196000
H	5.778026000	0.327200000	0.587992000
C	4.487264000	-2.923869000	2.282117000
H	2.625642000	-2.567987000	1.216556000
C	5.780650000	-2.465777000	2.537578000
H	7.253105000	-0.938238000	2.130156000
H	4.126921000	-3.840796000	2.757186000
H	6.434336000	-3.022506000	3.215389000
C	-1.431938000	0.357243000	2.596806000
C	-0.668628000	1.176970000	1.948248000
C	-1.838642000	-0.894843000	3.139839000
C	-3.176366000	-1.176759000	3.458015000
C	-0.862436000	-1.900904000	3.267889000
C	-3.529201000	-2.449332000	3.888583000

H	-3.927462000	-0.390702000	3.360405000
C	-1.235873000	-3.175739000	3.667477000
H	0.173447000	-1.688684000	2.987072000
C	-2.566098000	-3.453772000	3.981267000
H	-4.571758000	-2.664164000	4.139818000
H	-0.479713000	-3.962798000	3.727386000
H	-2.853192000	-4.459693000	4.299856000
C	-1.035299000	2.580952000	1.983158000
C	-0.429835000	3.655814000	1.425860000
C	-2.296978000	2.733119000	2.723590000
O	-2.793547000	1.715320000	3.203654000
C	-2.936576000	4.077516000	2.798140000
H	-3.605225000	4.120736000	3.670834000
H	-3.585238000	4.148887000	1.900934000
C	-0.952668000	5.038636000	1.589923000
H	-1.474837000	5.307670000	0.647294000
H	-0.112218000	5.749652000	1.657362000
C	-1.890519000	5.181869000	2.779637000
H	-2.379172000	6.168019000	2.769090000
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Structure IIb

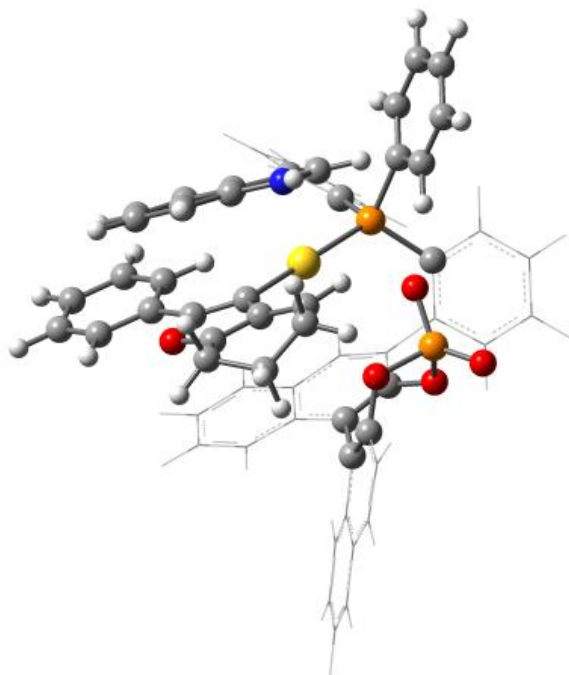


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C	4.340038000	0.419555000	3.225169000
C	5.367701000	-1.158230000	1.670901000
C	4.040024000	-2.359374000	0.038164000
C	5.555341000	0.610926000	3.840499000
H	3.453093000	0.932481000	3.607851000
C	6.608635000	-0.929099000	2.318004000
C	5.254195000	-2.101424000	0.616492000
C	6.709172000	-0.058943000	3.376964000
H	5.625944000	1.280358000	4.703009000
H	7.487686000	-1.476387000	1.960583000
H	6.151795000	-2.638789000	0.293074000
H	7.671505000	0.102482000	3.871174000
C	1.710118000	0.054689000	1.792343000
C	1.606929000	1.481817000	1.730424000
C	0.571439000	-0.684086000	2.099426000

