Supporting Information for

Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization

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Computational Details

All calculations were performed using the software package Gaussian '09.[1] All geometry optimizations and NBO analysis were performed at the (IEFPCM=toluene)/(U-BS)PBE0/6-311+G(d,p)/Def2-TZVP[2] (including Effective Core Potential (ECP)) level of theory (labeled as 'PBE0[3]'). In order to evaluate the solvent effect, we performed calculations with the aforementioned level of theory, varying solvents (*vacuum*, toluene, THF, MeCN, DCM, DCE) with PCM (*i.e.*, IEFPCM=solvent). PBE0 is known to provide sufficiently accurate description of gold complexes.[4] For the uncatalyzed reactions, we adopted an open-shell, broken-spin symmetry approach. (SMD=toluene)/CCSD(T)/6-311++G(d,p)/Def2-TZVP+ECP single-point corrections for the Distortion-Interaction analysis. The minimum energy pathway (MEP) was traced using the intrinsic reaction coordinate (IRC) method to ensure that each TS structure correctly links two minima. Frequency calculations were carried for all structures to confirm them as either a minimum or a TS. Electronic structures and properties were analyzed by the Natural Bond Orbitals (NBO) method at the PBE0 level of theory. Since they resulted in a good estimate for both the barrier and reaction energy for the parent Bergman Cyclization, relaxed scans (at the (SMD=toluene)/(U-BS)B2PLYP-D3BJ/6-311++G(d,p) level of theory for the uncatalyzed BC and (IEFPCM=toluene)/PBE0/6-311+G(d,p)/Def2-TZVP+ECP for the catalyzed one) were performed in order to evaluate the dynamic electronic changes throughout its MEPs. Three-dimensional structures were produced with both CYLView 1.0.1[5] and Chemcraft 1.8.

Screening Methodologies

Table S1: Methodology screening.

method	$\Delta E^{\ddagger}$	ΔE	$\Delta E^{\ddagger}$	ΔE
experimental[*]	30.1±0.5	7.8±1.0	—	—
(U)M06-2X	36.5	12.3	21.1	4.5
(U)ωB97XD	35.4	8.4	18.9	-1.5
(U)B3LYP	34.1	10.7	16.2	-1.6
(U)B2PLYP-D3	39.7	15.2	18.9	0.4
(U)B2PLYP-D3BJ[a]	38.8	10.7	14.8	-3.7
(U)PBE0	**30.3**	**4.6**	**15.7**	**-6.6**
(U)PBE0-D3BJ	29.5	1.2	15.9	-6.3
(U)BLYP	28.0	15.4	15.7	-2.1
CCSD(T)	*27.1*	*13.2*	*15.8*	*-1.7*
CCSD(T)[a]	*29.2*	*11.2*	*15.8*	*-1.7*

Energies are ZPE corrected and in kcal/mol. Solvent: IEFPCM = toluene
Basis set: C, P, H = 6-311+G(d,p); Au = Def2-TZVP with ECP
The broken-spin symmetry approach was used for the parent system.

[*]: see ref. 24 in the main paper
[a]: *C, P, H = 6-311++G(d,p), SMD = toluene*
CCSD(T) single-point calculations from PBE0 geometries

We evaluated 9 DFT functionals and also performed single-point corrections with CCSD(T). Since our goal was not reproduce the experimental data but rather get the correct reasonable trends, our choice of DFT method must comply with that idea. Comparing the activation enthalpy and reaction energy for the parent BC with the screened functionals, PBE0 seems to be the most reasonable as correctly describes the reaction as endothermic and is ~2 kcal/mol off on the barrier. PBE0 is know to accuretly describe Au-complex geometries, reaction energies and barriers for Au-catalyzed reactions. We used the PBE0 functional in all of our calculations, with 6-311+G(d,p) basis set for C, P and H and the Def2-TZVP with ECP for Au. The addition of dispersion (PBE0-D3BJ) for that specific functional does not change the trend, but it brings some unrealistic overstabilization

to *p*-benzyne; on the other hand, it does improve significantly the results for the double-hybrid B2PLYP functional. Overall, most functionals correctly describe the Au-catalyzed reaction as exothermic, with a significantly lower activation barrier than its uncatalyzed version and thus properly indicating the aborted pericyclic behavior of this reaction.

In order to confirm such paramount result, we turned to CCSD(T) single point corrections on the PBE0 geometries. The (SMD=toluene)/CCSD(T)/6-311++G(d,p)/Def2-TZVP+ECP provided values very close to the experimental ones and so it was chosen to be used for the Distortion-Interaction Analysis. For the uncatalyzed reaction, the (SMD=toluene)/B2PLYP-D3BJ/6-311++G(d,p) resulted in a very accurate description of the PES through a relaxed scan calculation, being then the method of choice for that analysis. Unfortunately, such a high level of theory displayed itself too computationally expensive for our resources to be used for the Au-catalyzed reaction and therefore we turned ourselves to the same PBE0 method for that relaxed scan.

Au-Catalyzed Bergman Cyclization Mechanism

The mechanism for this reaction is seemingly straightforward, with $[Au]^+$ first complexing to the top of one of the alkyne moieties with subsequent rotation to the productive geometry complex and then its cyclization step.

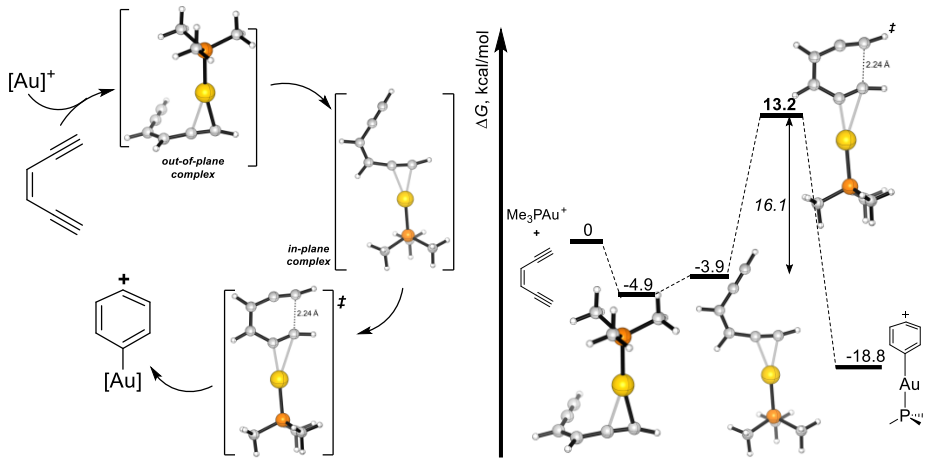


Figure S1: Mechanism for the Au-catalyzed Bergman Cyclization. Gibbs Free Energies at the PBE0 level of theory.

NBO scans for 1

We performed NBO calculations on-the-fly with relaxed scans for minimum energy pathways for the referred examples.

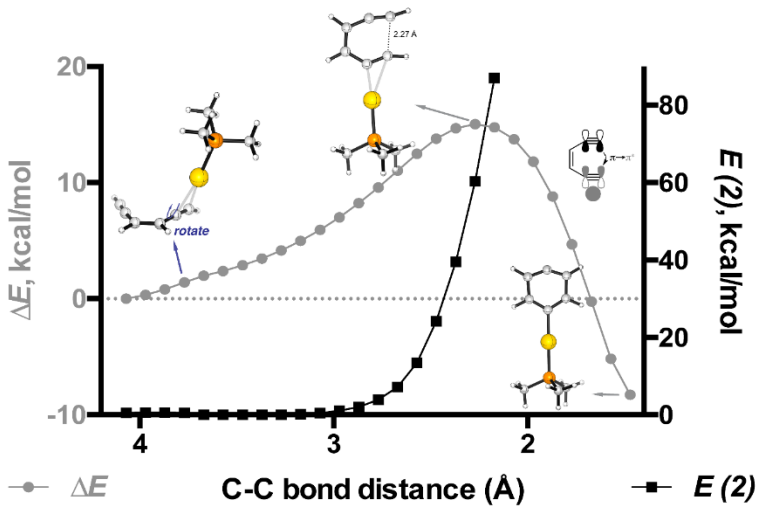


Figure S2: Scanning $\pi_{in} \rightarrow \pi^*_{in}$ interactions. Energies at the PBE0 level of theory.

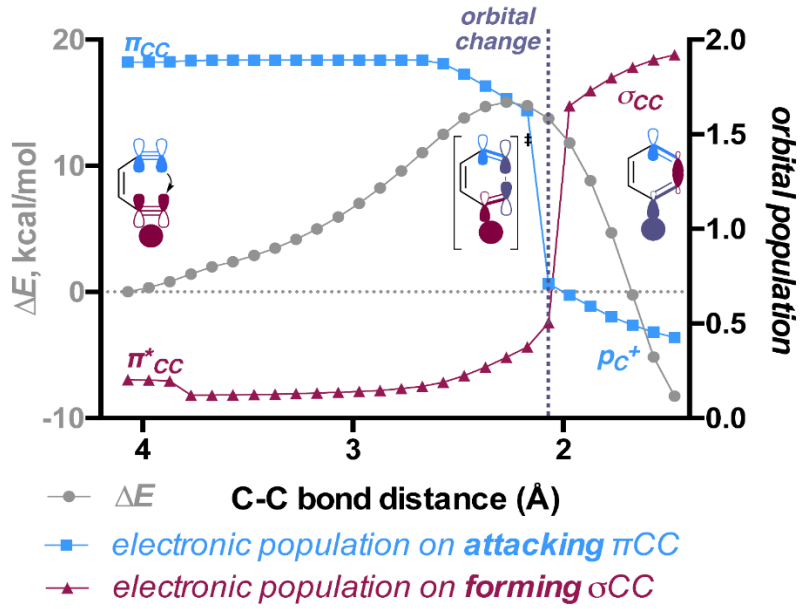


Figure S3: Scanning orbital populations at the PBE0 level of theory.

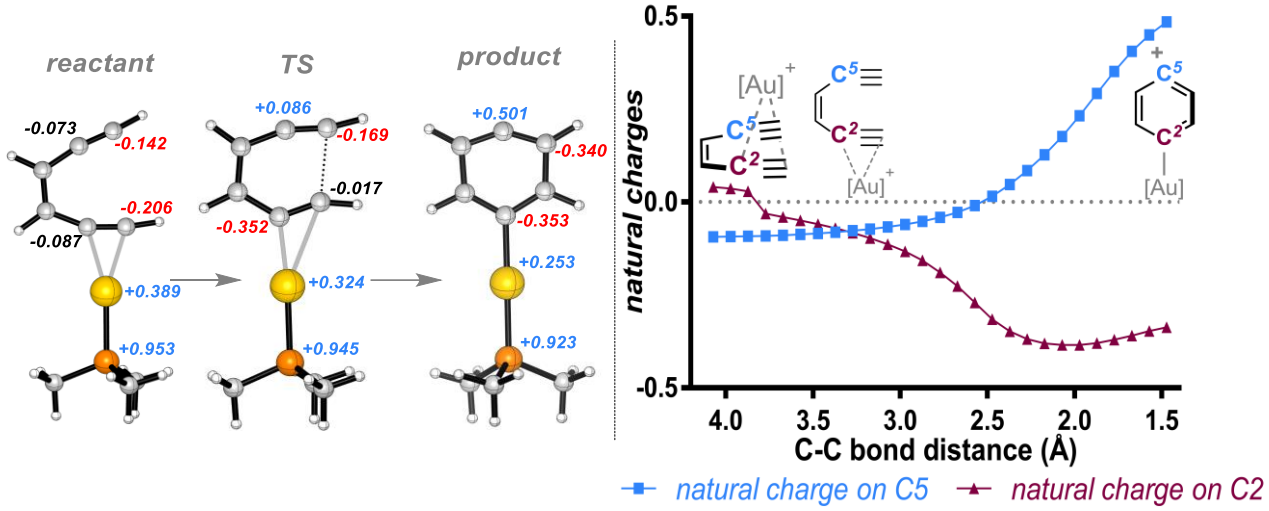


Figure S4: Scanning natural charges at the PBE0 level of theory.

