10.1071/CH10085_AC
CSIRO 2010
Australian Journal of Chemistry, 2010, 63(8), 1189-1194

A Computational Study of the Radical Ring-Opening Polymerization of Diphosphetanes

Michelle L. Coote,[1] Mansoor Namazian and S. Bruce Wild

ARC Centre of Excellence for Free-radical Chemistry and Biotechnology,

Research School of Chemistry, Australian National University, Canberra ACT

0200, Australia

Supporting Information

[1] Correspondence author: mcoote@rsc.anu.edu.au

1. Optimised geometries:

1.1 Optimised geometries at B3LYP/6-31G(d) level presented as Gaussian Archives: (For the structure of studied species see Figure 1s)

Monomer 2:


```
1\1\GINC-AC15\FOpt\RB3LYP\6-31G(d)\C4H10P2\MXN501\08-Sep-2006\0\\# B3L
 YP/6-31G* FOPT INT=ULTRAFINE MAXDISK=134217728\\e\\0,1\C,-0.6477635675
 ,-0.6630372644,-2.5068159503\P,-0.6813789495,-0.8372553161,-0.65004688
 82\C,1.131971496,-0.6007267794,-0.17869591\P,0.7827187311,0.9543229718
 ,0.8508553334\C,0.2581012538,0.1615390405,2.4622625328\C,-0.8763267539
 ,0.9492978973,-0.0698639801\H,1.585795748,-1.4326168319,0.3677799168\H
 ,-1.7563636076,1.146781231,0.5491602608\H,1.7756091122,-0.3550440223,-
 1.0307932097\H,-0.8587932597,1.6780678954,-0.8879459666\H,-1.668572681
 9,-0.510651927,-2.87503077\H,-0.0222048751,0.1713556846,-2.8459419399\
 H,-0.2696237127,-1.5905227953,-2.951359829\H,-0.2445421848,0.915206420
 2,3.0784591833\H,-0.4110975038,-0.6966539164,2.3397117492\H,1.15380167
 13,-0.1643739377,3.0025137723\\Version=IA64L-G03RevC.02\State=1-A\HF=-
 841.1392251\RMSD=8.169e-09\RMSF=6.226e-06\Dipole=-0.0609403,-0.0640297
 ,-0.2115286\PG=C01 [X(C4H10P2)]\\@
```


Monomer 3:


```
1\1\GINC-AC50\FOpt\RB3LYP\6-31G(d)\C10H22P2\MXN501\28-Apr-2007\0\\# B3
 LYP/6-31G* Fopt=(maxcyc=200) Int=UltraFine SCF=Tight Freq=Noraman maxd
 isk=671088640\\p2_tbu2\\0,1\C,0.0005948419,0.0018471888,-0.0456435806\
 P,-0.1290276856,-0.172430419,1.8500000161\C,1.6477846973,0.0411115554,
 2.4636117027\P,1.3673337137,1.8078184914,3.0795164944\C,1.2375440366,1
 .6332925821,4.9751087456\C,-0.4094529837,1.5943140515,2.4657633778\H,1
 .9038184372,-0.6939729383,3.2324674803\H,-1.1855173135,1.638437738,3.2
 357176469\H,2.4237689719,-0.0028499819,1.693570638\H,-0.6653019315,2.3
 293717132,1.6968188654\C,-1.4398035169,0.1837102951,-0.5640180172\C,0.
 8771885948,1.1635509884,-0.541286957\C,0.5692601218,-1.3331716398,-0.5
 660990964\C,0.6687862849,2.9682245471,5.4956824411\C,0.360930682,0.471
 4881429,5.4704949496\C,2.6778978821,1.4514012489,5.4935922653\H,2.6834
 220524,1.4181268856,6.5914215985\H,3.12369482,0.5157911617,5.135004804
 8\H,3.3269523918,2.2767379371,5.1792486964\H,0.3492835647,0.4545329998
 ,6.5692510762\H,-0.6781885159,0.5649109027,5.137278376\H,0.7349417758,
 -0.5019692092,5.1357926638\H,0.6367153751,2.9633207356,6.5935505949\H,
 1.2843755878,3.8188305588,5.1813839071\H,-0.3536177156,3.1410753096,5.
 1386128592\H,0.8887298311,1.1803287799,-1.6400468807\H,0.5032336419,2.
 1370752758,-0.2067166062\H,1.9163411372,1.0701621663,-0.2081652383\H,-
 1.4454364538,0.2168594112,-1.6618514995\H,-2.0888448633,-0.6415761789,
 -0.2495168823\H,-1.8855450552,1.1193715461,-0.2054948957\H,0.60122643,
 -1.3284207995,-1.6639718047\H,1.5916932342,-1.5060068129,-0.2091057219
 \H,-0.0463270736,-2.1837146007,-0.2516263778\\Version=IA64L-G03RevD.01
 \State=1-A\HF=-1077.0111365\RMSD=8.452e-09\RMSF=4.928e-06\Thermal=0.\D
 ipole=-0.0000167,-0.0000253,-0.0000489\PG=C01 [X(C10H22P2)]\\@
```