C	2.673364000	2.310879000	1.287609000
C	0.373975000	2.114522000	2.080304000
C	-0.666643000	-0.055974000	2.423889000
C	2.547665000	3.681187000	1.253875000
H	3.611359000	1.843467000	0.974605000
C	0.270811000	3.528418000	2.029752000
C	-0.740073000	1.317156000	2.438803000
C	1.337800000	4.303474000	1.639266000
H	3.395813000	4.294557000	0.930136000
H	-0.683082000	3.988417000	2.311989000
H	-1.682556000	1.812256000	2.701759000
H	1.251329000	5.394614000	1.620302000
O	1.717888000	-1.921114000	-0.148187000
O	0.613746000	-2.032637000	2.093895000
P	0.550508000	-2.853488000	0.616160000
O	1.057908000	-4.222303000	0.864717000
O	-0.731694000	-2.504357000	-0.079314000
C	-1.843019000	-0.909462000	2.720811000
C	-2.928662000	-1.014140000	1.832895000
C	-1.864031000	-1.650459000	3.907012000
C	-4.012215000	-1.839270000	2.160923000
C	-2.945885000	-2.461502000	4.228325000
C	-4.026773000	-2.553137000	3.354593000
H	-4.855275000	-1.932063000	1.468094000
H	-4.880065000	-3.193383000	3.594819000
H	-2.941219000	-3.031857000	5.161295000
H	-1.002414000	-1.586918000	4.578701000
H	3.908456000	-3.102932000	-0.754052000
P	-2.933991000	-0.100404000	0.241458000
Au	-0.914271000	0.309076000	-0.961653000
C	-3.804428000	1.470413000	0.626069000
C	-4.615602000	1.624763000	1.755633000
C	-3.646020000	2.549077000	-0.253331000
C	-5.253496000	2.839716000	2.001745000
H	-4.746276000	0.792610000	2.455509000
C	-4.291879000	3.758787000	-0.010889000
H	-3.007828000	2.432067000	-1.138391000
C	-5.093362000	3.907025000	1.120585000
H	-5.880745000	2.951613000	2.890704000
H	-4.166116000	4.592944000	-0.707284000
H	-5.594561000	4.859257000	1.316578000
C	-4.109206000	-1.037941000	-0.801551000
C	-5.385477000	-0.566925000	-1.122409000
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C	-6.221079000	-1.327280000	-1.940538000
H	-5.735070000	0.396066000	-0.734944000
C	-4.513326000	-3.026167000	-2.110609000
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C	-5.787110000	-2.555377000	-2.432986000
H	-7.218985000	-0.955716000	-2.191269000
H	-4.172482000	-3.991632000	-2.495500000
H	-6.444922000	-3.150646000	-3.073132000
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C	0.743779000	0.914181000	-2.048139000
C	1.957977000	-1.151795000	-3.091073000
C	3.194357000	-1.549284000	-3.623890000
C	0.964898000	-2.121633000	-2.883709000

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H	3.979832000	-0.807798000	-3.789260000
C	1.213322000	-3.454979000	-3.174900000
H	0.006755000	-1.832598000	-2.441140000
C	2.447092000	-3.844618000	-3.698202000
H	4.402238000	-3.182890000	-4.338397000
H	0.438604000	-4.199867000	-2.972306000
H	2.640342000	-4.897198000	-3.924060000
C	1.165526000	2.303798000	-2.141577000
C	0.673050000	3.482804000	-1.658033000
C	2.399887000	2.329313000	-2.857685000
O	2.739700000	1.143473000	-3.196973000
C	3.210369000	3.531432000	-3.096756000
H	3.828293000	3.419308000	-4.000859000
H	3.919099000	3.613307000	-2.245110000
C	1.330266000	4.779017000	-1.950889000
H	1.867827000	5.067062000	-1.021331000
H	0.564973000	5.563888000	-2.073898000
C	2.281635000	4.741153000	-3.141863000
H	2.870041000	5.669023000	-3.188092000
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Structure II'a

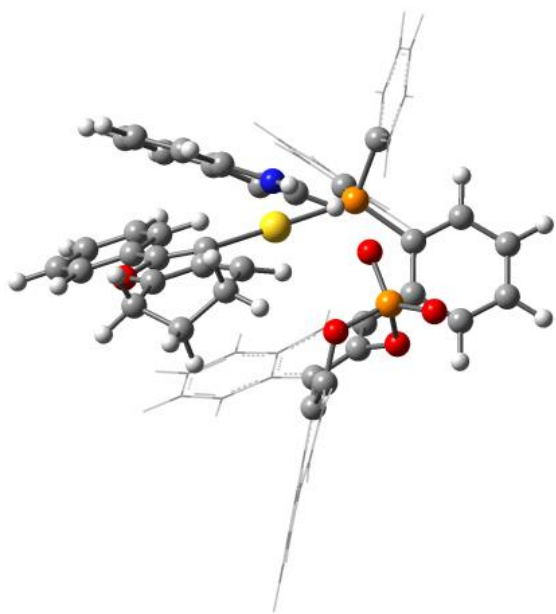


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C	4.523880000	-3.418581000	1.242486000
C	5.699454000	-2.476537000	-0.676857000
C	4.517795000	-1.235571000	-2.386662000
C	5.691439000	-4.003623000	1.673688000
H	3.600373000	-3.581846000	1.803642000
C	6.890097000	-3.081167000	-0.199015000
C	5.684215000	-1.767999000	-1.905653000
C	6.894448000	-3.824507000	0.956274000
H	5.685024000	-4.620392000	2.577120000

