

Supporting Information

A P-H Functionalized Al/P-Based Frustrated Lewis Pair – Hydrophosphination of Nitriles, Ring Opening with Cyclopropanones and Evidence of P=C Double Bond Formation[†]

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[†]Electronic supplementary information (ESI) available. CCDC 1xxxxxx–1xxxxxx. For ESI, crystallographic data in CIF or results of quantum chemical calculations see DOI:

DFT Calculations

All calculations were performed using the GAUSSIAN 09 D01 package of programs.¹ The structures were fully optimized for the gas phase using the TPSS² functional including the dispersion correction GD3BJ.³ The triple zeta basis set (def2-TZVP)⁴ was used in all calculations. Zero point vibrational energies and free enthalpy contributions were determined analytically.

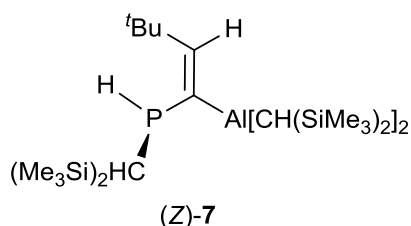
Table S1. DFT-calculated total electronic energies E after geometry optimization using the keyword TPSSTPSS, total free energies G_{298} , including the dispersion correction GD3BJ [a.u.] and the respective relative energies E_{rel} [kcal/mol]. The def2-TZVP basis set was used in all calculations.

Species	E [a.u.]	E_{rel} [kcal/mol]	G_{298} [a.u.]	E_{rel} [kcal/mol]
6 conformer 1 (gauche)	-1.433,66915	0,00	-1.433,34890	0,00
6 conformer 2 (gauche)	-1.433,66691	1,41	-1.433,34508	2,40
6 conformer 3 (trans)	-1.433,66621	1,85	-1.433,34419	2,96
FLP (Z)-7	-3391.87341	0,00	-3.391,10272	0,00
FLP (E)-7	-3391.86735	3,81	-3.391,09701	3,58
Invertomer to(E)-7	-3391.86653	4,32	-3.391,09597	4,24
Invertomer to(Z)-7	-3391.87299	0,27	-3.391,10250	0,14
TS for P-Inversion	-3391.83492	24,15	-3.391,06754	22,07
		Heat of formation		Heat of formation
(E)-13	-4045.15859	-68,76	-4.044,19977	-48,92
(E)-13a	-4.045,10219	-33,37	-4.044,14551	-14,87
(Z)-13	-4045.14177	-58,21	-4.044,18157	-37,50
(Z)-13a	-4045.08987	-25,63	-4.044,13248	-6,69
(E)-14	-4368.11226	-61,18	-4.367,15375	-40,60
(E)-14a	-4368.07154	-35,63	-4.367,11464	-16,06
(Z)-14	-4368.09841	-52,48	-4.367,14308	-33,90
(Z)-14a	-4368.05406	-24,65	-4.367,09842	-5,88
		Barrier		Barrier
TS (E)-13a-(E)-13	-4.045,05611	28,91	-4.044,10455	25,71
TS (Z)-13a-(Z)-13	-4045.06733	14,14	-4.044,11544	10,69
TS (E)-14a-(E)-14	-4368.02436	29,61	-4.367,07247	26,46
TS (Z)-14a-(Z)-14	-4368.01674	23,42	-4.367,06371	21,78

GAUSSIAN 09 Archive Entries

Structural formula, Heat of formation [au], Number of imaginary frequencies (with negative frequency for transition states), Cartesian coordinates

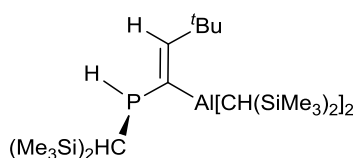
FLP's and starting materials



HF=-3391.873413 au (0)

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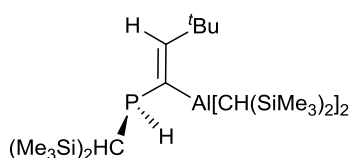
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HF=-3391.8673475 au (0)

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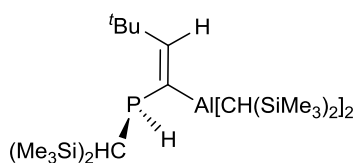