Monomer 4:


```
1\1\GINC-AC44\FOpt\RB3LYP\6-31G(d)\C6H14P2\MXN501\15-Sep-2006\0\\# B3L
 YP/6-31G* FOPT INT=ULTRAFINE MAXDISK=134217728\\title\\0,1\C,-0.775220
 8367,-0.768328816,-2.4528455963\P,-0.6330485447,-0.9288623035,-0.59775
 19486\C,1.2001858203,-0.6318418254,-0.1850218454\P,0.7731908895,0.8112
 661152,0.9856059823\C,0.308533081,-0.1378651739,2.5310846485\C,-0.8806
 392146,0.8342432072,0.0320520718\H,1.6167137316,-1.4893071877,0.354838
 7657\C,-2.1705523677,1.1678342976,0.7766569542\C,2.1621696179,-0.21880
 62056,-1.302723372\H,-0.7365327643,1.5523587072,-0.7865563949\H,-1.836
 5964215,-0.6646627697,-2.7061411478\H,-0.2321761739,0.0860078111,-2.87
 03995963\H,-0.4130154636,-1.6851295875,-2.9313775457\H,-0.2192010551,0
```

.530454149,3.2199175609\H,-0.3118127817,-1.0216770662,2.3517382417\H,1
.2344581381,-0.4535096199,3.0246900774\H,3.1548211502,0.0017842356,-0.
8907462631\H,2.2791881766,-1.0155603424,-2.0477025937\H,1.8258167787,0
.6810269086,-1.8299663629\H,-2.1326217811,2.1773801988,1.2062387545\H,
-3.0348696956,1.131535111,0.1012093636\H,-2.3631636131,0.4618293737,1.
5912294686\\Version=IA64L-G03RevC.02\State=1-A\HF=-919.7633316\RMSD=9.
147e-09\RMSF=1.658e-05\Dipole=-0.0598476,-0.0537001,-0.2591586\PG=C01
[X(C6H14P2)]\\@

Monomer 5:

1\1\GINC-AC53\FOpt\RB3LYP\6-31G(d)\C8H18P2\MXN501\15-Sep-2006\0\\# B3L
YP/6-31G* FOPT INT=ULTRAFINE MAXDISK=134217728\\title\\0,1\C,-0.840422
1957,-0.7406583935,-2.4727486872\P,-0.7698956737,-0.8510328348,-0.6089
905627\C,1.069552915,-0.7496885787,-0.1207780382\P,0.7233173247,0.7516
440285,1.03194058\C,0.1714675793,-0.0692560363,2.6200617976\C,-0.92440
50186,0.9290309114,0.0541018915\C,1.5798925374,-2.0266337076,0.5568683
828\C,-2.192058125,1.1490007392,0.8877181601\C,2.0623758242,-0.3314349
047,-1.2166651963\C,-0.7901077019,2.0700682988,-0.9664845774\H,-1.8814
04086,-0.5734240829,-2.7717524713\H,-0.2190297412,0.0434798104,-2.9147
800228\H,-0.5349742871,-1.7069696212,-2.8898317482\H,-0.2881450314,0.6
915672095,3.2598678126\H,-0.5349716495,-0.8953190551,2.4948683078\H,1.
0590932354,-0.4426673562,3.1417246373\H,3.0609649872,-0.1850375013,-0.
7838198028\H,2.1460613929,-1.1089283019,-1.9876161042\H,1.788941893,0.
6028465787,-1.7155327618\H,-2.1478540941,2.1032366891,1.4307499445\H,-
3.0745812083,1.188625934,0.2344796191\H,-2.3618456416,0.3503413307,1.6
149989633\H,2.5642328268,-1.8638981636,1.0172993263\H,0.8988873034,-2.
3947504913,1.329101759\H,1.6975799894,-2.8292881752,-0.1841001263\H,-1
.6454062496,2.0830916295,-1.6550762287\H,-0.7672113161,3.0378919798,-0
.4480633331\H,0.1205620239,2.0074637082,-1.5692104274\\Version=IA64L-G
03RevC.02\State=1-A\HF=-998.3851972\RMSD=9.576e-09\RMSF=1.483e-05\Dipo
le=-0.0602132,-0.0480042,-0.2257153\PG=C01 [X(C8H18P2)]\\@