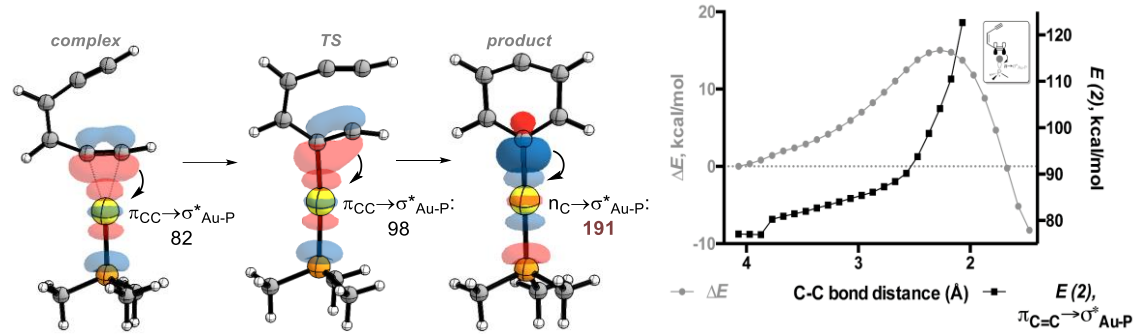


Figure S5: Scanning $\pi_{CC} \rightarrow \sigma^*_{Au-P}$ interactions. Energies at the PBE0 level of theory, in kcal/mol.

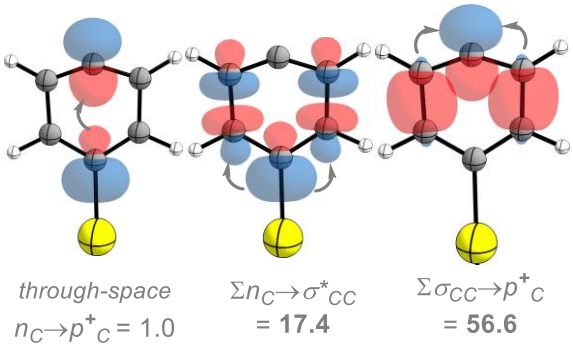


Figure S6: Stabilizing positive charge through hyperconjugation. Energies at the PBE0 level of theory, in kcal/mol.

NBO scans for 3

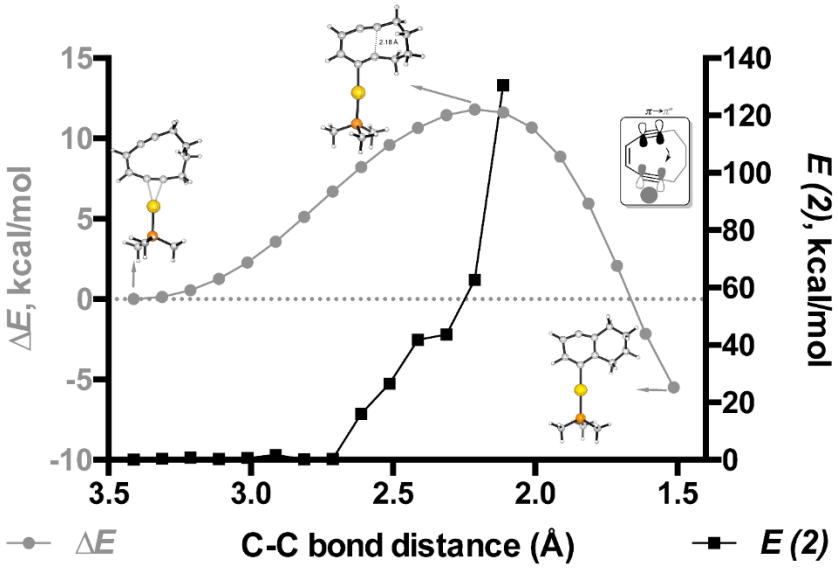


Figure S7: Scanning $\pi_{in} \rightarrow \pi_{in}^{*}$ interactions. Energies at the PBE0 level of theory.

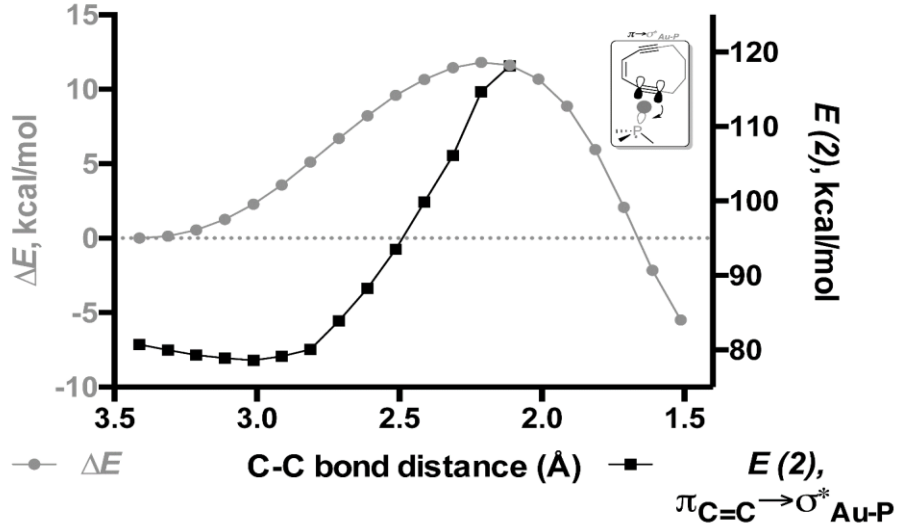


Figure S8: Scanning $\pi_{CC} \rightarrow \sigma_{Au-P}^{*}$ interactions. Energies at the PBE0 level of theory, in kcal/mol.

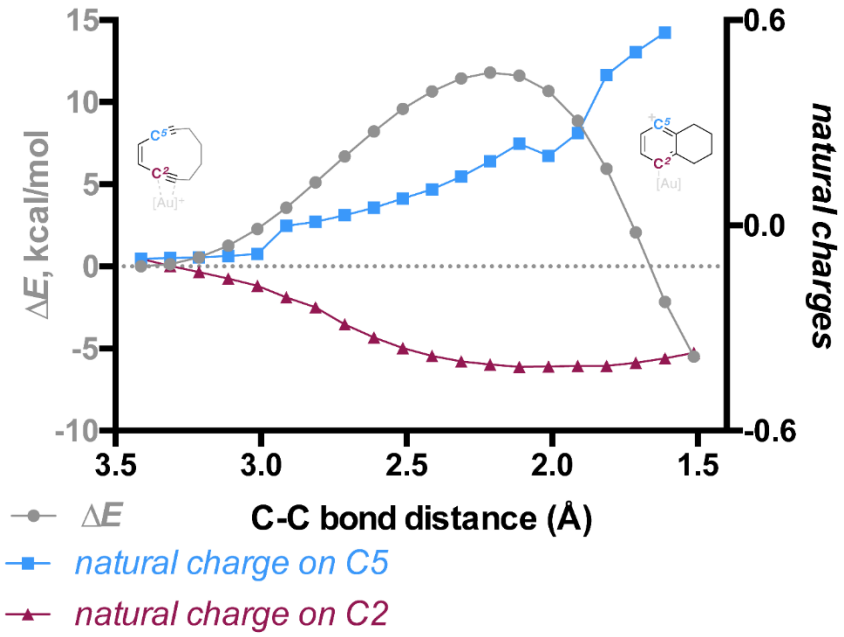


Figure S9: Scanning natural charges at the PBE0 level of theory.

Transition State control by hyperconjugative assistance for 3

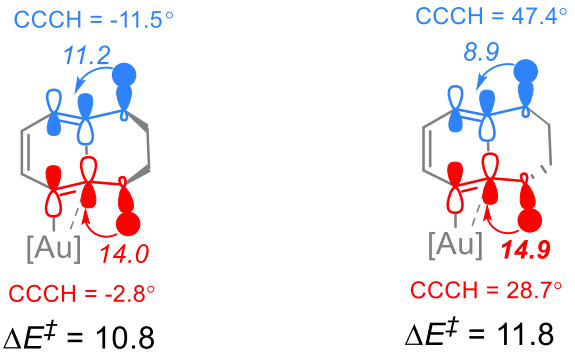


Figure S10: Geometric and electronic differences between two transition states for cyclization of **3**. Energies at the PBE0 level of theory, in kcal/mol

Figure S10 displays the TS control by hyperconjugative assistance presented from the vicinal top C-H bond donating into the π*-orbital that will evolve into an empty p^+-orbital. This minor but not negligible effect lowers the activation energy in about 1 kcal/mol.

NBO scans for 4

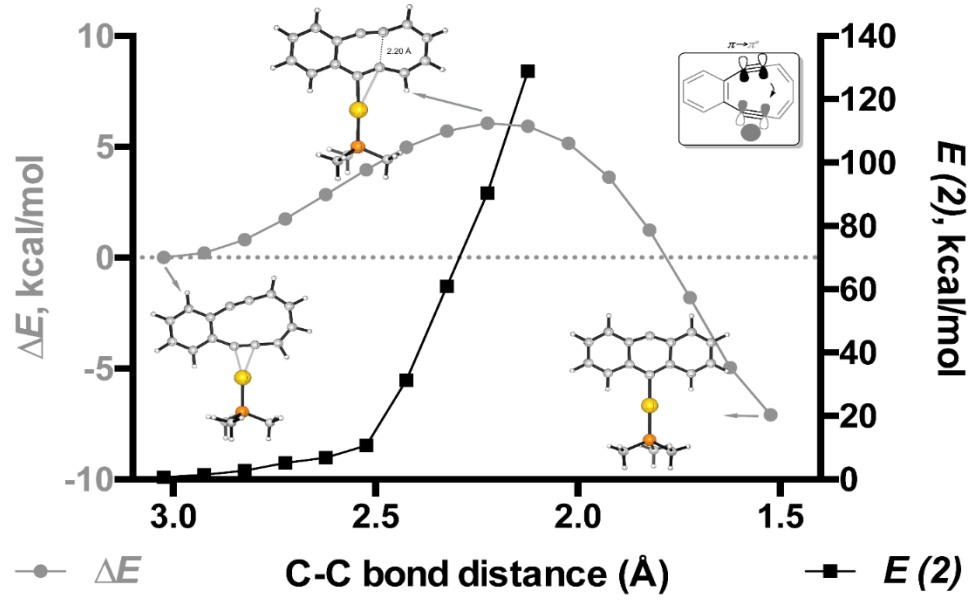


Figure S11: Scanning $\pi_{in} \rightarrow \pi_{in}^{*}$ interactions. Energies at the PBE0 level of theory.

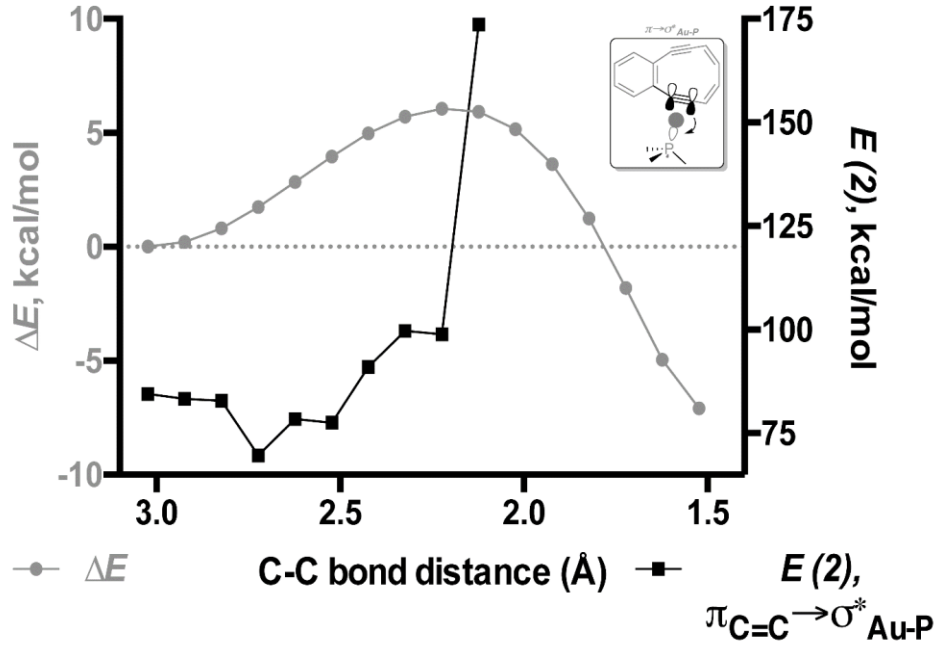


Figure S12: Scanning $\pi_{CC} \rightarrow \sigma_{Au-P}^{*}$ interactions. Energies at the PBE0 level of theory, in kcal/mol.