Invertomer to (E)-7

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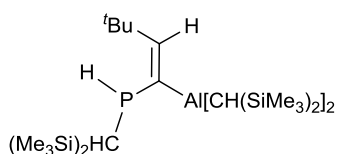
Invertomer to (Z)-7

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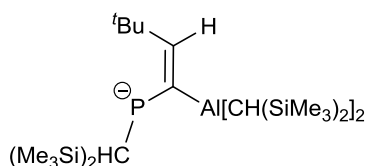


TS-(Z)-7 (P-Inversion)

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(Z)-7-Anion

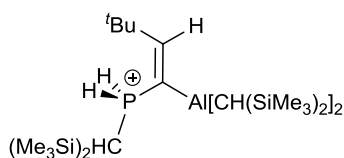
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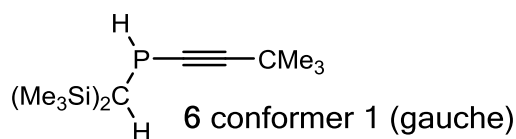
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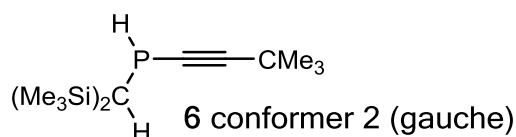
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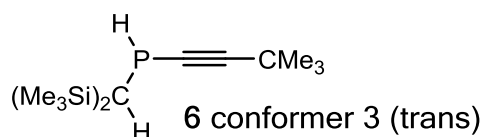
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HF=-1433.666906 au (1, -18,38 cm⁻¹)

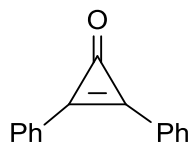
1\1\GINC-LUPUS09\FOpt\RTPSSTPSS\def2TZVP\C13H29P1Si2\WURTHWE\28-May-2018\0\# TPSSTPSS\def2tzvp opt=(verytight) pop=nbo freq nosym emp=gd3bj int=(grid=ultrafine,acc2e=11)\ Alkynylphosphine conformer 2\0,1\C,-0.0012888882,-0.00662336 22,0.0124945267\Si,0.0380649075,0.1043747875,1.9070876912\C,1.8174894846,0.1551444684,2.5265345438\Si,-1.6625490028,0.298432919,-0.8564420905\C,-3.1085789062,-0.4648375807,0.083670685\P,1.2618987453,1.1869331423,-0.6843137565\C,2.7031583038,0.1799365232,-0.7718243812\C,3.748808179,-0.4424555393,-0.7185532528\C,4.9989295035,-1.2046190765,-0.6548857047\C,5.0419296819,-2.2319022318,-1.8095232012\C,-1.9719624921,2.1475870576,-1.0515826652\C,-1.5914507713,-0.5128132149,-2.5576143531\C,6.1987242051,-0.236436021,-0.7746833674\C,5.0652766381,-1.9451478106,0.7014300782\C,-0.7833540737,-1.423027221,2.6482013215\C,-0.8367082889,1.6710201191,2.4829533052\H,4.9897936498,-1.7262412723,-2.7782851092\H,4.2013004443,-2.9284756063,-1.7378356684\H,5.9762620424,-2.8030742705,-1.7623244926\H,7.1361737753,-0.8020495796,-0.7231442112\H,6.1856921318,0.4963823567,0.0373833691\H,6.1668878399,0.3018417465,-1.7265745243\H,5.9975769033,-2.5180264412,0.7618577164\H,4.2234454811,-2.6363719506,0.8063245738\H,5.03608863,-1.234398628,1.5324448952\H,0.9238732938,1.102775141,-2.0643269902\H,0.3019665544,-1.0254656536,-0.2707949585\H,-4.0346574969,-0.316612144,-0.4862507269\H,-3.2530482024,-0.0116563174,1.070327153\H,-2.9761765518,-1.5436769714,0.2239500453\H,-1.1788521829,2.6405402361,-1.6256360683\H,-2.0406099761,2.6525435561,-0.0823395039\H,-2.9164834072,2.3151065495,-1.5840839824\H,-2.5185461324,-0.3297798603,-3.1147186599\H,-1.4660672336,-1.5987341704,-2.468523578\H,-0.7604022423,-0.1305766963,-3.1607163116\H,1.8303762282,0.2227104381,3.6219290256\H,2.3657540877,1.017426507,2.130724333\H,2.3673951863,-0.745992382,2.2349160611\H,-0.2988907987,-2.3391680404,2.2886025017\H,-1.8481510361,-1.4902199275,2.4055508798\H,-0.6902102286,-1.409270155,3.7413340464\H,-1.9056871496,1.6641710227,2.2422977318\H,-0.3918132256,2.5577336531,2.0162240056\H,-0.742758551,1.7848270784,3.5697904033\Version=AS64L-G09RevD.01\HF=-1433.666906\RMSD=9.619e-09\RMSF=2.808e-07\Dipole=0.0772879,-0.5792768,0.0485571\Quadrupole=4.7286743,-3.147359,-1.5813152,-4.2421335,0.4587705,0.2003947\PG=C01 [X(C13H29P1Si2)]\@