H	7.807320000	-2.952318000	-0.783617000
H	6.614152000	-1.683625000	-2.477290000
H	7.818133000	-4.290316000	1.311178000
C	2.001226000	-2.087615000	0.326762000
C	1.852584000	-1.656983000	1.684373000
C	0.891574000	-2.595862000	-0.338748000
C	2.868910000	-0.949039000	2.378651000
C	0.618604000	-1.894387000	2.362278000
C	-0.350340000	-2.819100000	0.325004000
C	2.688239000	-0.538220000	3.679070000
H	3.803508000	-0.717928000	1.858663000
C	0.469905000	-1.477244000	3.709573000
C	-0.453277000	-2.500171000	1.660993000
C	1.483150000	-0.816911000	4.361068000
H	3.480970000	0.018711000	4.187938000
H	-0.485634000	-1.668520000	4.210978000
H	-1.393450000	-2.688087000	2.194578000
H	1.349306000	-0.479983000	5.393320000
O	2.205045000	-0.766884000	-2.134279000
O	0.979289000	-2.918665000	-1.652313000
P	0.973182000	-1.714263000	-2.815447000
O	1.453627000	-2.326838000	-4.074296000
O	-0.246650000	-0.853558000	-2.662992000
C	-1.480855000	-3.420770000	-0.424576000
C	-2.703599000	-2.757842000	-0.646708000
C	-1.325105000	-4.720694000	-0.926705000
C	-3.733170000	-3.414484000	-1.338168000
C	-2.352698000	-5.364131000	-1.602706000
C	-3.568121000	-4.711776000	-1.804670000
H	-4.678736000	-2.892519000	-1.522685000
H	-4.382374000	-5.207648000	-2.340000000
H	-2.202773000	-6.379549000	-1.979824000
H	-0.367116000	-5.226685000	-0.775630000
H	4.464198000	-0.730267000	-3.355409000
P	-2.987206000	-1.020471000	-0.133471000
Au	-1.092922000	0.344951000	0.269608000
C	-4.081670000	-1.106408000	1.332746000
C	-4.655987000	-2.296238000	1.790331000
C	-4.330507000	0.086752000	2.026234000
C	-5.471526000	-2.290377000	2.922139000
H	-4.463659000	-3.237576000	1.265316000
C	-5.154998000	0.091136000	3.146821000
H	-3.874027000	1.022079000	1.678637000
C	-5.724655000	-1.099915000	3.598277000
H	-5.911996000	-3.226876000	3.275828000
H	-5.348304000	1.028654000	3.675863000
H	-6.365507000	-1.098846000	4.484563000
C	-4.026593000	-0.335464000	-1.474878000
C	-5.380683000	-0.027998000	-1.318695000
C	-3.387050000	-0.102915000	-2.702484000
C	-6.096558000	0.515318000	-2.385753000
H	-5.884141000	-0.211258000	-0.363209000
C	-4.114115000	0.432649000	-3.761868000
H	-2.321912000	-0.352926000	-2.823890000
C	-5.465150000	0.745572000	-3.605439000
H	-7.156043000	0.756988000	-2.260574000
H	-3.619330000	0.605793000	-4.722076000

H	-6.029314000	1.170727000	-4.440736000
C	1.082999000	2.157423000	1.680956000
C	0.564346000	1.530341000	0.591958000
C	0.665579000	2.349659000	3.060814000
C	1.482740000	3.023861000	3.982218000
C	-0.576432000	1.861952000	3.499911000
C	1.073909000	3.191032000	5.302558000
H	2.451589000	3.412744000	3.658848000
C	-0.980938000	2.034438000	4.817226000
H	-1.220815000	1.329341000	2.791489000
C	-0.157584000	2.697648000	5.728426000
H	1.726802000	3.715780000	6.006372000
H	-1.951472000	1.643709000	5.138075000
H	-0.477341000	2.832263000	6.765721000
C	1.504527000	1.835623000	-0.469126000
C	1.475551000	1.611172000	-1.829813000
C	2.524151000	2.631481000	0.083475000
O	2.305286000	2.823085000	1.348567000
C	3.621998000	3.255269000	-0.670366000
H	4.533554000	3.334224000	-0.056722000
H	3.303117000	4.298095000	-0.892022000
C	2.532089000	2.181292000	-2.693887000
H	2.096867000	3.117767000	-3.112802000
H	2.688849000	1.525867000	-3.565741000
C	3.839048000	2.467451000	-1.960273000
H	4.535939000	3.004958000	-2.620760000
H	4.316733000	1.500517000	-1.714915000
H	0.623783000	1.076209000	-2.274340000
C	-1.135356000	3.412831000	-2.249448000
C	-0.784021000	3.614538000	-3.559559000
C	-0.396677000	4.363626000	-1.470692000
H	-1.836071000	2.662107000	-1.880399000
N	0.140004000	4.631703000	-3.642602000
C	0.400284000	5.110646000	-2.377318000
H	-1.123781000	3.099257000	-4.457429000
C	-0.305517000	4.639328000	-0.096410000
C	0.574916000	5.620743000	0.335403000
H	-0.912609000	4.076215000	0.620161000
H	0.663590000	5.830868000	1.406087000
C	1.281134000	6.108395000	-1.947039000
C	1.358916000	6.349630000	-0.580841000
H	1.884467000	6.678458000	-2.660085000
H	2.037087000	7.124326000	-0.210489000
H	0.525480000	5.003390000	-4.502406000