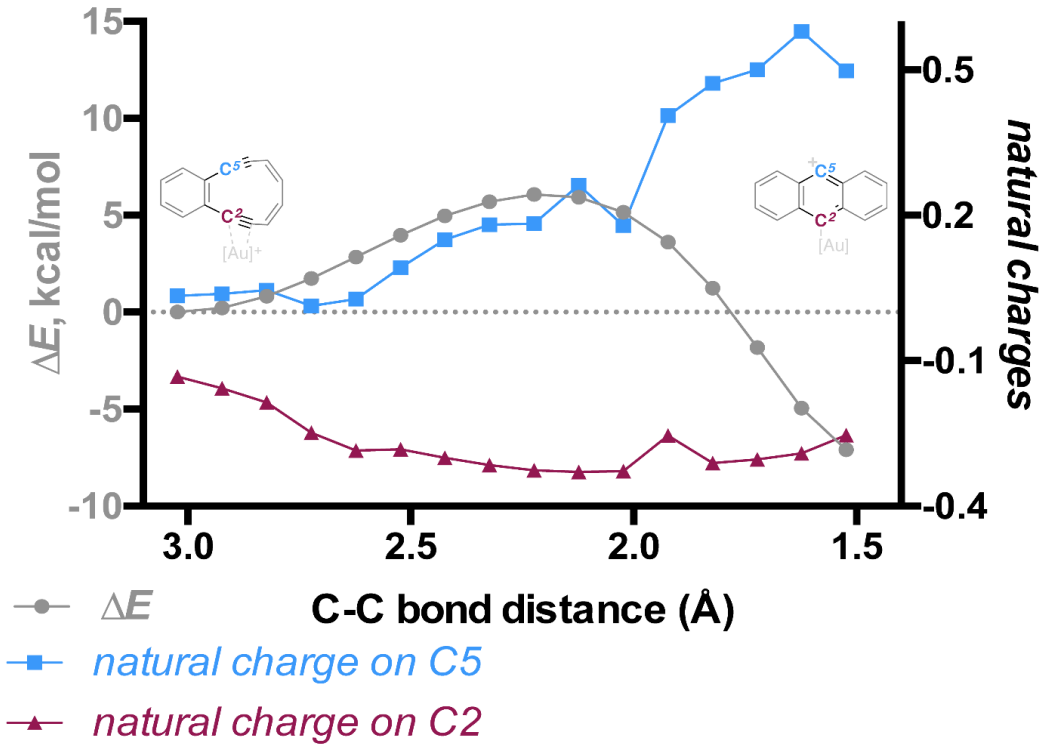


Figure S13: Scanning natural charges at the PBE0 level of theory.

Distortion-Interaction Model

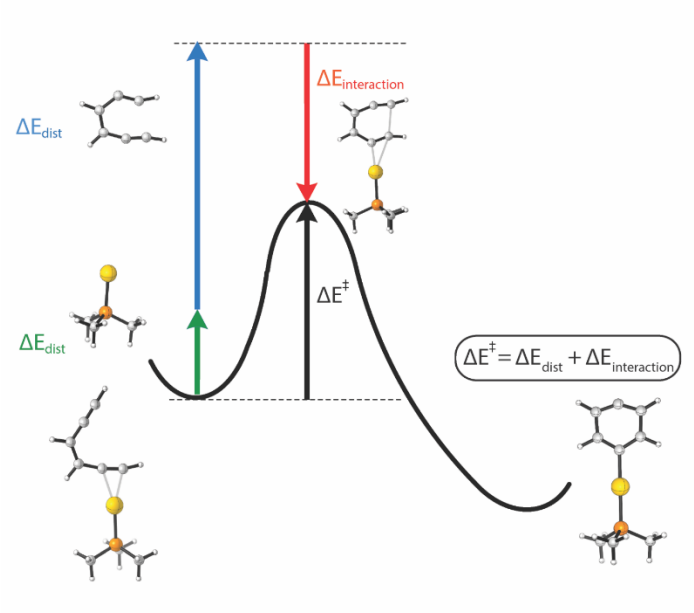
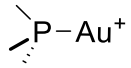
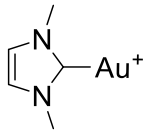


Figure S14: Simplified Distortion-Interaction Analysis model.

Correlations for different catalysts and substrates with Distortion-Interaction Analysis

Table S2. Computational analysis of three Au-catalyzed Bergman cyclizations of the parent enediyne. Calculations at (IEFPCM=toluene)/(U)PBE0/6-311+G(d,p)/Def2-TZVP+ECP level of theory. (SMD=toluene)/CCSD(T)/6-311++G(d,p)/Def2-TZVP+ECP single point corrections are given in parenthesis. All energies are in kcal/mol.

Catalyst	$E^{comp\,a}$	$E_{dist}(comp)$	$E_{int}(comp)$	$E_{dist}(TS)$	$E_{int}(TS)$	$\Delta E_{int}{}^{c}$	$\Delta\Delta E^{\ddagger\,d}$	$\Delta E_{cat}^{\ddagger\ b}$	$\Delta E_{rxn\ cat}{}^{b}$
	-29.4 (-30.5)	4.5 (3.6)	-33.9 (-34.1)	34.0 (31.5)	-48.6 (-47.3)	-14.7 (-13.2)	16.4 (13.4)	14.6 (15.8)	-7.3 (-1.7)
	-34.6	5.0	-39.6	34.3	-50.8	-11.2	14.5	16.5	-6.3
AuCl	-38.9	7.0	-45.9	34.9	-55.3	-9.4	10.6	20.4	-0.5

a: relative to isolated reactant and catalyst. **b**: relative to reactant-catalyst complex. **c**: between TS and reactant complex (catalyzed reaction). **d**: barrier lowering relative to the non-catalyzed reaction.

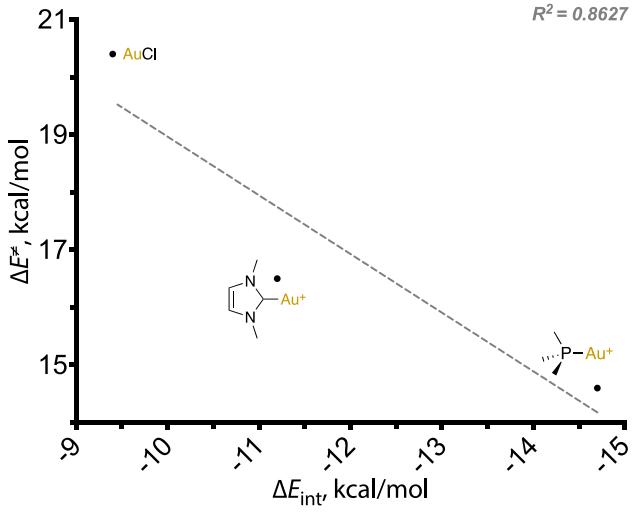
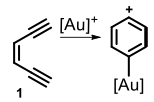
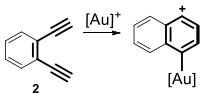
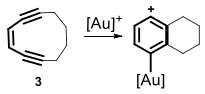
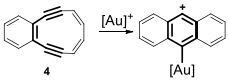


Figure S15: $\Delta E^{\neq}$ vs ΔE_{int} plot for the evaluated catalysts.

Table S3. Computational analysis of the Au-catalyzed and non-catalyzed BC for a broader range of substrates. (IEFPCM=toluene)/(U)PBE0/6-311+G(d,p)/Def2-TZVP+ECP level of theory. (SMD=toluene)/CCSD(T)/6-311++G(d,p)/Def2-TZVP+ECP single point corrections in parenthesis. Energies in kcal/mol.

[a]: relative to isolated reactant and catalyst. [b]: relative to reactant-catalyst complex. [c]: between TS and reactant complex (catalyzed reaction). [d]: between non-catalyzed and catalyzed reactions.

Reaction	E^{comp}[a]	$E_{dist}(comp)$	$E_{int}(comp)$	$\Delta E^{\ddagger}_{cat}$ [b]	$E_{dist}(TS)$	$E_{int}(TS)$	$\Delta E^{b}_{rxn\,cat}$	ΔE_{int} [c]	$\Delta\Delta E^{\ddagger}$ [d]	$\Delta E^{\ddagger}_{rxn\,noncat}$
 1	-29.4 (-30.5)	4.5 (3.6)	-33.9 (-34.1)	**14.6 (15.8)**	34.0 (31.5)	-48.6 (-47.3)	**-7.3 (-1.7)**	-14.7 (-13.2)	16.4 (13.4)	**31.0 (29.2)**
 2	-32.1	3.2	-35.3	**13.7**	34.4	-52.8	**-0.6**	-17.5	18.2	**31.9**
 3	-37.0	2.9	-39.9	**10.9**	33.0	-59.1	**-6.1**	-19.2	16.7	**27.6**
 4	-33.5	3.1	-36.6	**6.1**	25.8	-53.2	**-7.3**	-16.6	15.5	**21.6**

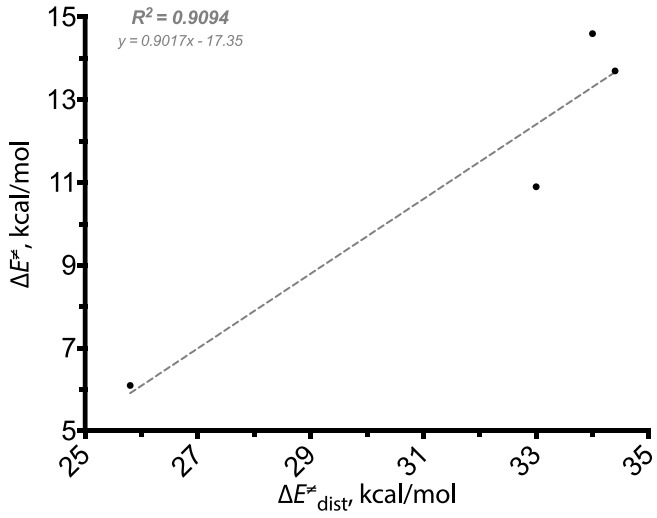
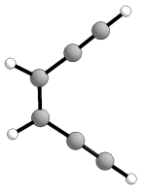


Figure S16: $\Delta E^{\neq}$ vs $\Delta E^{\neq}_{dist}$ plot for the evaluated substrates.

GEOMETRIES

Calculated geometries with their respective energies (in hartree) and number of imaginary frequencies.