HF=-1433.6662067 au (1, -6,25 cm⁻¹)

1\1\GINC-LUPUS08\FOpt\RTPSSTPSS\def2TZVP\C13H29P1Si2\WURTHWE\28-May-2018\0\# TPSSTPSS\def2tzvp opt=(verytight) pop=nbo freq nosym emp=gd3bj int=(grid=ultrafine,acc2e=11)\ Alkynylphosphine conformer 3\0,1\C,-0.0046830207,0.0010679614,0.0027973941\Si,0.0006264969,-0.0013107899,1.9074246424\C,1.7734279819,-0.0011592008,2.5487825502\P,1.152643031,1.3943314739,-0.4958467701\C,0.6081177498,1.804007832,-2.11735726\C,0.1711776169,2.2448454746,-3.1657789498\C,-0.3417577093,2.736836567,-4.4472014517\C,0.852234073,3.1208282867,-5.352372

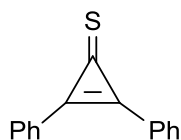
0183\Si,0.2842453997,-1.6389534664,-0.9002632596\C,-1.2494758181,-2.72
88054179,-0.7405654934\C,1.7733551141,-2.5246119106,-0.1532767766\C,0.
6039281728,-1.3983458644,-2.740344398\C,-1.1727051734,1.6262874723,-5.
1309647705\C,-1.2308641721,3.9787354984,-4.2065031367\C,-0.8704391543,
1.5654922967,2.4873875671\C,-0.909489073,-1.4922733212,2.6189483636\H,
-0.6580433456,4.7759013919,-3.7237708122\H,-2.0808664477,3.7271349596,
-3.5651137221\H,-1.6131780942,4.3507127411,-5.1640223758\H,0.479089633
6,3.4893919054,-6.3146741971\H,1.4937873583,2.2535243937,-5.5338730077
\H,1.4542643673,3.9059459523,-4.8857264644\H,-1.561694616,1.9922680139
,-6.0880383018\H,-2.0177539615,1.3322251385,-4.5009421324\H,-0.5560370
074,0.7424760969,-5.3184520742\H,2.2801043365,0.6084007074,-0.86347175
12\H,-1.003040338,0.3680229462,-0.2826755897\H,-0.9479549539,-1.411610
2409,3.7127020291\H,-0.4140496831,-2.4387022553,2.3761877137\H,-1.9417
967309,-1.5492587,2.2551370673\H,2.3312285537,0.867837327,2.179746376\H,
2.3197120914,-0.9032821958,2.2540163169\H,1.7771108114,0.0480974847,
3.6447347183\H,-0.8469638064,1.6490352499,3.5808229399\H,-1.9219932582
,1.5731486956,2.1752930311\H,-0.3892269674,2.4578994175,2.0712437105\H
,0.7666222682,-2.3777035002,-3.2091358272\H,1.4841438175,-0.7777862064
,-2.9360966815\H,-0.2487250546,-0.92243486,-3.235233855\H,-2.131659642
8,-2.2209259326,-1.1497819752\H,-1.4712788581,-2.9995557853,0.29606372
72\H,-1.1143818885,-3.6588486411,-1.3069932313\H,1.6012968188,-2.81453
85137,0.8893345016\H,2.6719900917,-1.8970476803,-0.1822038806\H,1.9922
74187,-3.4385171782,-0.7189191309\Version=AS64L-G09RevD.01\HF=-1433.6
662067\RMSD=1.814e-09\RMSF=2.068e-07\Dipole=-0.3635098,-0.1607584,-0.3
956468\Quadrupole=-2.2186586,-2.7633239,4.9819825,-2.2008523,1.3155282
,-3.6295626\PG=C01 [X(C13H29P1Si2)]\@