Monomer 5a:

1\1\GINC-AC17\FOpt\RB3LYP\6-31G(d)\C7H16P2\MXN501\10-Oct-2007\0\\# B3L
YP/6-31G* Fopt=(maxcyc=200) Int=UltraFine SCF=Tight Freq=Noraman maxdi
sk=134217728\\p2_tbu2\\0,1\C,-0.2276347739,-0.2098459975,0.237207499\P
,-0.1953459169,0.2636559346,2.0745412703\C,1.6173059025,-0.2915828317,
1.9909765646\P,1.6540131384,-0.2341415295,0.1058007181\C,2.1339178036,
-1.9836794426,-0.4804513628\C,1.4088458219,-3.1381523365,0.2285409564\
C,3.6534741335,-2.1131993177,-0.2548004986\C,1.8275806758,-2.032612183
2,-1.9905782185\C,0.0178903254,2.1172577343,1.9365831917\H,1.721650367
2,-1.2896161614,2.4283102649\H,2.3353122442,0.3733562904,2.4799536491\
H,-0.7200525667,0.508887052,-0.4243919278\H,-0.7156956083,-1.181554468
4,0.1115232087\H,4.0134631361,-3.0769727433,-0.6395881193\H,4.20656749
11,-1.3187294189,-0.7686984949\H,3.9095361146,-2.0683691078,0.81079299
37\H,2.1492458302,-2.9945987303,-2.412021325\H,0.753806263,-1.92933927
91,-2.1891192835\H,2.3495020128,-1.2366314277,-2.5339062019\H,1.751778
7816,-4.1000236307,-0.1771354863\H,1.6078958209,-3.153756867,1.3057225
259\H,0.3235568644,-3.0967643372,0.0848983339\H,0.3291514269,2.5091998
356,2.9112257648\H,0.7488584393,2.4254661666,1.18200207\H,-0.951694904
9,2.5659374431,1.6936574818\\Version=IA64L-G03RevD.01\State=1-A\HF=-95
9.0753927\RMSD=6.082e-09\RMSF=6.853e-06\Thermal=0.\Dipole=0.1606587,-0
.1909745,-0.1778944\PG=C01 [X(C7H16P2)]\\@

Attacking radical 2′:

1\1\GINC-AC58\FOpt\UB3LYP\6-31G(d)\C6H14P1(2)\MXN501\27-Apr-2007\0\\#
UB3LYP/6-31G* Fopt=(maxcyc=200) Int=UltraFine SCF=Tight Freq=Noraman m