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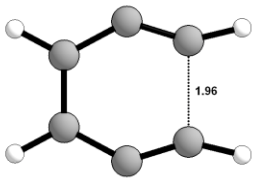
E = -230.652454849
symmetry c1

C	-2.203024000	-1.039340000	-0.000006000
C	-1.482535000	-0.071470000	-0.000003000
C	-0.674108000	1.087280000	0.000000000
H	-1.191846000	2.042585000	0.000002000
C	0.674185000	1.087243000	0.000000000
H	1.191952000	2.042531000	0.000000000
C	1.482523000	-0.071491000	0.000002000
C	2.202959000	-1.039392000	0.000005000
H	2.829362000	-1.901091000	-0.000029000
H	-2.829468000	-1.901007000	0.000037000



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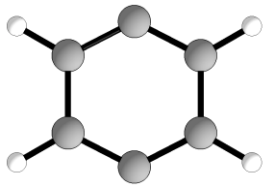
C	0.000000000	-1.220935000	0.698083000
H	0.000000000	-2.177155000	1.208015000
C	0.000000000	-1.220935000	-0.698083000
H	0.000000000	-2.177155000	-1.208015000

C	0.000000000	0.003336000	-1.352512000
C	0.000000000	1.205535000	-0.981475000
H	0.000000000	2.249544000	-1.231148000
H	0.000000000	2.249544000	1.231148000



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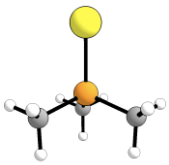
C	0.000000000	-1.330672000	0.000018000
C	1.218877000	-0.707128000	0.000010000
C	1.218877000	0.707128000	-0.000009000
H	-2.160434000	1.246954000	-0.000017000
H	-2.160434000	-1.246954000	0.000016000
H	2.160434000	-1.246954000	0.000017000
H	2.160434000	1.246954000	-0.000016000



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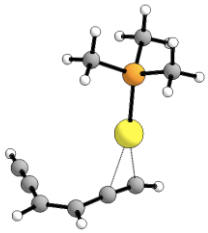
Au	0.938670000	-0.000114000	-0.000139000
P	-1.308517000	-0.000045000	-0.000123000
C	-1.973068000	1.566665000	-0.616938000
H	-1.621764000	1.745506000	-1.634331000
H	-3.065679000	1.516806000	-0.614031000
H	-1.644684000	2.386314000	0.024171000

C	-1.972567000	-0.247987000	1.665226000
H	-3.065370000	-0.238736000	1.620091000
H	-1.633736000	-1.207279000	2.059203000
H	-1.630289000	0.551546000	2.324033000
C	-1.975221000	-1.317607000	-1.047105000
H	-3.067809000	-1.270748000	-1.026572000
H	-1.625894000	-1.191306000	-2.073040000
H	-1.646780000	-2.288826000	-0.673786000



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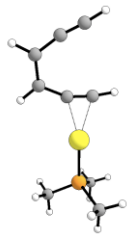
H	-4.055310000	1.104871000	1.939451000
C	-3.620770000	1.432015000	-0.122121000
C	-2.144296000	-1.077569000	0.173315000
C	-1.604599000	-1.684597000	-0.752471000
H	-1.481330000	-2.355056000	-1.580036000
C	-3.726766000	2.083549000	-1.131517000
H	-3.828530000	2.654530000	-2.026769000
Au	0.102217000	-0.480365000	-0.138144000
P	2.158023000	0.533317000	0.124942000
C	2.090009000	2.035324000	1.147193000
H	1.717609000	1.790313000	2.143370000
H	3.091184000	2.466925000	1.230145000
H	1.419227000	2.764153000	0.688963000

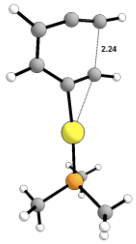
C	2.893021000	1.049509000	-1.453828000
H	3.867500000	1.511029000	-1.273983000
H	3.019333000	0.182918000	-2.105039000
H	2.236607000	1.768427000	-1.947463000
C	3.388763000	-0.543410000	0.916217000
H	4.335242000	-0.007071000	1.022811000
H	3.032615000	-0.848549000	1.901928000
H	3.545449000	-1.435867000	0.307405000



# of imaginary frequencies: 0
E = -827.136791722
symmetry c1

C	2.712994000	1.397032000	0.015052000
H	2.180024000	2.338110000	0.031703000
C	4.064187000	1.335524000	-0.012601000
H	4.652066000	2.247787000	-0.018303000
C	4.709825000	0.084365000	-0.033942000
C	2.019953000	0.157497000	0.020426000
C	1.871182000	-1.067558000	0.014115000
H	1.900651000	-2.137621000	0.014396000
C	5.070566000	-1.066612000	-0.048659000
H	5.466655000	-2.056858000	-0.063541000
Au	-0.165161000	-0.164401000	0.019641000
P	-2.467575000	0.116775000	-0.016043000
C	-2.946620000	1.857896000	-0.218750000
H	-2.545674000	2.244727000	-1.157243000
H	-4.036655000	1.937737000	-0.231019000
H	-2.551329000	2.450563000	0.608048000

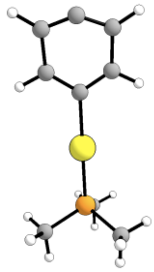
C	-3.297708000	-0.454128000	1.495131000
H	-4.375786000	-0.294932000	1.407436000
H	-3.100978000	-1.517465000	1.643303000
H	-2.917837000	0.098082000	2.356492000
C	-3.261809000	-0.776842000	-1.383750000
H	-4.338945000	-0.592158000	-1.368909000
H	-2.848441000	-0.437271000	-2.335077000
H	-3.077796000	-1.847710000	-1.280429000



# of imaginary frequencies: 1
E = -827.118094816
symmetry c1

C	-2.731907000	1.354363000	-0.000139000
H	-2.280282000	2.337777000	-0.001214000
C	-4.086599000	1.207149000	0.002865000
H	-4.760210000	2.055634000	0.004297000
C	-4.556054000	-0.104378000	0.004018000
C	-1.944974000	0.156660000	-0.001520000
C	-2.350735000	-1.053742000	-0.000427000
H	-2.234930000	-2.120927000	-0.000206000
C	-4.571401000	-1.326566000	0.004093000
H	-4.812841000	-2.367802000	0.004536000
Au	0.146139000	-0.012847000	-0.002639000
P	2.458906000	-0.012450000	0.001618000
C	3.157192000	1.661032000	-0.142139000
H	2.821000000	2.272455000	0.697355000
H	4.249450000	1.616860000	-0.141640000
H	2.815561000	2.122499000	-1.070458000

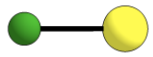
C	3.195140000	-0.964731000	-1.362223000
H	4.285957000	-0.925866000	-1.300232000
H	2.868295000	-2.004527000	-1.301809000
H	2.871516000	-0.550243000	-2.318758000
C	3.183474000	-0.709368000	1.517433000
H	4.274584000	-0.668335000	1.464244000
H	2.841463000	-0.140718000	2.384114000
H	2.867009000	-1.747682000	1.632235000



# of imaginary frequencies: 0
E = -827.155196611
symmetry c1

C	-2.660282000	1.186120000	-0.000487000
H	-2.196837000	2.169848000	-0.001975000
C	-4.102977000	1.245812000	0.003079000
H	-4.644637000	2.180483000	0.004398000
C	-4.512263000	-0.006501000	0.004375000
C	-1.939961000	0.001160000	-0.001698000
C	-2.653470000	-1.187921000	0.000401000
H	-2.184305000	-2.168919000	-0.000655000
C	-4.095801000	-1.256395000	0.003972000
H	-4.631654000	-2.194418000	0.005587000
Au	0.120152000	0.004310000	-0.002870000
P	2.445372000	-0.001719000	0.001615000
C	3.196997000	1.567230000	-0.537211000
H	2.874205000	2.375189000	0.122026000
H	4.287230000	1.492200000	-0.509622000
H	2.877004000	1.799132000	-1.554835000

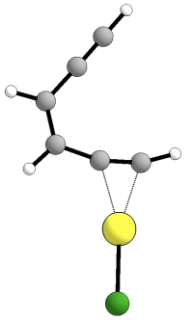
C	3.179123000	-1.263741000	-1.088086000
H	4.270299000	-1.209564000	-1.050242000
H	2.855971000	-2.256542000	-0.768993000
H	2.845065000	-1.102689000	-2.114837000
C	3.175198000	-0.323992000	1.639590000
H	4.266691000	-0.320331000	1.577516000
H	2.851318000	0.445297000	2.343377000
H	2.837677000	-1.295007000	2.007150000



# of imaginary frequencies: 0
E = -595.812585716

symmetry c1

Au	0.000000000	0.000000000	0.395670000
Cl	0.000000000	0.000000000	-1.838700000

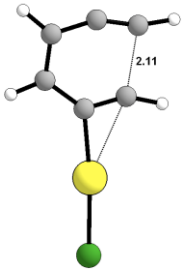


# of imaginary frequencies: 0
E = -826.527040229

symmetry c1

C	-2.081779000	-1.231088000	0.002247000
H	-1.529906000	-2.163036000	0.003844000
C	-3.430811000	-1.254622000	0.000154000
H	-3.928652000	-2.220477000	0.000152000
C	-4.254911000	-0.109782000	-0.001989000
C	-1.341727000	-0.016842000	0.002612000
C	-1.016830000	1.184885000	0.003273000
H	-1.070328000	2.255368000	0.004453000

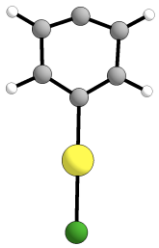
C	-4.981050000	0.853617000	-0.003846000
H	-5.621327000	1.705688000	-0.005476000
Au	0.806251000	0.132652000	0.000345000
Cl	3.005824000	-0.389065000	-0.002642000



# of imaginary frequencies: 1
E = -826.494512288

symmetry c1

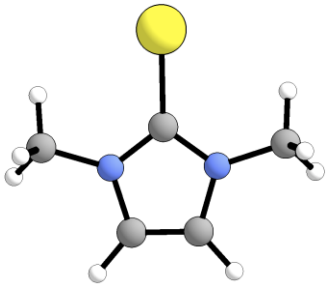
C	-2.121871000	1.353077000	-0.000002000
H	-1.697283000	2.349191000	-0.000007000
C	-3.479443000	1.182789000	0.000000000
H	-4.164656000	2.021181000	-0.000003000
C	-3.911728000	-0.137716000	0.000006000
C	-1.294941000	0.190117000	0.000001000
C	-1.671110000	-1.040279000	0.000004000
H	-1.469747000	-2.095376000	0.000007000
C	-3.761722000	-1.357289000	-0.000006000
H	-3.947289000	-2.410121000	-0.000013000
Au	0.728695000	-0.010807000	0.000000000
Cl	3.009234000	-0.009134000	-0.000001000



# of imaginary frequencies: 0
E = -826.527836430

symmetry c1

C	2.007881000	-1.186744000	-0.000285000
H	1.537367000	-2.167304000	-0.000618000
C	3.451093000	-1.246017000	0.000500000
H	3.979698000	-2.187854000	0.000909000
C	3.887857000	0.000244000	0.000558000
C	1.291931000	-0.000072000	-0.000517000
C	2.007610000	1.186767000	-0.000246000
H	1.536864000	2.167215000	-0.000702000
C	3.450805000	1.246405000	0.000531000
H	3.979161000	2.188382000	0.000753000
Au	-0.713330000	-0.000115000	-0.000217000
Cl	-3.015474000	0.000303000	0.000795000

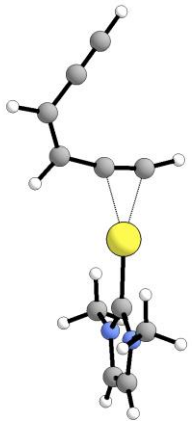


# of imaginary frequencies: 0
E = -440.123024751

symmetry c1

Au	-1.152659000	0.000001000	-0.000023000
C	0.815610000	-0.000003000	-0.017160000
C	2.934620000	0.676931000	0.001407000
C	2.934668000	-0.676903000	0.001403000
H	3.749274000	1.382292000	0.001169000
H	3.749341000	-1.382247000	0.001178000
N	1.619345000	-1.078416000	-0.012627000
N	1.619372000	1.078404000	-0.012624000
C	1.190689000	-2.468324000	0.014163000
H	1.819676000	-3.048899000	-0.659942000
H	1.270144000	-2.864989000	1.027390000

H	0.156594000	-2.525663000	-0.321252000
C	1.190679000	2.468306000	0.014163000
H	1.820196000	3.049038000	-0.659306000
H	0.156849000	2.525732000	-0.322053000
H	1.269351000	2.864739000	1.027542000