Structure **TS-II'-IIIa**

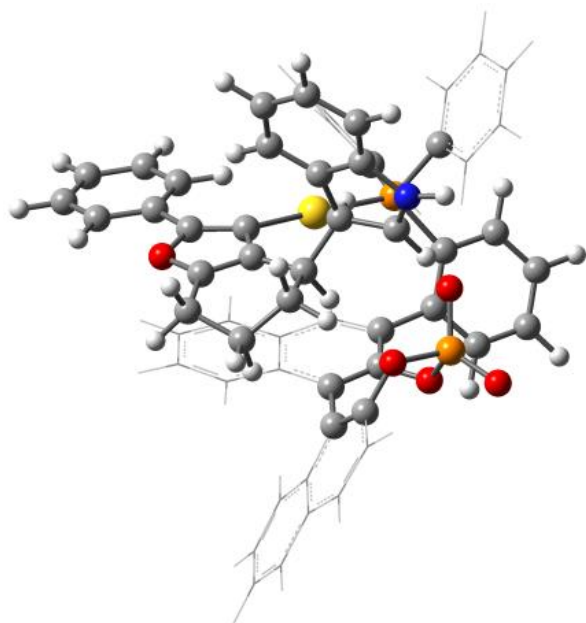


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C	4.309850000	-3.002455000	2.371216000
C	5.842688000	-2.474910000	0.550732000
C	5.026403000	-1.688610000	-1.585804000
C	5.365127000	-3.444242000	3.134969000
H	3.294635000	-3.067392000	2.770428000
C	6.911952000	-2.922127000	1.367880000
C	6.072868000	-2.055177000	-0.783994000
C	6.685946000	-3.391843000	2.638801000
H	5.176127000	-3.848006000	4.133968000
H	7.925488000	-2.897573000	0.953290000
H	7.097557000	-2.059512000	-1.169676000
H	7.518097000	-3.739945000	3.257251000
C	2.038223000	-1.932018000	0.761430000
C	1.698826000	-1.214974000	1.957649000
C	1.023284000	-2.574481000	0.062661000
C	2.605451000	-0.345484000	2.619764000
C	0.377115000	-1.324256000	2.485525000
C	-0.306084000	-2.670701000	0.570551000
C	2.228284000	0.358868000	3.741007000
H	3.615713000	-0.225308000	2.216816000
C	0.028842000	-0.616966000	3.663696000
C	-0.589966000	-2.086986000	1.784726000
C	0.930511000	0.215822000	4.279973000
H	2.940035000	1.040344000	4.217314000
H	-0.992893000	-0.716061000	4.047765000
H	-1.595452000	-2.181879000	2.214264000
H	0.638938000	0.783469000	5.169266000
O	2.734070000	-1.233655000	-1.911277000
O	1.292862000	-3.154354000	-1.133968000
P	1.460652000	-2.179232000	-2.481923000
O	1.917752000	-3.038549000	-3.596587000
O	0.319873000	-1.200213000	-2.550489000
C	-1.336518000	-3.406648000	-0.198362000
C	-2.550768000	-2.827803000	-0.617652000
C	-1.096174000	-4.753189000	-0.514183000