axdisk=671088640\\radp2_tbu2\\0,2\C,-0.1348872334,0.0165486611,-0.0826
473494\P,1.6327267188,-0.0884301104,-0.1359244039\C,2.1334621899,1.703
289931,0.0146176128\C,2.1443369365,-0.8822334593,1.528186858\C,1.60591
4398,-2.3256180048,1.5259720434\C,1.596584395,-0.1239111003,2.74796413
63\C,3.6837464475,-0.9154162144,1.5712624311\H,1.7342323628,2.19034295
15,0.9094682197\H,3.2241720835,1.7885854975,0.0135155534\H,1.759780539
5,2.2340868207,-0.8673723613\H,-0.6387751769,0.8440649035,-0.576652064
2\H,-0.7344618318,-0.8769835617,0.0695135343\H,1.9459956575,-2.8524236
416,2.4276241754\H,0.5106158215,-2.351590646,1.5254683206\H,1.96107248
88,-2.8887849788,0.6551358843\H,1.881487298,-0.6426650868,3.674116403\
H,1.9968630629,0.894098834,2.8100526233\H,0.5042544261,-0.0566291358,2
.716697039\H,4.0219615626,-1.430042951,2.480573696\H,4.1006004668,-1.4
487590373,0.7092839737\H,4.1149573866,0.0922603288,1.5874636746\\Versi
on=IA64L-G03RevD.01\State=2-A\HF=-578.3695368\S2=0.756665\S2-1=0.\S2A=
0.750027\RMSD=3.809e-09\RMSF=1.583e-06\Thermal=0.\Dipole=0.0798074,0.1
811966,0.349686\PG=C01 [X(C6H14P1)]\\@

Attacking radical 3′:

1\1\GINC-AC58\FOpt\UB3LYP\6-31G(d)\C6H14P1(2)\MXN501\27-Apr-2007\0\\#
UB3LYP/6-31G* Fopt=(maxcyc=200) Int=UltraFine SCF=Tight Freq=Noraman m
axdisk=671088640\\radp2_tbu2\\0,2\C,-0.1348872334,0.0165486611,-0.0826
473494\P,1.6327267188,-0.0884301104,-0.1359244039\C,2.1334621899,1.703
289931,0.0146176128\C,2.1443369365,-0.8822334593,1.528186858\C,1.60591
4398,-2.3256180048,1.5259720434\C,1.596584395,-0.1239111003,2.74796413
63\C,3.6837464475,-0.9154162144,1.5712624311\H,1.7342323628,2.19034295
15,0.9094682197\H,3.2241720835,1.7885854975,0.0135155534\H,1.759780539
5,2.2340868207,-0.8673723613\H,-0.6387751769,0.8440649035,-0.576652064
2\H,-0.7344618318,-0.8769835617,0.0695135343\H,1.9459956575,-2.8524236
416,2.4276241754\H,0.5106158215,-2.351590646,1.5254683206\H,1.96107248
88,-2.8887849788,0.6551358843\H,1.881487298,-0.6426650868,3.674116403\
H,1.9968630629,0.894098834,2.8100526233\H,0.5042544261,-0.0566291358,2
.716697039\H,4.0219615626,-1.430042951,2.480573696\H,4.1006004668,-1.4
487590373,0.7092839737\H,4.1149573866,0.0922603288,1.5874636746\\Versi
on=IA64L-G03RevD.01\State=2-A\HF=-578.3695368\S2=0.756665\S2-1=0.\S2A=
0.750027\RMSD=3.809e-09\RMSF=1.583e-06\Thermal=0.\Dipole=0.0798074,0.1
811966,0.349686\PG=C01 [X(C6H14P1)]\\@

Attacking radical 4′:

1\1\GINC-AC57\FOpt\UB3LYP\6-31G(d)\C4H10P1(2)\MXN501\16-Feb-2007\0\\#
UB3LYP/6-31G* OPT INT=ULTRAFINE MAXDISK=134217728\\title\\0,2\C,-1.220
5149745,0.0343376776,-0.2950109736\P,0.5615131433,-0.0587812486,-0.454
7825576\C,1.0310037959,1.7461771988,-0.4143371804\C,1.1257494321,-0.60
74386177,1.2419681249\H,0.7839342153,-1.6291577266,1.4348977454\H,0.75
36671591,0.0475117233,2.0374086264\H,2.220748851,-0.6158259941,1.26490
84375\H,2.1214632064,1.838574413,-0.4498630548\H,0.6253541637,2.245975
3104,-1.3002643686\H,-1.7080768874,0.8452195344,-0.8377327661\C,-2.084
6452012,-1.1334047662,0.077630046\H,-2.9866251554,-0.7998792305,0.6088
681745\H,-2.4335848827,-1.6947501643,-0.8055044413\H,-1.5668430466,-1.
8491274369,0.7265043061\H,0.6577069124,2.2551493448,0.4810156042\\Vers
ion=IA64L-G03RevC.02\State=2-A\HF=-499.7498716\S2=0.755798\S2-1=0.\S2A
=0.750023\RMSD=5.158e-09\RMSF=5.832e-06\Dipole=-0.0805969,0.2168552,0.
3431724\PG=C01 [X(C4H10P1)]\\@