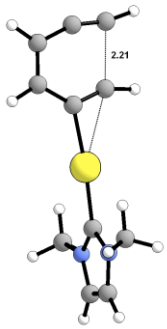


# of imaginary frequencies: 0
E = -670.830566165

symmetry c1

C	-2.818208000	-0.001757000	1.282086000
H	-2.159602000	-0.003373000	2.142088000
C	-4.155946000	0.002075000	1.459852000
H	-4.536727000	0.003400000	2.477723000
C	-5.107643000	0.004354000	0.420452000
C	-2.235691000	-0.003979000	-0.013231000
C	-1.977490000	-0.005914000	-1.221457000
H	-2.027528000	-0.008323000	-2.291736000
C	-5.945277000	0.006179000	-0.447204000
H	-6.688186000	0.007853000	-1.212328000
Au	-0.024538000	-0.002268000	-0.286588000
C	1.965137000	0.001299000	0.081209000
C	4.066264000	-0.671742000	0.449205000
C	4.063562000	0.683600000	0.447663000
H	4.870732000	-1.374659000	0.591740000
H	4.865188000	1.390066000	0.588729000

N	2.772710000	-1.071111000	0.223493000
N	2.768424000	1.077254000	0.221017000
C	2.358112000	-2.462351000	0.147069000
H	2.844321000	-2.948556000	-0.699782000
H	2.625363000	-2.977316000	1.070562000
H	1.278355000	-2.498337000	0.013501000
C	2.348040000	2.466580000	0.141531000
H	2.612235000	2.984475000	1.064290000
H	2.832992000	2.953180000	-0.705814000
H	1.268243000	2.497661000	0.006850000

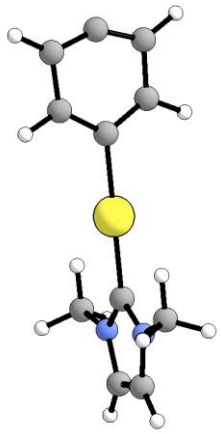


# of imaginary frequencies: 1
E = -670.804261007

symmetry c1

C	2.983507000	-0.110069000	1.347498000
H	2.561831000	-0.186070000	2.341344000
C	4.333186000	-0.095567000	1.159665000
H	5.034201000	-0.157455000	1.983196000
C	4.757822000	0.008737000	-0.162390000
C	2.158277000	-0.017833000	0.181009000
C	2.530006000	0.076956000	-1.038508000
H	2.371029000	0.158304000	-2.097200000
C	4.716090000	0.103892000	-1.381357000
H	4.919170000	0.181898000	-2.427956000
Au	0.085962000	0.004054000	0.007734000
C	-1.945404000	-0.001248000	-0.024274000

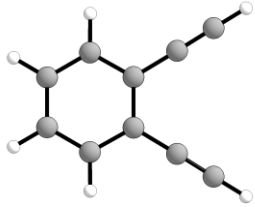
C	-4.082725000	0.674664000	-0.019768000
C	-4.081609000	-0.678383000	-0.065661000
H	-4.899038000	1.378100000	-0.011916000
H	-4.896445000	-1.382937000	-0.102271000
C	-2.336719000	2.456121000	0.081437000
H	-2.658117000	2.895558000	1.027052000
H	-1.249895000	2.486039000	0.022310000
H	-2.761190000	3.020899000	-0.749509000
C	-2.335962000	-2.461842000	-0.068286000
H	-2.470435000	-2.897872000	0.923270000
H	-2.921383000	-3.022643000	-0.797012000
H	-1.283370000	-2.504303000	-0.342726000
N	-2.766103000	1.070490000	0.006418000
N	-2.764782000	-1.073687000	-0.068666000



# of imaginary frequencies: 0
E = -670.840694321
symmetry c1

C	-2.873080000	0.000202000	-1.186548000
H	-2.405678000	0.000400000	-2.168655000
C	-4.315236000	0.000059000	-1.251630000
H	-4.854877000	0.000134000	-2.187375000
C	-4.726776000	-0.000155000	0.000033000
C	-2.152718000	0.000091000	0.000006000
C	-2.873059000	-0.000139000	1.186577000

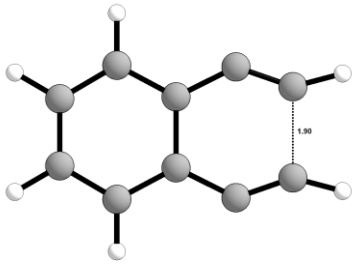
H	-2.405636000	-0.000222000	2.168674000
C	-4.315212000	-0.000307000	1.251689000
H	-4.854835000	-0.000504000	2.187444000
Au	-0.104009000	0.000096000	-0.000018000
C	1.938003000	-0.000037000	-0.000017000
C	4.079577000	0.676375000	0.000094000
C	4.079471000	-0.676787000	0.000000000
H	4.895226000	1.380809000	0.000159000
H	4.895006000	-1.381357000	-0.000016000
N	2.761292000	1.071313000	0.000079000
N	2.761123000	-1.071516000	-0.000069000
C	2.329880000	2.457542000	0.000127000
H	2.701996000	2.964621000	-0.891555000
H	1.241008000	2.478583000	0.000022000
H	2.701825000	2.964512000	0.891943000
C	2.329510000	-2.457682000	-0.000135000
H	1.240638000	-2.478572000	-0.000313000
H	2.701615000	-2.964762000	-0.891822000
H	2.701323000	-2.964761000	0.891675000



# of imaginary frequencies: 0
E = -384.162871657
symmetry c1

C	-1.294722000	-1.439319000	0.000081000
C	-1.296151000	1.438745000	-0.000081000
C	-2.320324000	2.074110000	-0.000126000
H	-3.229936000	2.628464000	-0.000177000
C	-2.318507000	-2.075268000	0.000196000
H	-3.227769000	-2.630192000	0.000310000

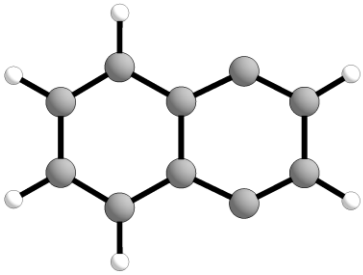
C	-0.075890000	0.706746000	-0.000003000
C	1.146326000	-1.389396000	-0.000271000
C	2.346307000	-0.695422000	-0.000059000
H	3.283590000	-1.241403000	-0.000054000
C	2.345899000	0.696720000	0.000179000
H	3.282863000	1.243261000	0.000426000
C	1.145492000	1.389972000	0.000117000
H	1.136334000	2.474082000	0.000130000
H	1.137861000	-2.473512000	-0.000539000
C	-0.075589000	-0.707004000	-0.000050000



# of imaginary frequencies: 1
E = -384.108836508
symmetry c1

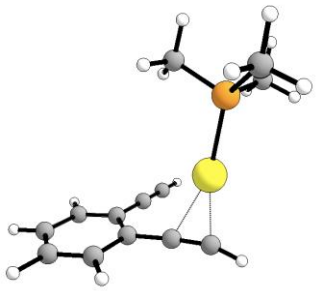
C	2.470242000	-0.948492000	0.000000000
C	1.281124000	-1.360170000	-0.000012000
C	0.029735000	-0.737680000	-0.000005000
C	0.029734000	0.737680000	-0.000011000
C	1.281123000	1.360171000	0.000002000
C	2.470241000	0.948492000	0.000013000
H	3.508900000	1.221258000	0.000029000
H	3.508902000	-1.221255000	-0.000006000
C	-1.207014000	1.393917000	-0.000004000
C	-2.401044000	0.696781000	-0.000001000
H	-3.339323000	1.241197000	-0.000021000
C	-2.401043000	-0.696782000	0.000009000
H	-3.339326000	-1.241192000	0.000051000
C	-1.207012000	-1.393918000	0.000003000

H	-1.207833000	-2.477269000	0.000000000
H	-1.207835000	2.477268000	-0.000008000



# of imaginary frequencies: 0
E = -384.143934523
symmetry cs

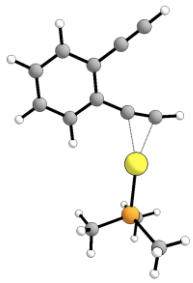
C	2.492101000	0.713458000	0.000000000
C	1.283061000	1.323903000	0.000000000
C	0.020644000	0.718186000	0.000000000
C	0.020643000	-0.718184000	0.000000000
C	1.283061000	-1.323901000	0.000000000
C	2.492101000	-0.713455000	0.000000000
H	3.425047000	-1.269433000	0.000000000
H	3.425048000	1.269435000	0.000000000
C	-1.215054000	1.406759000	0.000000000
C	-2.393593000	0.706177000	0.000000000
H	-3.338584000	1.239340000	0.000000000
C	-2.393593000	-0.706181000	0.000000000
H	-3.338583000	-1.239344000	0.000000000
C	-1.215052000	-1.406761000	0.000000000
H	-1.209420000	-2.491694000	0.000000000
H	-1.209425000	2.491692000	0.000000000



# of imaginary frequencies: 0
E = -980.656660303
symmetry c1

C	2.346022000	-1.972687000	-0.621188000
C	1.462544000	0.695946000	-1.191639000
C	0.636133000	0.945522000	-2.069421000
H	0.240789000	1.213804000	-3.029176000
C	1.864583000	-2.930629000	-1.171161000
H	1.452735000	-3.781536000	-1.664132000
Au	-0.751132000	0.322477000	-0.511909000
P	-2.562413000	-0.238559000	0.801474000
C	-2.080894000	-0.969156000	2.395194000
H	-1.470353000	-0.259966000	2.956894000
H	-2.975219000	-1.214349000	2.974190000
H	-1.499514000	-1.877053000	2.224821000
C	-3.655784000	-1.456423000	0.011923000
H	-4.499544000	-1.683263000	0.668847000
H	-4.030535000	-1.059003000	-0.933011000
H	-3.098085000	-2.372835000	-0.189024000
C	-3.615717000	1.184539000	1.210402000
H	-4.448651000	0.865173000	1.842267000
H	-3.028045000	1.936324000	1.740144000
H	-4.007710000	1.627457000	0.292995000
C	2.486501000	0.461844000	-0.234391000
C	3.961185000	-1.036679000	0.958387000
C	4.536378000	0.052813000	1.597243000

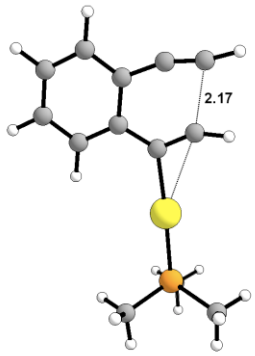
H	5.338669000	-0.109331000	2.308680000
C	4.094872000	1.346579000	1.331094000
H	4.550720000	2.193426000	1.830970000
C	3.071403000	1.552142000	0.421270000
H	2.719141000	2.553396000	0.200978000
H	4.308681000	-2.042010000	1.165090000
C	2.929857000	-0.855062000	0.033654000



# of imaginary frequencies: 0
E = -980.652845924
symmetry c1

C	-4.202821000	-1.380252000	-0.019493000
C	-1.442905000	-0.795592000	0.016481000
C	-0.870338000	-1.885610000	0.022865000
H	-0.598735000	-2.921738000	0.031715000
C	-4.596361000	-2.518879000	-0.029251000
H	-4.953021000	-3.523501000	-0.038056000
Au	0.815172000	-0.481655000	0.008946000
P	2.931368000	0.454590000	-0.010822000
C	2.900010000	2.260916000	-0.209194000
H	2.359785000	2.715596000	0.623005000
H	3.924120000	2.643292000	-0.225858000
H	2.402622000	2.524625000	-1.144208000
C	3.963569000	-0.174863000	-1.366983000
H	4.944033000	0.307802000	-1.341743000
H	4.089695000	-1.253978000	-1.262110000
H	3.482074000	0.031133000	-2.324621000

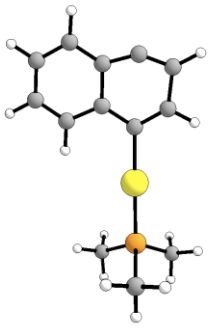
C	3.865826000	0.138438000	1.514356000
H	4.851665000	0.605906000	1.450554000
H	3.325600000	0.548102000	2.369775000
H	3.985787000	-0.937146000	1.655910000
C	-2.376533000	0.285082000	0.008495000
C	-4.682440000	1.015597000	-0.014037000
C	-4.260603000	2.336393000	-0.003809000
H	-4.996053000	3.133156000	-0.008196000
C	-2.902657000	2.640858000	0.011927000
H	-2.573811000	3.673701000	0.019652000
C	-1.966354000	1.619857000	0.018054000
H	-0.906274000	1.848611000	0.029991000
H	-5.739121000	0.775325000	-0.026569000
C	-3.756304000	-0.031782000	-0.008353000