HF=-653.175601 au (0)

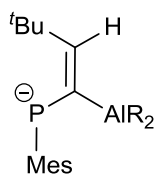
1\1\GINC-LUPUS06\FOpt\RTPSSTPSS\def2TZVP\C15H10O1\WURTHWE\28-Jan-2018\
0\# tpsstps/def2tzvp Opt=(readfc,tight) Pop=NBO Freq emp=gd3bj geom=
check guess=read\Diphenylcyclopropenone\0,1\C,-0.0056352119,-0.001565
7067,0.5940328071\O,-0.0079683236,-0.0039818411,1.8124825781\C,0.47407
49737,-0.493289098,-0.6618230283\C,-0.4805361753,0.4951380409,-0.66169
09273\C,-2.2369968541,2.1983413273,-0.6823782177\C,-3.0775263541,3.080
2808758,-1.3529073446\C,-3.0229770084,3.1762410343,-2.7453483827\C,-2.
123453986,2.3873438709,-3.4678705818\C,-1.2843643318,1.5002562813,-2.8
03148401\C,-1.3321991115,1.3934442542,-1.4008692889\C,2.2306149306,-2.
1964102852,-0.6825381533\C,1.3285692514,-1.3886632177,-1.4012911987\C,
1.2861058162,-1.4899127633,-2.8041557929\C,2.1277416809,-2.3743635367,
-3.4691725731\C,3.0244971193,-3.1661267673,-2.7463452074\C,3.073712829
7,-3.0756900392,-1.3533358607\H,-2.2652186416,2.1154215271,0.399882876
8\H,-3.7748559818,3.6957822152,-0.7921600047\H,-3.67867866,3.866672310
6,-3.2682198488\H,-2.0797116002,2.4666749948,-4.5503520311\H,-0.579265
4809,0.8944198762,-3.3629134813\H,2.2546912431,-2.1177834749,0.4001434
227\H,0.5831512172,-0.881855804,-3.3642099425\H,2.0881457004,-2.449400

7072,-4.5521197062\H,3.6822015998,-3.854483945,-3.2694358167\H,3.76889
 45741,-3.6934156934,-0.7923675496\\Version=AS64L-G09RevD.01\State=1-A\
 HF=-653.175601\RMSD=8.922e-09\RMSF=8.239e-07\Dipole=0.0038413,0.003978
 ,-2.0060879\Quadrupole=4.2619032,4.3347405,-8.5966438,-10.6174612,0.00
 35679,0.0053119\PG=C02 [C2(C1O1),X(C14H10)]\\@



HF=-976.1413538 au (0)

1\1\GINC-LUPUS08\FOpt\RTPSS\def2TZVP\C15H10S1\WURTHWE\28-Jan-2018\
 0\#\# tpsstps/def2tzvp Opt=(readfc,tight) geom=check guess=read Pop=NB
 O Freq emp=gd3bj\Diphenylcyclopropenethione\\0,1\C,0.1044527617,-0.242
 0114617,-0.086289566\C,0.0517284949,-0.1070841886,1.3253831193\C,1.255
 1898861,-0.3909491493,0.6290308237\S,-0.774105869,0.1682359801,2.71122
 89749\C,-0.6279387371,-0.216184562,-1.3191337698\C,-2.0113615056,0.043
 9456021,-1.2656058496\C,-2.7586570941,0.0779093986,-2.4377546866\C,-2.
 1385171782,-0.1458392399,-3.6693891589\C,-0.7656461293,-0.4047269023,-
 3.7308007868\C,-0.0115000061,-0.4404412894,-2.5641810472\C,3.252794719
 6,-0.6374985867,2.0067165501\C,2.6638126711,-0.6422207625,0.7270801383
 \C,3.4634069658,-0.8900452452,-0.4041415577\C,4.8244308469,-1.12808298
 11,-0.2559338863\C,5.4017082788,-1.1217339769,1.0177535072\C,4.6154792
 737,-0.8766231296,2.1461705668\H,-2.4738316783,0.2151529069,-0.2980900
 297\H,-3.8250510881,0.2786122937,-2.3944308934\H,-2.7241973269,-0.1188
 535397,-4.5838857381\H,-0.2883233815,-0.5780237774,-4.6909005473\H,1.0
 545641269,-0.6409691329,-2.6060652264\H,2.6238303666,-0.444840176,2.87
 07559389\H,3.0100933703,-0.8937976346,-1.390524415\H,5.4401236233,-1.3
 19178847,-1.1300420889\H,6.4660757607,-1.308306156,1.128956704\H,5.067
 6946508,-0.872570006,3.1335102133\\Version=AS64L-G09RevD.01\State=1-A\
 HF=-976.1413538\RMSD=7.473e-09\RMSF=1.001e-07\Dipole=1.1689863,-0.3897
 215,-1.9616947\Quadrupole=8.735549,-7.2166511,-1.5188979,-2.0726886,10
 .368284,-1.3853259\PG=C01 [X(C15H10S1)]\\@