Attacking radical 5′:

1\1\GINC-AC46\FOpt\UB3LYP\6-31G(d)\C5H12P1(2)\MXN501\16-Feb-2007\0\\#
UB3LYP/6-31G* GEOM=CHECKPOINT OPT=CALCFC FREQ=NORAMAN MAXDISK=13421772
8\\title\\0,2\C,-0.950930284,-0.0881461686,-0.1940168104\P,0.851575396
4,-0.1315941846,-0.3353865528\C,1.3427536392,1.6277437797,0.0759008403

\C,1.3932509491,-0.9796789836,1.2367115705\H,1.1684021311,-2.049332544
4,1.1897065426\H,0.9263041034,-0.5552639683,2.132866914\H,2.4801554098
,-0.8764424002,1.3233527612\C,-1.7244611617,0.8327627352,-1.0993200182
\C,-1.7279932856,-1.2401354021,0.3795677055\H,2.4363477202,1.689298547
7,0.0927870308\H,0.9870346525,2.3106849121,-0.7012715324\H,0.949404957
1,1.9573693404,1.0437937704\H,-2.5907214963,1.2590811074,-0.5715036324
\H,-1.127873078,1.6681320877,-1.4805419772\H,-2.1304444543,0.299201706
8,-1.9762146991\H,-2.6711284038,-0.884622029,0.8200768631\H,-2.0117489
243,-1.9757533586,-0.394154818\H,-1.1850827049,-1.7837163956,1.1588413
421\\Version=IA64L-G03RevC.02\State=2-A\HF=-539.066642\S2=0.755497\S2-
1=0.\S2A=0.750022\RMSD=6.180e-09\RMSF=3.345e-06\Dipole=-0.124786,0.146
7171,0.3934773\PG=C01 [X(C5H12P1)]\\@

Attacking radical 4a':

1\1\GINC-AC55\FOpt\UB3LYP\6-31G(d)\C3H8P1(2)\MXN501\11-Apr-2007\0\\# U
B3LYP/6-31G* Fopt=(maxcyc=200) Int=UltraFine SCF=Tight Freq=Noraman ma
xdisk=134217728\\Untitled-1\\0,2\C,-0.0137059501,-0.0381359122,-0.0184
94596\P,1.7957299894,-0.1618762375,-0.0475291337\H,2.1164416698,1.2155
309791,-0.2311617792\H,2.0469280146,-0.171416914,1.3563844189\C,-0.715
8485635,0.6603228012,-1.1471461743\C,-0.8005445002,-1.0293575753,0.789
6519655\H,-1.6835861205,1.0591398138,-0.8116747499\H,-0.132915659,1.49
49958135,-1.5534285464\H,-0.9357857576,-0.0205143736,-1.9884039861\H,-
1.7661796602,-0.6004350094,1.0924967707\H,-1.0336198314,-1.9447597102,
0.2175159978\H,-0.2745436312,-1.3437736754,1.6984898126\\Version=IA64L
-G03RevD.01\State=2-A\HF=-460.4271496\S2=0.754732\S2-1=0.\S2A=0.750018
\RMSD=3.528e-09\RMSF=1.091e-05\Thermal=0.\Dipole=-0.3684678,0.1522743,
0.1169485\PG=C01 [X(C3H8P1)]\\@