# of imaginary frequencies: 1
E = -980.630970861
symmetry c1

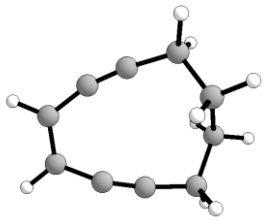
C	3.704834000	-1.670418000	0.004988000
C	1.298790000	-0.621196000	-0.002296000
C	1.384711000	-1.899809000	-0.000874000
H	0.935435000	-2.875114000	-0.000464000
C	3.343340000	-2.836822000	0.005502000
H	3.248725000	-3.901230000	0.006536000
Au	-0.761641000	-0.229037000	-0.004566000
P	-3.008133000	0.320532000	0.001910000

C	-3.337002000	1.979624000	0.671975000
H	-2.824976000	2.731001000	0.067912000
H	-4.411640000	2.180007000	0.663510000
H	-2.966689000	2.041500000	1.696993000
C	-4.027561000	-0.804736000	1.004696000
H	-5.072711000	-0.485403000	0.979003000
H	-3.950222000	-1.820080000	0.611382000
H	-3.673182000	-0.800542000	2.037203000
C	-3.770043000	0.310660000	-1.649950000
H	-4.824809000	0.589489000	-1.580284000
H	-3.251400000	1.018108000	-2.299559000
H	-3.688292000	-0.687084000	-2.085040000
C	2.398745000	0.314001000	-0.000772000
C	4.841108000	0.538696000	0.004728000
C	4.697198000	1.916557000	0.002302000
H	5.579660000	2.546185000	0.003418000
C	3.428974000	2.494329000	-0.001610000
H	3.329963000	3.574091000	-0.003525000
C	2.289492000	1.702960000	-0.002933000
H	1.307491000	2.161048000	-0.005945000
H	5.823843000	0.083403000	0.007775000
C	3.702487000	-0.268751000	0.003107000



# of imaginary frequencies: 0
E = -980.653852895
symmetry c1

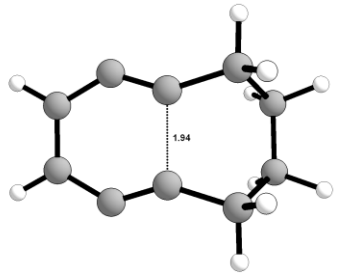
C	1.584385000	-2.103694000	-0.000391000
H	0.842807000	-2.898036000	-0.000969000
C	2.958376000	-2.643614000	0.001245000
H	3.154562000	-3.705374000	0.002054000
C	3.725597000	-1.597756000	0.001036000
C	1.280349000	-0.772242000	-0.001276000
C	2.341567000	0.173141000	-0.000927000
C	3.769604000	-0.257776000	0.000752000
Au	-0.716601000	-0.234753000	-0.000662000
P	-2.966637000	0.338826000	0.002023000
C	-4.056295000	-0.936212000	-0.708696000
H	-3.949844000	-1.867442000	-0.149082000
H	-5.098340000	-0.607828000	-0.669545000
H	-3.774466000	-1.119176000	-1.747424000
C	-3.349446000	1.844655000	-0.949398000
H	-4.421757000	2.054244000	-0.911276000
H	-2.801568000	2.692969000	-0.534361000
H	-3.045335000	1.708053000	-1.988986000
C	-3.648516000	0.656767000	1.661066000
H	-4.707334000	0.920056000	1.591649000
H	-3.537780000	-0.235433000	2.280415000
H	-3.102487000	1.476286000	2.132318000
C	2.170728000	1.576922000	-0.001793000
C	3.215479000	2.464723000	-0.000977000
H	3.011443000	3.529283000	-0.001763000
C	4.547173000	2.013157000	0.000773000
H	5.362123000	2.727789000	0.001435000
C	4.825834000	0.673512000	0.001576000
H	5.842352000	0.302452000	0.002857000
H	1.147620000	1.935758000	-0.003337000



# of imaginary frequencies: 0
E = -386.562439359

symmetry c1

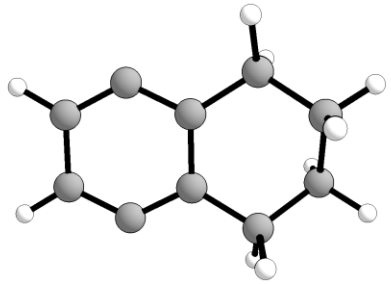
C	-0.144673000	1.673439000	-0.108690000
C	-1.313124000	1.356921000	-0.121321000
C	-2.551222000	0.675117000	-0.068743000
C	-2.551509000	-0.674510000	0.068789000
C	-1.313669000	-1.356802000	0.121185000
C	-0.145241000	-1.673439000	0.108726000
C	1.292522000	1.865263000	-0.003072000
H	1.501910000	2.688693000	0.689762000
C	1.291933000	-1.865474000	0.003283000
H	1.501273000	-2.689172000	-0.689247000
C	2.002118000	-0.591229000	-0.494570000
H	3.034326000	-0.866261000	-0.733310000
C	2.002556000	0.590787000	0.494362000
H	1.537477000	0.290064000	1.439072000
H	1.704395000	-2.170888000	0.973183000
H	1.536636000	-0.290374000	-1.439036000
H	3.034971000	0.865502000	0.732582000
H	1.705080000	2.170985000	-0.972838000
H	-3.487367000	-1.220940000	0.126761000
H	-3.486847000	1.221959000	-0.126624000



# of imaginary frequencies: 1
E = -386.518508657

symmetry c1

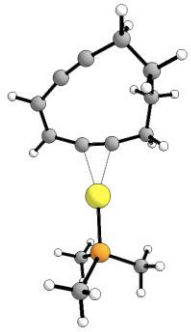
C	0.190934000	0.969602000	-0.246443000
C	1.382929000	1.351953000	-0.026337000
C	2.582334000	0.693408000	0.199043000
C	2.577663000	-0.702444000	0.210917000
C	1.373796000	-1.356617000	-0.003203000
C	0.185277000	-0.969429000	-0.233434000
C	-1.207100000	1.382534000	-0.481969000
H	-1.503263000	1.120176000	-1.505396000
C	-1.210466000	-1.375063000	-0.492499000
H	-1.250106000	-2.466034000	-0.439212000
C	-2.219075000	-0.767901000	0.488957000
H	-2.015410000	-1.168631000	1.485445000
C	-2.192722000	0.771527000	0.519877000
H	-3.186850000	1.172002000	0.301431000
H	3.515177000	-1.216494000	0.390542000
H	3.523039000	1.204221000	0.371086000
H	-1.240215000	2.473212000	-0.419057000
H	-1.926409000	1.125259000	1.519415000
H	-3.213639000	-1.125089000	0.206233000
H	-1.483737000	-1.104036000	-1.519946000



# of imaginary frequencies: 0
E = -386.563229394

symmetry c2

C	-0.000067000	0.707415000	2.621131000
C	-0.001669000	1.316872000	1.398628000
C	0.000067000	0.711596000	0.163229000
C	-0.000067000	-0.711596000	0.163229000
C	0.001669000	-1.316872000	1.398628000
C	0.000067000	-0.707415000	2.621131000
C	-0.021677000	1.497858000	-1.126521000
C	0.373290000	0.663530000	-2.338240000
H	1.453930000	0.472309000	-2.320619000
C	-0.373290000	-0.663530000	-2.338240000
H	-0.167057000	-1.226723000	-3.253564000
C	0.021677000	-1.497858000	-1.126521000
H	-0.630918000	-2.369801000	-1.023184000
H	-1.036441000	1.891974000	-1.270226000
H	-0.000503000	-1.255035000	3.558230000
H	0.000503000	1.255035000	3.558230000
H	0.630918000	2.369801000	-1.023184000
H	0.167057000	1.226723000	-3.253564000
H	-1.453930000	-0.472309000	-2.320619000
H	1.036441000	-1.891974000	-1.270226000

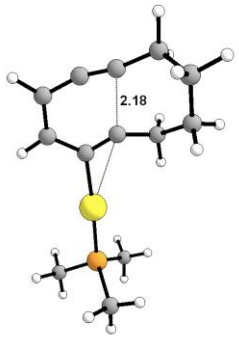


# of imaginary frequencies: 0
E = -983.063330433

symmetry c1

C	1.380077000	-0.378737000	-0.404842000
C	1.259927000	0.854473000	-0.374493000
C	1.562302000	2.245553000	-0.322525000
C	2.831295000	2.632786000	-0.052091000
C	3.828161000	1.672417000	0.203232000
C	4.513290000	0.697494000	0.411911000
C	1.823872000	-1.764505000	-0.583824000
H	1.378615000	-2.146265000	-1.509101000
C	5.151475000	-0.582594000	0.651631000
H	5.689924000	-0.557004000	1.605231000
C	4.102941000	-1.707430000	0.669451000
H	4.610432000	-2.637542000	0.939632000
C	3.356778000	-1.890460000	-0.664563000
H	3.724641000	-1.179788000	-1.411302000
Au	-0.797128000	0.071516000	-0.101677000
P	-3.077827000	-0.157574000	0.207388000
C	-3.644631000	0.355788000	1.855838000
H	-3.410672000	1.409844000	2.015127000
H	-4.724016000	0.207629000	1.942953000
H	-3.136306000	-0.235660000	2.619567000
C	-3.633781000	-1.877597000	0.010120000
H	-4.715086000	-1.934784000	0.161101000

H	-3.390675000	-2.231850000	-0.993277000
H	-3.133909000	-2.515146000	0.741498000
C	-4.056277000	0.808846000	-0.980738000
H	-3.797088000	0.509474000	-1.997861000
H	-5.123179000	0.638258000	-0.814505000
H	-3.838299000	1.871532000	-0.861111000
H	5.905387000	-0.771907000	-0.122137000
H	3.392921000	-1.498124000	1.476626000
H	3.558964000	-2.887392000	-1.065125000
H	1.437138000	-2.387669000	0.229621000
H	3.074855000	3.690760000	-0.034534000
H	0.784279000	2.973316000	-0.515407000

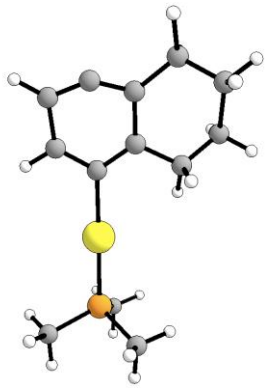


# of imaginary frequencies: 1
E = -983.045991591

symmetry c1

C	2.031651000	0.025369000	0.257350000
C	1.153225000	-0.908920000	0.033328000
C	1.475923000	-2.291688000	-0.189905000
C	2.789881000	-2.645662000	-0.169827000
C	3.665902000	-1.590033000	0.053180000
C	4.153901000	-0.474808000	0.214842000
C	2.279929000	1.410018000	0.676948000
H	2.755542000	1.402907000	1.664560000
C	4.974724000	0.723368000	0.268671000
H	5.995380000	0.436042000	-0.002412000

C	4.428004000	1.776732000	-0.704323000
H	4.372710000	1.320658000	-1.696054000
C	3.057110000	2.319427000	-0.285477000
H	3.175434000	3.276329000	0.230730000
Au	-0.827638000	-0.237053000	0.010329000
P	-3.055104000	0.370825000	-0.027318000
C	-3.572724000	1.237973000	-1.541526000
H	-3.396841000	0.600560000	-2.409907000
H	-4.635831000	1.487104000	-1.484400000
H	-2.992825000	2.155367000	-1.658826000
C	-3.538973000	1.480858000	1.332232000
H	-4.604613000	1.715649000	1.265588000
H	-3.333470000	1.001191000	2.290893000
H	-2.962481000	2.406045000	1.272656000
C	-4.179619000	-1.054945000	0.100072000
H	-3.995289000	-1.588668000	1.034438000
H	-5.219332000	-0.718346000	0.074019000
H	-4.000524000	-1.737420000	-0.733034000
H	3.139446000	-3.655782000	-0.343089000
H	0.706513000	-3.031054000	-0.373730000
H	1.280580000	1.829542000	0.839061000
H	2.446942000	2.513364000	-1.170950000
H	5.148610000	2.594673000	-0.772632000
H	5.016410000	1.110503000	1.293489000