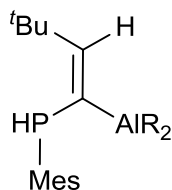
3-anion: R = CH(SiMe₃)₂

HF=-2883.5883187au (0)

1\1\GINC-PALMA316\FOpt\RTPSS\def2TZVP\C29H59Al1P1Si4(1-)\WURTHWE\1
 6-Mar-2018\0\#\# tpsstps/def2tzvp opt=(gdiis,maxstep=2) int=(Acc2e=11,
 grid=ultrafine) freq pop=nbo emp=gd3bj geom=check guess=read\
 FLP: Anion\\-1,1\C,4.3487194902,1.5653635989,1.5778149
 078\C,4.785241567,0.6493036754,0.6118413832\C,4.0647980204,-0.50006789

31,0.3001710112\C,2.8117209856,-0.7748810671,0.9317367426\C,2.44117881
34,0.0846419641,2.0153563595\C,3.196836749,1.2318013384,2.2906929087\P
,1.9053234247,-2.2864852757,0.4758160902\C,0.1890410034,-1.7611553428,
0.6738804412\C,-0.8837604942,-2.5537650641,0.9967036322\C,-0.903369249
6,-4.0180096149,1.4445071215\C,-0.3063226308,-4.9451515588,0.367561851
8\C,4.6423621389,-1.4735584218,-0.6948688946\C,1.3692893236,-0.3070474
353,3.0082422872\C,5.0940651041,2.8496245771,1.8402062018\A1,-0.557035
7643,-0.1333488907,-0.1128950269\C,-2.0218669551,0.7104623928,0.961866
3325\Si,-1.7148913525,2.2421446684,2.0053977908\C,-2.0457013644,1.7750
600669,3.8105598928\Si,-3.6900340107,0.5921207606,0.1298448012\C,-4.00
42137265,1.9235019343,-1.1767594599\C,-5.098228949,0.6729893249,1.4006
52501\C,-3.9042009622,-1.0658934969,-0.7584120127\C,-0.4325278994,0.42
30277662,-2.0165825366\Si,-0.0307326504,-0.9551036919,-3.230648987\C,-
0.7815412012,-0.542547946,-4.9271727075\Si,0.5037074433,2.0286648565,-
2.2625656965\C,0.9743512368,2.4175234906,-4.0612587963\C,2.0959251707,
2.0568879395,-1.2661577426\C,-0.6251382751,3.4651890958,-1.7588950436\
C,1.8229209,-1.219303592,-3.385646195\C,-0.7742785899,-2.6168852443,-2
.738225947\C,0.0393204785,2.9263837334,1.8986878458\C,-2.8376316559,3.
7258887679,1.6215031496\C,-0.0906583018,-4.1653061742,2.7484790728\C,-
2.3606165605,-4.4346253438,1.7080706309\H,-1.4860037208,0.6933424938,-
2.2190319949\H,-2.073003428,-0.0774698516,1.740806503\H,0.2014919663,3
.6649708185,2.6954439793\H,0.2269948492,3.4295963948,0.9448282556\H,0.
8010846012,2.149202822,2.0121710395\H,-3.9055873191,3.4913087774,1.686
8753452\H,-2.6457809407,4.1474538854,0.6286586747\H,-2.6267258814,4.51
55216265,2.3556598536\H,-3.0794412245,1.4317933429,3.9425729713\H,-1.8
829825766,2.6259693543,4.4846742803\H,-1.382332561,0.9622900923,4.1292
029051\H,-3.1153641043,-1.2412818832,-1.4990206564\H,-4.8658317759,-1.
0902647341,-1.2888067411\H,-3.8843775812,-1.9104216605,-0.0607917413\H
,-3.9638474644,2.9378690426,-0.7697907901\H,-5.0014990527,1.7753252206
,-1.6119548671\H,-3.2769793946,1.8660678698,-1.9938612181\H,-4.9881335
448,-0.1303348426,2.1401444334\H,-6.0758138972,0.5475286728,0.91637667
13\H,-5.115345838,1.6226231733,1.9471909264\H,1.9433581299,1.878319532
7,-0.195232249\H,2.607743192,3.0228152117,-1.3678826358\H,2.7849056038
,1.2770714493,-1.6069028724\H,-1.4124978766,3.6111609488,-2.5091938631
\H,-0.0660240125,4.4059368431,-1.6749988601\H,-1.1214175339,3.28272568
31,-0.8018181266\H,1.6242835569,1.6569832124,-4.5069737655\H,1.5139837
575,3.3741143439,-4.0923438217\H,0.087093423,2.5170669341,-4.697808935
7\H,2.3809295863,-0.309338099,-3.6304595153\H,2.0504857959,-1.97515515
28,-4.1482456917\H,2.1755654104,-1.5945363471,-2.4154688024\H,-1.87031
11025,-2.5974833683,-2.7073899446\H,-0.4106162107,-2.924037763,-1.7528
943316\H,-0.4778937756,-3.3844865298,-3.4660549578\H,-1.8617628548,-0.
365129741,-4.839598908\H,-0.641555844,-1.383297412,-5.6198798971\H,-0.
3342247873,0.3460459264,-5.3839074865\H,-1.8876353839,-2.1117056261,0.
9751467217\H,0.9380795304,-3.8252498333,2.5844676529\H,-0.0709891176,-
5.215146842,3.0739473876\H,-0.5360182212,-3.5608447443,3.5474093757\H,
-2.8154851935,-3.79373719,2.4742688656\H,-2.4136164467,-5.4742723707,2
.0559779728\H,-2.9605623738,-4.3486561233,0.7930338413\H,-0.8928243468
,-4.8923833785,-0.5566519414\H,-0.3053985015,-5.9873315186,0.718511326
\H,0.7240446439,-4.6531565292,0.1392060396\H,3.9328732917,-1.691728363
2,-1.4999155154\H,4.858573375,-2.4376811137,-0.2150768648\H,5.57154635
5,-1.0828650844,-1.1261132883\H,5.7167559555,0.841573828,0.0771088333\