1.2. Standard orientation of studied transition states at B3LYP/6-31G(d) level (based on IRC calculations):

Transition state of 2′ + 2:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.215009	0.452710	1.246346
2	15	0	-0.535219	0.303400	0.311158
3	6	0	-0.368833	2.076944	-0.242431
4	15	0	-3.225905	0.164709	-0.315841
5	6	0	-4.090184	-1.447065	0.055195
6	6	0	-1.595069	-0.428005	-1.066264
7	6	0	1.636322	-0.507431	-0.810460
8	15	0	3.031569	0.282607	0.046908
9	6	0	3.094836	-0.767726	1.586776
10	6	0	4.498178	-0.450458	-0.871894
11	1	0	-3.428694	-2.188748	0.518833
12	1	0	-4.934314	-1.258856	0.727818
13	1	0	-4.492219	-1.865863	-0.874217
14	1	0	-1.377734	-0.044766	-2.067357
15	1	0	-1.496261	-1.519547	-1.088029
16	1	0	-2.317413	-0.346416	1.988334
17	1	0	-2.379981	1.413272	1.743222
18	1	0	-1.303577	2.485672	-0.640314
19	1	0	0.412621	2.155903	-1.002775
20	1	0	-0.058189	2.682757	0.615415
21	1	0	1.370815	-0.110775	-1.790655
22	1	0	1.457601	-1.577878	-0.697992
23	1	0	4.530221	-0.048654	-1.889928
24	1	0	4.458894	-1.544828	-0.925219
25	1	0	5.424086	-0.153160	-0.365082
26	1	0	3.985325	-0.512363	2.171312
27	1	0	3.118603	-1.841100	1.360523
28	1	0	2.212087	-0.559199	2.199119

Transition state of 3′ + 3:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.974361	0.448192	-1.336464
2	15	0	0.447029	0.741940	-0.195681
3	6	0	0.248530	2.648683	-0.224405
4	15	0	3.163386	0.242646	0.107262
5	6	0	3.596484	-1.616440	0.127947
6	6	0	1.638643	0.383533	1.216664
7	6	0	-1.483420	-0.086165	1.196573
8	15	0	-3.118123	0.191456	0.445607
9	6	0	-3.417253	-1.372868	-0.611593
10	6	0	-4.216439	-0.109068	1.941790
11	6	0	2.407976	-2.575467	-0.047514
12	6	0	4.607802	-1.835823	-1.014555
13	6	0	4.281646	-1.887501	1.481974
14	1	0	1.730221	1.181710	1.959982
15	1	0	1.354801	-0.529113	1.750315
16	1	0	1.823278	-0.445865	-1.948725
17	1	0	2.240297	1.269276	-2.008593
18	6	0	1.586588	3.405362	-0.141577
19	6	0	-0.644003	3.105264	0.945495
20	6	0	-0.455711	2.977535	-1.557045
21	1	0	-1.270352	0.549585	2.055886
22	1	0	-1.096427	-1.098333	1.312243
23	1	0	-4.019984	0.689463	2.665331
24	1	0	-4.036692	-1.070273	2.434948
25	1	0	-5.272690	-0.043069	1.658650
26	6	0	-4.881670	-1.316302	-1.091950
27	6	0	-3.173571	-2.700423	0.124810
28	6	0	-2.489968	-1.288492	-1.839762
29	1	0	-0.739472	4.199262	0.920960
30	1	0	-1.649737	2.682086	0.880118
31	1	0	-0.213651	2.839307	1.918548
32	1	0	-0.608597	4.061793	-1.642105
33	1	0	0.140102	2.661261	-2.421650
34	1	0	-1.436088	2.493280	-1.620296
35	1	0	1.394577	4.486679	-0.173665
36	1	0	2.121974	3.198260	0.791213
37	1	0	2.257463	3.171684	-0.973458
38	1	0	2.761077	-3.615850	-0.027087
39	1	0	1.668872	-2.470879	0.754419
40	1	0	1.893430	-2.428432	-1.003332
41	1	0	4.960864	-2.875918	-1.014291
42	1	0	4.159063	-1.640973	-1.996062
43	1	0	5.482630	-1.184140	-0.908560
44	1	0	4.628979	-2.928476	1.529917
45	1	0	5.150528	-1.236370	1.631232
46	1	0	3.594892	-1.731520	2.322784
47	1	0	-2.684888	-2.132227	-2.516346
48	1	0	-2.655098	-0.362401	-2.402701
49	1	0	-1.433384	-1.319930	-1.554625
50	1	0	-5.076694	-2.133620	-1.799353
51	1	0	-5.591166	-1.425112	-0.263871
52	1	0	-5.100827	-0.371860	-1.603765
53	1	0	-3.385107	-3.545292	-0.545643