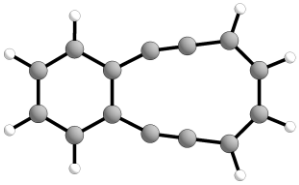


# of imaginary frequencies: 0
E = -983.073092180

symmetry c1

C	1.417926000	-2.230087000	0.063822000
C	1.176761000	-0.861306000	0.016461000
C	2.265449000	0.021266000	0.001369000
C	3.648442000	-0.412238000	-0.033807000
C	3.526522000	-1.723015000	0.031887000
C	2.748694000	-2.789562000	0.072193000
C	2.047880000	1.516432000	0.179579000
C	3.278901000	2.410829000	0.341660000
H	3.495234000	2.590215000	1.399198000
C	4.524602000	1.922098000	-0.384153000
H	5.365794000	2.527393000	-0.033391000
C	4.872034000	0.471317000	-0.087054000
H	5.492876000	0.072275000	-0.895146000
H	1.427388000	1.836888000	-0.665305000
Au	-0.794847000	-0.243458000	-0.002241000
P	-3.031992000	0.381812000	-0.024900000
C	-3.655229000	0.948967000	1.591382000
H	-3.082377000	1.817310000	1.921825000
H	-4.712799000	1.218231000	1.527158000
H	-3.530894000	0.151869000	2.327649000
C	-4.170825000	-0.958994000	-0.504737000
H	-5.204593000	-0.602755000	-0.499287000
H	-3.918265000	-1.314661000	-1.505723000
H	-4.072816000	-1.792148000	0.193706000
C	-3.424176000	1.739983000	-1.175600000
H	-3.150075000	1.449645000	-2.191725000
H	-4.492188000	1.970575000	-1.144109000
H	-2.854467000	2.630431000	-0.902222000

H	2.970653000	-3.840330000	-0.014103000
H	0.644827000	-2.989867000	-0.012052000
H	1.407786000	1.610722000	1.059489000
H	3.026804000	3.393863000	-0.062536000
H	4.466873000	2.093246000	-1.462552000
H	5.451132000	0.348945000	0.831654000

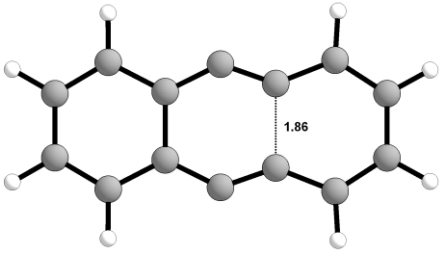


# of imaginary frequencies: 0
E = -537.639167232

symmetry c1

C	1.204829000	1.506757000	0.000000000
C	-0.006634000	1.350560000	0.000000000
C	-1.251935000	0.719414000	0.000000000
C	-1.251357000	-0.718633000	0.000000000
C	-0.005710000	-1.348982000	0.000000000
C	1.205574000	-1.506376000	0.000000000
C	-2.484230000	1.401230000	0.000000000
C	-3.670502000	0.701381000	0.000000000
H	-4.612682000	1.238948000	0.000000000
C	-3.669913000	-0.702973000	0.000000000
H	-4.611606000	-1.241382000	0.000000000
C	-2.482972000	-1.401647000	0.000000000
H	-2.478515000	-2.485736000	0.000000000
H	-2.480858000	2.485331000	0.000000000
C	2.580601000	1.677609000	0.000000000
H	2.930450000	2.708123000	-0.000001000
C	2.581231000	-1.677879000	0.000000000
H	2.930971000	-2.708435000	0.000001000
C	3.558498000	-0.713987000	0.000000000

H	4.564720000	-1.126094000	0.000000000
C	3.558090000	0.713970000	0.000000000
H	4.564099000	1.126584000	0.000000000

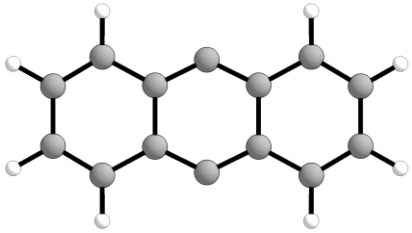


# of imaginary frequencies: 1
E = -537.604651887

symmetry c1

C	-1.208646000	0.930727000	-0.000004000
C	0.011658000	1.358744000	-0.000011000
C	1.233513000	0.752028000	-0.000005000
C	1.233511000	-0.752027000	0.000002000
C	0.011657000	-1.358747000	0.000013000
C	-1.208647000	-0.930727000	0.000000000
C	2.491928000	1.401413000	0.000000000
C	3.671477000	0.704135000	0.000003000
H	4.612726000	1.243197000	0.000009000
C	3.671477000	-0.704136000	-0.000001000
H	4.612725000	-1.243199000	-0.000002000
C	2.491927000	-1.401413000	-0.000002000
H	2.495832000	-2.484623000	-0.000004000
H	2.495834000	2.484624000	0.000001000
C	-2.519611000	1.446585000	0.000004000
H	-2.584318000	2.529679000	0.000008000
C	-2.519612000	-1.446584000	-0.000005000
H	-2.584320000	-2.529678000	-0.000012000
C	-3.665031000	-0.706740000	-0.000003000
H	-4.615957000	-1.228440000	-0.000007000
C	-3.665030000	0.706742000	0.000006000

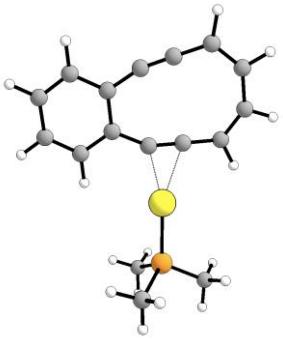
H	-4.615956000	1.228442000	0.000012000



# of imaginary frequencies: 0
E = -537.639716176

symmetry cs

C	-0.732406000	-1.233264000	0.000000000
C	-1.340352000	-0.000001000	0.000000000
C	-0.732405000	1.233264000	0.000000000
C	0.732357000	1.233326000	0.000000000
C	1.340396000	0.000000000	0.000000000
C	0.732356000	-1.233326000	0.000000000
C	1.409400000	2.486087000	0.000000000
C	0.709938000	3.658370000	0.000000000
H	1.241871000	4.603864000	0.000000000
C	-0.709947000	3.658309000	0.000000000
H	-1.241860000	4.603819000	0.000000000
C	-1.409372000	2.486019000	0.000000000
H	-2.493846000	2.484769000	0.000000000
C	1.409400000	-2.486086000	0.000000000
C	0.709939000	-3.658369000	0.000000000
H	1.241874000	-4.603864000	0.000000000
C	-0.709947000	-3.658309000	0.000000000
H	-1.241859000	-4.603821000	0.000000000
C	-1.409372000	-2.486020000	0.000000000
H	-2.493847000	-2.484771000	0.000000000
H	2.493880000	2.484829000	0.000000000
H	2.493878000	-2.484827000	0.000000000

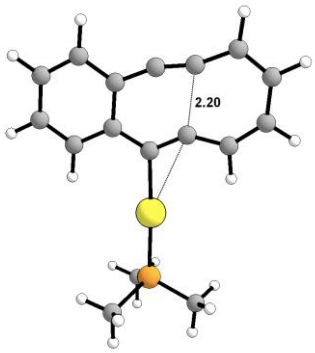


# of imaginary frequencies: 0
E = -1134.13451684

symmetry c1

C	1.107709000	-1.144122000	-0.069354000
C	1.138950000	0.110255000	-0.053851000
C	1.790091000	1.361199000	-0.034696000
C	3.220839000	1.350305000	0.025036000
C	3.854787000	0.111887000	0.055391000
C	4.126235000	-1.076439000	0.072992000
C	1.116655000	2.595818000	-0.067808000
C	1.824271000	3.776607000	-0.043713000
H	1.293736000	4.721742000	-0.071715000
C	3.226466000	3.767083000	0.016951000
H	3.770948000	4.704442000	0.036539000
C	3.914589000	2.575652000	0.050886000
H	4.996991000	2.559563000	0.097174000
H	0.033683000	2.608140000	-0.114219000
C	1.085897000	-2.538315000	-0.099527000
H	0.087255000	-2.961346000	-0.176414000
C	4.420915000	-2.427134000	0.094039000
H	5.472152000	-2.698469000	0.155675000
C	3.512684000	-3.449543000	0.040649000
H	3.951442000	-4.442757000	0.066212000
C	2.092071000	-3.472069000	-0.050646000
H	1.701776000	-4.485214000	-0.094736000

Au	-1.016683000	-0.184011000	-0.027305000
P	-3.314698000	0.070929000	0.044970000
C	-3.884549000	0.878663000	1.569309000
H	-3.440707000	1.872752000	1.649295000
H	-4.973674000	0.968797000	1.552958000
H	-3.582947000	0.288531000	2.436395000
C	-4.211542000	-1.508366000	-0.039636000
H	-5.287627000	-1.320355000	0.005792000
H	-3.973750000	-2.020782000	-0.973563000
H	-3.921047000	-2.144555000	0.798338000
C	-3.967903000	1.081538000	-1.316541000
H	-3.726553000	0.614517000	-2.272950000
H	-5.053075000	1.173638000	-1.220807000
H	-3.519154000	2.076203000	-1.288316000

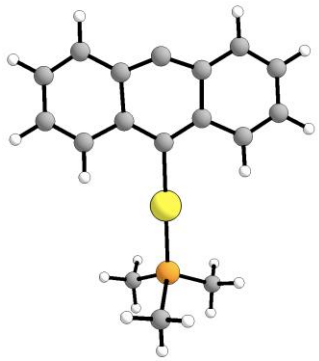


# of imaginary frequencies: 1
E = -1134.12486191

symmetry c1

C	-1.632517000	-1.084229000	0.005533000
C	-1.066662000	0.107285000	0.007200000
C	-1.749159000	1.351051000	0.003838000
C	-3.185690000	1.307045000	-0.003692000
C	-3.702732000	0.034748000	-0.005950000
C	-3.827798000	-1.198429000	-0.007277000
C	-1.132938000	2.617366000	0.006858000
C	-1.888632000	3.766690000	0.002483000

H	-1.396043000	4.732669000	0.005040000
C	-3.293954000	3.707149000	-0.005427000
H	-3.871020000	4.624920000	-0.009046000
C	-3.942645000	2.496170000	-0.008445000
H	-5.024287000	2.440403000	-0.014431000
H	-0.050305000	2.671784000	0.012751000
C	-1.354105000	-2.455464000	0.009419000
H	-0.277580000	-2.619691000	0.018148000
C	-4.345074000	-2.486998000	-0.011113000
H	-5.427681000	-2.568250000	-0.018335000
C	-3.559643000	-3.598428000	-0.006049000
H	-4.044724000	-4.568013000	-0.009722000
C	-2.144984000	-3.567527000	0.004425000
H	-1.628057000	-4.520258000	0.009359000
Au	1.031557000	-0.032315000	0.007131000
P	3.339031000	-0.076315000	-0.006147000
C	4.071767000	1.001193000	-1.276304000
H	3.755341000	2.033080000	-1.113506000
H	5.162628000	0.946617000	-1.230220000
H	3.734818000	0.684755000	-2.265206000
C	4.033286000	-1.728069000	-0.329350000
H	5.125635000	-1.681888000	-0.337707000
H	3.708685000	-2.422041000	0.448380000
H	3.680128000	-2.092877000	-1.295723000
C	4.094524000	0.454810000	1.561176000
H	3.760469000	-0.196877000	2.370482000
H	5.184092000	0.409019000	1.484762000
H	3.791135000	1.478047000	1.789891000