C	-3.484401000	-3.608289000	-1.319077000
C	-2.031235000	-5.517087000	-1.196960000
C	-3.237379000	-4.944710000	-1.599380000
H	-4.421195000	-3.153238000	-1.659762000
H	-3.978926000	-5.535196000	-2.144202000
H	-1.815639000	-6.565061000	-1.422703000
H	-0.146171000	-5.199440000	-0.207995000
H	5.167782000	-1.401822000	-2.631490000
P	-2.974488000	-1.058951000	-0.371741000
Au	-1.329788000	0.540810000	0.261909000
C	-4.328645000	-1.041025000	0.862833000
C	-4.860403000	-2.199811000	1.436561000
C	-4.805601000	0.210844000	1.280431000
C	-5.859226000	-2.107176000	2.406287000
H	-4.491501000	-3.184333000	1.131682000
C	-5.811415000	0.298934000	2.237110000
H	-4.382478000	1.126095000	0.847348000
C	-6.338256000	-0.862386000	2.804202000
H	-6.264390000	-3.019620000	2.852767000
H	-6.181439000	1.280259000	2.547608000
H	-7.122577000	-0.794021000	3.563329000
C	-3.740358000	-0.597203000	-1.968129000
C	-5.093938000	-0.288743000	-2.121375000
C	-2.873917000	-0.538335000	-3.070012000
C	-5.582213000	0.084449000	-3.373957000
H	-5.774798000	-0.339792000	-1.264902000
C	-3.373251000	-0.170138000	-4.315612000
H	-1.810386000	-0.796502000	-2.950239000
C	-4.724213000	0.145429000	-4.468981000
H	-6.642460000	0.326292000	-3.492174000
H	-2.698787000	-0.129295000	-5.176004000
H	-5.110268000	0.438597000	-5.449650000
C	0.247340000	2.785335000	1.857341000
C	0.091025000	1.943774000	0.790477000
C	-0.530578000	3.075828000	3.052982000
C	-0.028615000	3.925333000	4.051983000
C	-1.786665000	2.480037000	3.255815000
C	-0.753415000	4.158613000	5.217265000
H	0.946972000	4.397931000	3.913369000
C	-2.505951000	2.714274000	4.420686000
H	-2.189801000	1.810384000	2.487886000
C	-1.993394000	3.553405000	5.411715000
H	-0.341319000	4.821038000	5.984494000
H	-3.479306000	2.232815000	4.557010000
H	-2.559592000	3.735099000	6.329724000
C	1.308990000	2.115307000	0.033602000
C	1.790725000	1.459960000	-1.123539000
C	2.094802000	3.043841000	0.696671000
O	1.483549000	3.455972000	1.789888000
C	3.477119000	3.423567000	0.338101000
H	4.058614000	3.665597000	1.242618000
H	3.465169000	4.341368000	-0.285474000
C	3.164628000	1.828530000	-1.596858000
H	3.094800000	2.681385000	-2.302659000
H	3.594620000	0.986551000	-2.161111000
C	4.084088000	2.264202000	-0.453196000
H	5.067127000	2.548282000	-0.860637000

H	4.256494000	1.407318000	0.224770000
H	1.390483000	0.468282000	-1.365133000
C	0.337629000	2.197108000	-2.625339000
C	0.934628000	1.578694000	-3.728351000
C	0.659939000	3.598285000	-2.721826000
H	-0.465395000	1.742059000	-2.039535000
N	1.644521000	2.486955000	-4.425546000
C	1.513079000	3.744391000	-3.838099000
H	0.898918000	0.513962000	-3.975103000
C	0.393858000	4.706830000	-1.909259000
C	0.972436000	5.926371000	-2.243086000
H	-0.258742000	4.608731000	-1.035518000
H	0.772316000	6.806735000	-1.625933000
C	2.096061000	4.962452000	-4.180523000
C	1.810248000	6.052041000	-3.364316000
H	2.755744000	5.057129000	-5.047302000
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H	2.219749000	2.276891000	-5.235239000

Structure IIIa

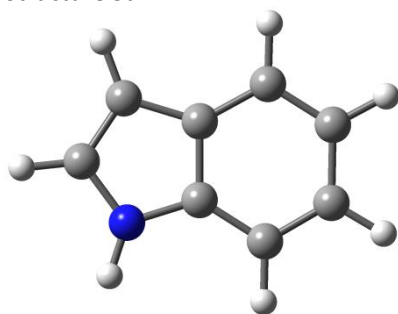


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C	4.890546000	-0.388314000	3.000986000
C	6.146670000	-1.150028000	1.055232000
C	5.026812000	-2.104062000	-0.864124000
C	6.067882000	-0.118120000	3.658663000
H	3.939720000	-0.229995000	3.515713000
C	7.343603000	-0.845383000	1.752573000
C	6.186136000	-1.749948000	-0.229021000
C	7.312120000	-0.331720000	3.026033000
H	6.038300000	0.258225000	4.685387000
H	8.298186000	-1.045487000	1.254141000
H	7.159453000	-1.954083000	-0.686811000
H	8.242050000	-0.106798000	3.555929000
C	2.333347000	-0.845005000	1.514034000
C	1.989308000	0.472106000	1.971626000
C	1.371997000	-1.846022000	1.589231000