54	1	0	-2.134900	-2.803567	0.456344
55	1	0	-3.821658	-2.811180	1.001094

Transition state of 4′ + 4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.003006	1.302424	0.542749
2	15	0	0.360124	0.279616	0.399158
3	6	0	0.180933	-0.223632	2.187374
4	15	0	3.054854	-0.262283	0.377380
5	6	0	4.106920	-0.011274	-1.145795
6	6	0	1.492794	-1.073372	-0.314429
7	6	0	-1.823069	-0.768879	-0.353772
8	15	0	-3.065993	0.249810	0.526294
9	6	0	-3.136928	1.786535	-0.531120
10	6	0	-4.666359	-0.563355	-0.029337
11	1	0	3.562143	0.400576	-2.001759
12	1	0	4.945780	0.652532	-0.909273
13	1	0	4.527688	-0.981349	-1.434320
14	6	0	1.258903	-2.540192	0.041555
15	1	0	1.460261	-0.953100	-1.405871
16	6	0	2.109109	2.400902	-0.515590
17	1	0	2.117122	1.741034	1.540280
18	1	0	1.124713	-0.551112	2.634673
19	1	0	-0.560408	-1.020463	2.286894
20	1	0	-0.191742	0.640751	2.746503
21	1	0	-1.644186	-1.716496	0.160163
22	6	0	-1.707393	-0.830538	-1.854976
23	1	0	-4.745826	-0.656187	-1.118831
24	1	0	-5.515318	0.028293	0.332781
25	1	0	-3.913361	2.450179	-0.135226
26	1	0	-3.360031	1.583815	-1.584845
27	1	0	-2.178269	2.311247	-0.468945
28	1	0	2.053412	-3.170136	-0.379138
29	1	0	1.258160	-2.699337	1.124942
30	1	0	0.306092	-2.909303	-0.356129
31	1	0	3.102999	2.865896	-0.520136
32	1	0	1.914250	2.024896	-1.526459
33	1	0	1.373697	3.191328	-0.319236
34	1	0	-2.622990	-1.228979	-2.322558
35	1	0	-1.531418	0.159980	-2.290463
36	1	0	-0.882959	-1.481646	-2.170771
37	1	0	-4.742066	-1.561272	0.415288

Transition state of 5′ + 5:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.035364	0.405880	-2.056409
2	15	0	-0.244571	0.232149	-0.219544
3	6	0	-1.485730	-1.240612	-0.131885
4	6	0	-1.475235	-1.920257	1.247475
5	6	0	-1.818912	1.370424	0.028612
6	6	0	-1.914610	2.597189	-0.882414
7	15	0	-2.945248	-0.059479	-0.478143
8	6	0	-4.153824	-0.323977	0.921512
9	6	0	-1.871641	1.821440	1.494626
10	6	0	-1.392806	-2.320245	-1.220461
11	6	0	2.018959	-0.748084	0.304239
12	15	0	3.078068	0.543415	-0.490086
13	6	0	4.777469	-0.056352	0.033621
14	6	0	2.924798	2.002687	0.666147
15	1	0	-3.716684	-0.300068	1.923683
16	1	0	-4.929057	0.447955	0.858763
17	1	0	-4.648162	-1.291475	0.777812
18	1	0	-0.890203	0.357258	-2.637393
19	1	0	0.713140	-0.378049	-2.401899
20	1	0	0.525722	1.363803	-2.250825
21	6	0	2.119841	-2.088177	-0.390340
22	6	0	1.950975	-0.820193	1.812110
23	1	0	4.854338	-0.239823	1.111730
24	1	0	3.600426	2.790141	0.313939
25	1	0	3.178092	1.768626	1.706046
26	1	0	1.904176	2.397021	0.635713
27	1	0	-2.263962	-2.986623	-1.151507
28	1	0	-1.389558	-1.901349	-2.230056
29	1	0	-0.498712	-2.942973	-1.105561
30	1	0	-2.829701	2.307120	1.724191
31	1	0	-1.736738	1.000296	2.205325
32	1	0	-1.075760	2.552198	1.693036
33	1	0	-2.822617	3.174854	-0.658429
34	1	0	-1.059702	3.270157	-0.725323
35	1	0	-1.949161	2.334456	-1.943070
36	1	0	-2.361654	-2.556359	1.369403
37	1	0	-0.597813	-2.569985	1.351173
38	1	0	-1.457647	-1.212365	2.081112
39	1	0	5.021305	-0.981609	-0.498447
40	1	0	5.527544	0.692386	-0.244952
41	1	0	3.099391	-2.564333	-0.203478
42	1	0	1.367530	-2.794937	-0.020724
43	1	0	2.013857	-2.012586	-1.479144
44	1	0	2.934330	-1.058282	2.251786
45	1	0	1.612725	0.121018	2.257193
46	1	0	1.262937	-1.606084	2.145499