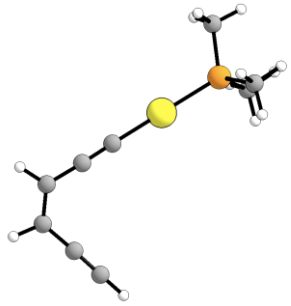


# of imaginary frequencies: 0
E = -1134.14618167

symmetry c1

C	-1.813934000	1.215016000	0.111894000
C	-1.105027000	0.000047000	0.114918000
C	-1.813198000	-1.215329000	0.112199000
C	-3.297585000	-1.257555000	-0.010090000
C	-3.725395000	-0.000769000	0.147000000
C	-3.298324000	1.256272000	-0.010234000
C	-1.199683000	-2.493529000	0.207305000
C	-1.890697000	-3.664606000	0.064608000
H	-1.365516000	-4.610402000	0.129635000
C	-3.285196000	-3.656598000	-0.160149000
H	-3.813739000	-4.593651000	-0.294320000
C	-3.983992000	-2.483291000	-0.176666000
H	-5.055647000	-2.461737000	-0.328092000
H	-0.133260000	-2.505265000	0.407900000
C	-1.201183000	2.493593000	0.206925000
H	-0.134693000	2.506124000	0.407353000
C	-3.985553000	2.481544000	-0.176788000
H	-5.057220000	2.459297000	-0.328030000
C	-3.287487000	3.655292000	-0.160527000
H	-3.816643000	4.591994000	-0.294736000
C	-1.892960000	3.664209000	0.064017000
H	-1.368361000	4.610345000	0.128814000

Au	0.963780000	0.000849000	0.015368000
P	3.286245000	0.000326000	-0.058060000
C	4.072070000	-0.331704000	1.551931000
H	3.757021000	-1.310028000	1.920103000
H	5.160815000	-0.315912000	1.453890000
H	3.763698000	0.426428000	2.274552000
C	4.013887000	1.577198000	-0.607739000
H	5.104774000	1.506546000	-0.616383000
H	3.659906000	1.817023000	-1.612222000
H	3.710367000	2.377919000	0.069291000
C	3.989626000	-1.248850000	-1.182424000
H	3.618801000	-1.081614000	-2.195486000
H	5.081254000	-1.188392000	-1.182019000
H	3.683894000	-2.246261000	-0.860487000

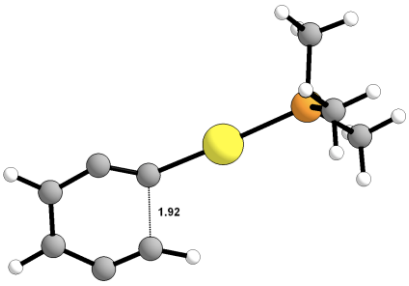


# of imaginary frequencies: 0
E = -826.730696481

symmetry c1

C	4.973248000	2.258163000	0.001741000
C	5.052327000	1.052985000	-0.001763000
C	5.188703000	-0.353212000	-0.005926000
H	6.202646000	-0.743772000	-0.009931000
C	4.158579000	-1.229488000	-0.005260000
H	4.406136000	-2.289440000	-0.008831000
C	2.789258000	-0.899689000	-0.000727000
C	1.589401000	-0.656524000	0.002779000
H	4.887846000	3.319519000	0.004938000
Au	-0.349272000	-0.227904000	0.003470000
P	-2.601623000	0.281468000	-0.002326000
C	-3.108608000	1.419224000	-1.335107000
H	-2.868835000	0.974722000	-2.303055000
H	-4.181982000	1.621026000	-1.283264000

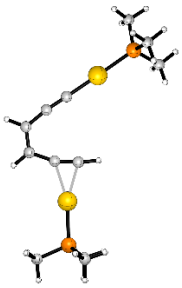
H	-2.557568000	2.357091000	-1.241367000
C	-3.198459000	1.089480000	1.520338000
H	-4.266383000	1.312378000	1.446034000
H	-3.022862000	0.432005000	2.374106000
H	-2.644164000	2.016381000	1.680294000
C	-3.705905000	-1.156569000	-0.203388000
H	-4.753302000	-0.842663000	-0.198877000
H	-3.481274000	-1.658209000	-1.146755000
H	-3.534666000	-1.862857000	0.611330000



# of imaginary frequencies: 1
E = -826.679406705

symmetry c1

C	2.744415000	-1.429762000	0.001141000
C	4.013991000	-1.321267000	-0.000677000
C	4.820545000	-0.187476000	-0.002467000
H	5.904849000	-0.222181000	-0.003720000
C	4.211351000	1.073604000	-0.002377000
H	4.843646000	1.954671000	-0.003594000
C	2.829862000	1.106276000	-0.000639000
C	1.864502000	0.280656000	0.001184000
H	1.931653000	-2.129757000	0.002564000
Au	-0.143374000	0.086862000	0.001217000
P	-2.445693000	-0.056454000	-0.001398000
C	-3.201513000	0.029249000	-1.658638000
H	-2.822603000	-0.788849000	-2.274341000
H	-4.290590000	-0.040945000	-1.590842000
H	-2.927239000	0.972895000	-2.134260000
C	-3.272704000	1.269185000	0.938693000
H	-4.358872000	1.148671000	0.901815000
H	-2.939433000	1.240043000	1.977970000
H	-3.000414000	2.238807000	0.517081000
C	-3.112012000	-1.595912000	0.714876000
H	-4.205052000	-1.592787000	0.684597000
H	-2.736938000	-2.452429000	0.151176000
H	-2.777724000	-1.690754000	1.749837000

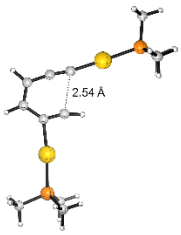


# of imaginary frequencies: 0
E = -1423.22956941

symmetry c1

C	-1.377501000	1.980103000	0.001086000
H	-2.241304000	2.633599000	0.001970000
C	-0.125348000	2.503075000	0.000732000
H	-0.047024000	3.588876000	0.001329000
C	1.071160000	1.775991000	-0.000153000
C	-1.587822000	0.581870000	0.000349000
C	-1.577444000	-0.652647000	0.000344000
H	-1.299021000	-1.686292000	0.000844000
C	2.144156000	1.183602000	-0.000863000
Au	-3.725299000	-0.220057000	-0.002401000
P	-6.032984000	-0.304485000	-0.002037000
C	-6.787142000	1.048211000	0.950169000
H	-6.510823000	2.008765000	0.511422000
H	-7.875636000	0.946395000	0.942100000
H	-6.429140000	1.015566000	1.980836000
C	-6.676704000	-1.836641000	0.734779000
H	-7.769644000	-1.820886000	0.725634000
H	-6.323924000	-2.698019000	0.164828000
H	-6.324654000	-1.926507000	1.763951000
C	-6.763330000	-0.211138000	-1.663304000
H	-7.853523000	-0.258287000	-1.598989000
H	-6.469281000	0.724723000	-2.141762000
H	-6.400724000	-1.042765000	-2.270171000
Au	3.913568000	0.280003000	-0.001110000
P	5.997350000	-0.730784000	0.000854000
C	6.035875000	-2.390353000	-0.753005000
H	7.045485000	-2.807727000	-0.709500000
H	5.348474000	-3.050606000	-0.220443000
H	5.715714000	-2.325674000	-1.794853000
C	6.704456000	-0.970362000	1.663759000
H	7.686535000	-1.445788000	1.596267000
H	6.803369000	-0.003316000	2.160762000
H	6.038193000	-1.598040000	2.258610000
C	7.271512000	0.208610000	-0.902661000
H	7.374964000	1.201134000	-0.459837000

H	8.233408000	-0.309290000	-0.860268000
H	6.968613000	0.325579000	-1.944980000

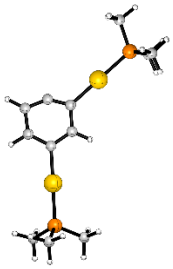


# of imaginary frequencies: 1
E = -1423.21615836

symmetry c1

C	-1.417241000	2.864273000	0.003663000
H	-2.298946000	3.490268000	0.005848000
C	-0.157785000	3.380901000	0.003791000
H	0.004329000	4.453963000	0.006121000
C	0.925790000	2.498323000	0.001028000
C	-1.490206000	1.433602000	0.000421000
C	-0.575992000	0.557490000	-0.002248000
H	-0.048917000	-0.373502000	-0.004913000
C	1.751505000	1.580847000	-0.001309000
Au	-3.155687000	0.152803000	-0.000364000
P	-5.106749000	-1.084692000	0.000082000
C	-6.599930000	-0.050405000	0.101843000
H	-6.637275000	0.626897000	-0.753454000
H	-7.492567000	-0.681351000	0.103038000
H	-6.575861000	0.542990000	1.017587000
C	-5.238921000	-2.248090000	1.392926000
H	-6.182919000	-2.796364000	1.334583000
H	-4.407820000	-2.955099000	1.362017000
H	-5.195797000	-1.698913000	2.335380000
C	-5.334958000	-2.100061000	-1.492202000
H	-6.281662000	-2.643491000	-1.433852000
H	-5.338708000	-1.459012000	-2.375639000
H	-4.513357000	-2.813046000	-1.581059000
Au	3.277948000	0.301206000	-0.001835000
P	5.094368000	-1.136604000	0.001577000
C	5.223251000	-2.168686000	1.497286000
H	4.331926000	-2.791880000	1.591662000
H	6.107993000	-2.808259000	1.442740000
H	5.294085000	-1.528166000	2.378449000
C	5.111886000	-2.323630000	-1.380568000
H	5.119035000	-1.781791000	-2.328387000
H	5.996986000	-2.962455000	-1.321640000
H	4.215134000	-2.945093000	-1.342097000
C	6.697492000	-0.279002000	-0.107447000
H	7.517410000	-1.002086000	-0.097971000

H	6.738549000	0.302440000	-1.030391000
H	6.806133000	0.403337000	0.737757000



# of imaginary frequencies: 0
E = -1423.25707141

symmetry c1

C	-0.068167000	0.325174000	0.001382000
H	-0.074530000	-0.759079000	0.001704000
C	1.227940000	0.975642000	0.004175000
C	1.012724000	2.248171000	0.003226000
C	-1.249852000	1.071767000	-0.001932000
C	-1.161891000	2.467698000	-0.002485000
H	-2.049646000	3.095324000	-0.004791000
C	0.069363000	3.191924000	0.000145000
H	0.134625000	4.269531000	0.000017000
Au	-3.087048000	0.144762000	-0.003541000
P	-5.173646000	-0.876375000	0.001317000
C	-5.160395000	-2.631883000	-0.491634000
H	-4.522766000	-3.198001000	0.190233000
H	-6.172801000	-3.043519000	-0.465130000
H	-4.757878000	-2.726299000	-1.502069000
C	-6.386255000	-0.102730000	-1.119431000
H	-7.348984000	-0.617047000	-1.055233000
H	-6.518674000	0.946247000	-0.846897000
H	-6.018558000	-0.149181000	-2.146403000
C	-6.002358000	-0.875680000	1.625562000
H	-6.979533000	-1.361045000	1.555350000
H	-5.384724000	-1.408059000	2.351519000
H	-6.133431000	0.151666000	1.970814000
Au	3.108655000	0.128616000	0.004316000
P	5.212403000	-0.832250000	-0.002807000
C	5.534284000	-1.906953000	1.430353000
H	4.793874000	-2.708396000	1.463476000
H	6.534587000	-2.341338000	1.353065000
H	5.460948000	-1.325841000	2.351597000
C	6.566285000	0.384220000	0.003149000
H	7.532916000	-0.126427000	-0.003125000
H	6.488976000	1.022110000	-0.879143000
H	6.493645000	1.010061000	0.894375000
C	5.528895000	-1.882620000	-1.454957000

H	5.451027000	-1.285813000	-2.365713000
H	6.530107000	-2.316700000	-1.389194000
H	4.789112000	-2.684065000	-1.498676000

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