C	2.817135000	1.607341000	1.765787000
C	0.739586000	0.674450000	2.632081000
C	0.088550000	-1.630095000	2.171441000
C	2.447492000	2.851522000	2.223551000
H	3.758441000	1.488674000	1.220513000
C	0.403217000	1.959458000	3.126923000
C	-0.181028000	-0.397657000	2.722898000
C	1.237959000	3.031186000	2.930088000
H	3.092660000	3.713792000	2.027372000
H	-0.561059000	2.087882000	3.631807000
H	-1.140213000	-0.222759000	3.226894000
H	0.952210000	4.025451000	3.287584000
O	2.666548000	-2.150617000	-0.983974000
O	1.661119000	-3.089927000	1.127386000
P	1.643301000	-3.398422000	-0.506316000
O	2.285258000	-4.714271000	-0.720976000
O	0.318498000	-2.976894000	-1.088546000
C	-0.915789000	-2.717758000	2.183842000
C	-2.203668000	-2.577026000	1.628488000
C	-0.578611000	-3.941262000	2.784146000
C	-3.110597000	-3.647359000	1.704294000
C	-1.486982000	-4.986708000	2.861565000
C	-2.764857000	-4.840151000	2.323041000
H	-4.107061000	-3.544057000	1.260194000
H	-3.487297000	-5.659291000	2.373428000
H	-1.195048000	-5.924869000	3.341513000
H	0.426015000	-4.059232000	3.198193000
H	5.024186000	-2.607966000	-1.834385000
P	-2.778840000	-1.084424000	0.724425000
Au	-1.321564000	0.654481000	-0.035053000
C	-4.061620000	-0.326437000	1.793203000
C	-4.445926000	-0.859671000	3.027466000
C	-4.632111000	0.881486000	1.362941000
C	-5.393251000	-0.201153000	3.811695000
H	-4.000747000	-1.792750000	3.386785000
C	-5.587176000	1.527779000	2.140857000
H	-4.322108000	1.319269000	0.405589000
C	-5.967649000	0.987177000	3.369665000
H	-5.682033000	-0.624235000	4.777945000
H	-6.030058000	2.464276000	1.790011000
H	-6.710770000	1.499770000	3.986963000
C	-3.670397000	-1.809336000	-0.703691000
C	-5.033157000	-1.624247000	-0.944426000
C	-2.891456000	-2.548433000	-1.607548000
C	-5.617983000	-2.169277000	-2.088456000
H	-5.648722000	-1.056636000	-0.238677000
C	-3.486614000	-3.093222000	-2.741319000
H	-1.821779000	-2.716514000	-1.407233000
C	-4.847414000	-2.901246000	-2.987273000
H	-6.686237000	-2.022621000	-2.272358000
H	-2.881993000	-3.682159000	-3.437981000
H	-5.309546000	-3.330319000	-3.881141000
C	0.195472000	3.435253000	-0.301177000
C	-0.020960000	2.128082000	-0.680385000
C	-0.542174000	4.379782000	0.524415000
C	-0.031378000	5.662687000	0.785106000
C	-1.766105000	4.024429000	1.116573000

C	-0.710431000	6.545113000	1.620380000
H	0.918830000	5.958677000	0.332706000
C	-2.438643000	4.905533000	1.953777000
H	-2.179698000	3.027546000	0.926497000
C	-1.915020000	6.172909000	2.215381000
H	-0.289748000	7.537268000	1.811690000
H	-3.384629000	4.597119000	2.410302000
H	-2.444210000	6.865755000	2.876049000
C	1.140402000	1.794488000	-1.453634000
C	1.502670000	0.501975000	-2.101016000
C	1.968189000	2.875703000	-1.460126000
O	1.405493000	3.893678000	-0.782724000
C	3.352702000	2.931515000	-1.986558000
H	4.001959000	3.489537000	-1.288017000
H	3.401792000	3.475548000	-2.951118000
C	2.810088000	0.630187000	-2.888014000
H	2.606110000	1.087278000	-3.877528000
H	3.221517000	-0.378005000	-3.079229000
C	3.839606000	1.490605000	-2.161180000
H	4.798495000	1.471971000	-2.704498000
H	4.036076000	1.046603000	-1.165034000
H	1.623359000	-0.272992000	-1.320515000
C	0.331967000	-0.000017000	-2.985451000
C	0.467081000	-1.382356000	-3.459584000
C	0.009834000	0.752466000	-4.236322000
H	-0.552808000	-0.026221000	-2.291456000
N	0.264502000	-1.441839000	-4.746565000
C	-0.016600000	-0.163080000	-5.293388000
H	0.623519000	-2.251683000	-2.789181000
C	-0.238377000	2.095871000	-4.495202000
C	-0.504684000	2.473965000	-5.812709000
H	-0.227036000	2.829177000	-3.683397000
H	-0.703125000	3.525052000	-6.038520000
C	-0.282813000	0.186498000	-6.608513000
C	-0.527232000	1.537450000	-6.851814000
H	-0.300410000	-0.554165000	-7.411686000
H	-0.741317000	1.868041000	-7.871438000
H	0.276253000	-2.306919000	-5.287373000