H,4.8811621042,3.2316796226,2.8455628747\H,4.8064364335,3.6351058249,1.1254133883\H,6.1788555148,2.7122712351,1.7498250613\H,2.8899154268,1.8696181481,3.1209589372\H,1.4535300762,-1.380402272,3.2204406309\H,0.3434104845,-0.1630197312,2.6536000182\H,1.4927931137,0.2651764647,3.9362101126\\Version=EM64L-G09RevD.01\State=1-A\HF=-2883.5883187\RMSD=8.835e-09\RMSF=1.720e-06\Dipole=-1.6727264,1.7459572,-0.536687\Quadrupole=-4.2331517,-1.3346885,5.5678402,5.9606244,-3.1057568,3.3734893\PG=C01[X(C29H59Al1P1Si4)]\@

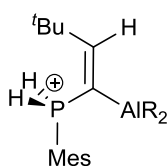


3: R = CH(SiMe₃)₂

HF=-2884.1497184 au (0)

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3-protonated: R = CH(SiMe₃)₂

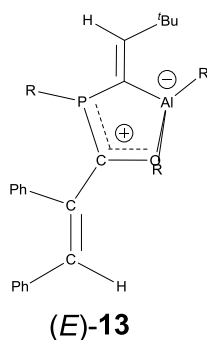
HF=-2884.5463282 au (0)

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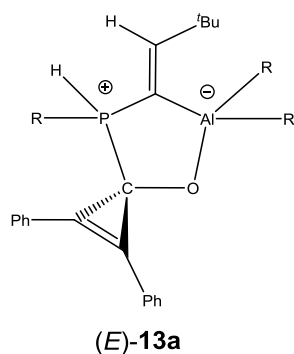
Adducts



HF = -4045.1585917 au (0)