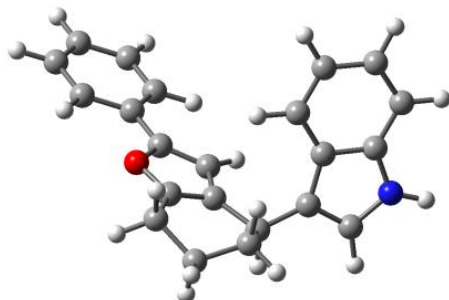
Structure 9a



C	-0.249254000	0.751594000	0.000010000
C	-0.251769000	-0.668662000	-0.000070000
C	0.930144000	-1.415997000	0.000020000
C	2.130231000	-0.720334000	0.000197000
C	2.156697000	0.688081000	0.000280000
C	0.983272000	1.426374000	0.000187000
C	-1.621843000	1.167653000	-0.000114000

C	-2.382256000	0.028092000	-0.000258000
H	0.907265000	-2.509926000	-0.000046000
H	3.073187000	-1.275142000	0.000271000
H	3.121437000	1.204124000	0.000420000
H	1.013488000	2.520417000	0.000254000
H	-1.998365000	2.189523000	-0.000098000
H	-3.465562000	-0.087725000	-0.000376000
H	-1.877250000	-2.039846000	-0.000269000
N	-1.563647000	-1.077463000	-0.000239000

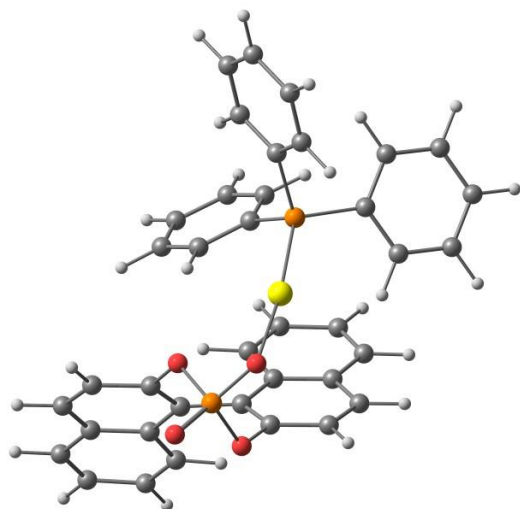
Structure 10a



C	1.957706000	0.391158000	-0.238417000
C	0.758385000	0.183862000	-0.870382000
C	3.207197000	-0.350712000	-0.214666000
C	4.309333000	0.105558000	0.524547000
C	3.331945000	-1.548365000	-0.937176000
C	5.498776000	-0.616532000	0.537545000
H	4.223160000	1.036255000	1.091321000
C	4.521769000	-2.265431000	-0.920786000
H	2.481771000	-1.920535000	-1.516932000
C	5.612822000	-1.803764000	-0.183384000
H	6.348081000	-0.246173000	1.119434000
H	4.599158000	-3.196708000	-1.489554000
H	6.548854000	-2.369289000	-0.171028000
C	-0.090387000	1.268588000	-0.496132000
C	-1.517604000	1.580624000	-0.845052000
C	0.655332000	2.056595000	0.332225000
O	1.892736000	1.538644000	0.496407000
C	0.235209000	3.304267000	1.008634000
H	1.027560000	4.070686000	0.947192000
H	0.073886000	3.120568000	2.089699000
C	-2.044165000	2.638734000	0.139829000
H	-2.251266000	2.147871000	1.110745000
H	-3.013926000	3.018041000	-0.224206000
C	-1.059052000	3.782884000	0.350592000
H	-1.519010000	4.579674000	0.957057000
H	-0.819351000	4.235627000	-0.630293000
H	-1.539824000	2.027689000	-1.861261000
C	-2.387249000	0.361098000	-0.882579000
C	-3.264247000	0.016360000	-1.879557000
C	-2.514851000	-0.653235000	0.133138000
H	0.499229000	-0.655051000	-1.516597000
N	-3.931063000	-1.141663000	-1.549363000
C	-3.492107000	-1.576657000	-0.322928000
H	-3.464458000	0.526643000	-2.822526000
C	-1.893150000	-0.881082000	1.373412000
C	-2.258604000	-1.993277000	2.116651000
H	-1.124097000	-0.193390000	1.740851000