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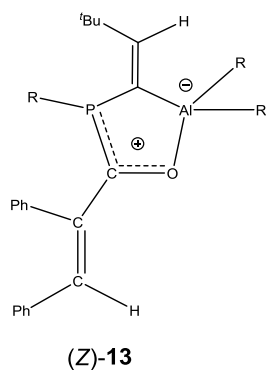
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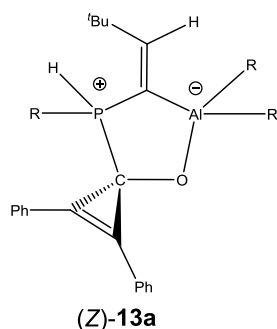
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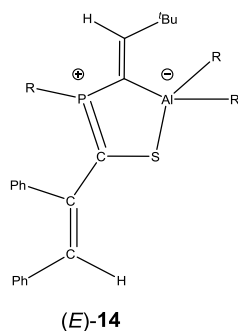
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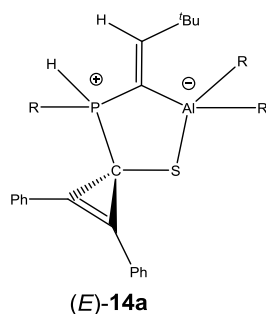
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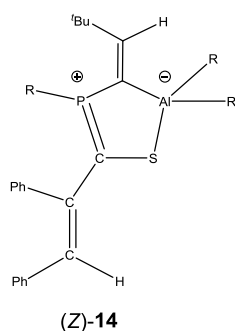
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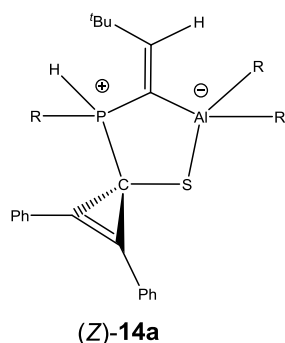
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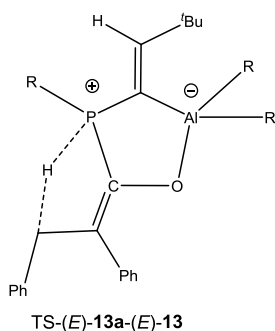


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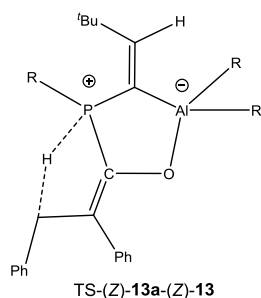
Transition states for 1,3-hydrogen shift



HF=-4045.0561116 au (1, -994.3075cm⁻¹)

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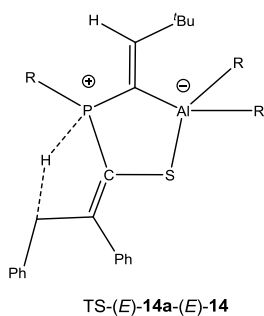
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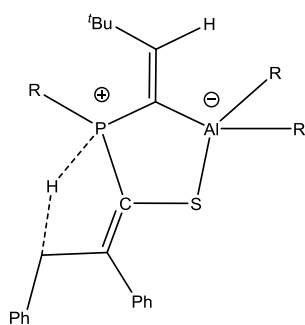
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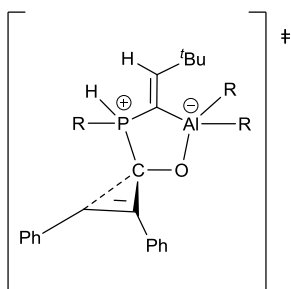
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TS for Carbene-formation to give (*E*)-**13**

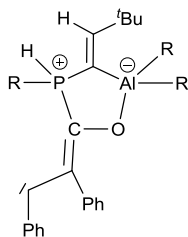
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1 [X(C42H78Al1O1P1Si6)]\@



(*E*)-Carbene for the formation of (*E*)-**13**

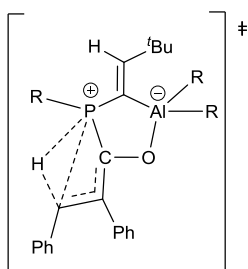
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1O1P1Si6)]\@



TS for the formation of (*E*)-**13** via Carbene

HF=-4045.0644177 au (1, -869.8075cm⁻¹)

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