H	-1.779385000	-2.180186000	3.082142000
C	-3.861417000	-2.699300000	0.424390000
C	-3.234672000	-2.893118000	1.646935000
H	-4.616693000	-3.399839000	0.055498000
H	-3.501339000	-3.762529000	2.255257000
H	-4.622621000	-1.606407000	-2.123560000

Structure 14



C	3.168245000	-0.245108000	-0.108811000
C	4.368111000	0.400213000	-0.558828000
C	2.801297000	-1.436833000	-0.720528000
C	4.920342000	1.532050000	0.098188000
C	5.072184000	-0.127502000	-1.685506000
C	3.508124000	-1.970768000	-1.819563000
C	6.070610000	2.131824000	-0.358322000
H	4.425780000	1.921253000	0.992081000
C	6.247585000	0.522660000	-2.141428000
C	4.606327000	-1.313676000	-2.308009000
C	6.737622000	1.633805000	-1.499483000
H	6.476973000	2.997012000	0.173426000
H	6.765589000	0.106641000	-3.011987000
H	5.158117000	-1.711375000	-3.165698000
H	7.648777000	2.121903000	-1.856599000
C	2.343952000	0.284385000	1.004682000
C	1.787625000	1.608226000	1.000896000
C	2.040033000	-0.547015000	2.074159000
C	1.916295000	2.491152000	-0.104037000
C	1.031204000	2.058228000	2.127833000
C	1.292588000	-0.103571000	3.187560000
C	1.352135000	3.745023000	-0.087232000
H	2.462368000	2.158276000	-0.990382000
C	0.474080000	3.362725000	2.120959000
C	0.817801000	1.181018000	3.222128000
C	0.626672000	4.193945000	1.038207000
H	1.462389000	4.397515000	-0.958650000
H	-0.090447000	3.690594000	3.000912000
H	0.246013000	1.540926000	4.084803000
H	0.188319000	5.195887000	1.044082000
O	1.691615000	-2.115369000	-0.301589000
O	2.474545000	-1.841551000	2.079451000
P	1.691957000	-2.948666000	1.139446000

O	2.470478000	-4.197772000	1.103074000
O	0.206333000	-2.939412000	1.529899000
C	-2.653800000	1.668016000	1.885341000
C	-3.210691000	1.292421000	0.658432000
C	-3.293628000	2.615533000	2.679813000
C	-4.417164000	1.864420000	0.237026000
C	-4.492399000	3.186587000	2.256310000
C	-5.053463000	2.810514000	1.036744000
H	-4.865111000	1.566804000	-0.717594000
H	-5.996977000	3.253691000	0.706549000
H	-4.997838000	3.925216000	2.884741000
H	-2.856736000	2.901929000	3.641103000
H	3.148373000	-2.908474000	-2.250402000
P	-2.315858000	0.088261000	-0.374681000
Au	-1.080432000	-1.478677000	0.727647000
C	-1.237823000	1.048136000	-1.490704000
C	-1.541715000	2.364174000	-1.855029000
C	-0.123320000	0.410157000	-2.050498000
C	-0.750074000	3.024317000	-2.792596000
H	-2.400956000	2.876966000	-1.409050000
C	0.664726000	1.076199000	-2.985422000
H	0.136424000	-0.612832000	-1.749316000
C	0.346759000	2.379985000	-3.362528000
H	-0.992193000	4.052037000	-3.078117000
H	1.537878000	0.572497000	-3.412142000
H	0.965644000	2.902645000	-4.097575000
C	-3.592469000	-0.650244000	-1.450789000
C	-3.699635000	-0.342351000	-2.809858000
C	-4.493613000	-1.550922000	-0.867967000
C	-4.707104000	-0.928004000	-3.576410000
H	-2.994483000	0.352604000	-3.277581000
C	-5.500042000	-2.126152000	-1.635617000
H	-4.403847000	-1.803863000	0.195226000
C	-5.606665000	-1.815158000	-2.991742000
H	-4.785467000	-0.687887000	-4.640319000
H	-6.201014000	-2.827888000	-1.175634000
H	-6.393804000	-2.273494000	-3.596885000
H	1.115961000	-0.815007000	3.998479000
H	-1.715101000	1.210354000	2.220059000