Transition state of propyl + 2:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.064923	0.350962	0.382985
2	6	0	-0.925020	-0.735874	-0.800004
3	15	0	-2.582219	0.095411	-0.426989
4	6	0	-1.697317	0.821309	1.065860
5	6	0	0.332797	1.879631	-0.658931
6	6	0	-3.557778	-1.307965	0.324199
7	1	0	-3.893682	-1.984013	-0.470177
8	1	0	-4.449271	-0.906055	0.818309
9	1	0	-2.978994	-1.884488	1.056497
10	1	0	0.595501	2.714448	0.000032
11	1	0	-0.557125	2.159587	-1.232011
12	1	0	1.163727	1.719553	-1.351757
13	1	0	-1.853848	1.891125	1.234014
14	1	0	-1.902136	0.286351	1.999435
15	1	0	-0.604943	-0.686080	-1.844826
16	1	0	-0.883233	-1.783615	-0.479544
17	6	0	2.216985	-0.728860	-0.250837
18	1	0	2.012396	-1.738203	0.107984
19	1	0	2.126290	-0.638830	-1.335921
20	6	0	3.382521	-0.021351	0.389966
21	6	0	4.752463	-0.646595	0.048043
22	1	0	3.393908	1.034176	0.083821
23	1	0	3.254085	-0.022533	1.480540
24	1	0	5.566323	-0.100105	0.541083
25	1	0	4.802514	-1.691907	0.374895
26	1	0	4.940010	-0.626772	-1.032092

Transition state of propyl + 3:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.876175	-0.855861	-1.236570
2	15	0	-1.958473	-0.753341	0.298675
3	6	0	-0.463451	0.044860	1.138414
4	15	0	0.697152	-0.183527	-0.328281
5	6	0	1.663771	-1.798618	0.055729
6	6	0	2.326333	-2.224917	-1.270267
7	6	0	0.779143	-2.945936	0.578134
8	6	0	2.756523	-1.514003	1.103059
9	6	0	-3.149760	0.702888	-0.026035
10	6	0	-3.807174	1.031879	1.328782
11	6	0	-2.502144	1.971290	-0.604705
12	6	0	-4.218701	0.178395	-1.004708
13	6	0	2.158499	1.673120	0.507851
14	6	0	3.276122	1.962897	-0.457791
15	6	0	4.095750	3.214231	-0.082851
16	1	0	2.861517	2.096019	-1.466328
17	1	0	-0.162456	-0.477627	2.051909
18	1	0	-0.572666	1.104087	1.391098
19	1	0	-1.155443	-0.183090	-2.053188
20	1	0	-0.800649	-1.866087	-1.650287
21	1	0	2.441536	1.319110	1.500443
22	1	0	1.362253	2.418556	0.539049
23	1	0	4.561707	3.101646	0.903294
24	1	0	3.458617	4.105960	-0.048342
25	1	0	4.893792	3.398797	-0.813390
26	1	0	3.310322	-2.438702	1.314987
27	1	0	3.476423	-0.767855	0.756067
28	1	0	2.331182	-1.163055	2.050290
29	1	0	2.923521	-3.134030	-1.118038
30	1	0	1.582452	-2.446541	-2.044382
31	1	0	2.992931	-1.446040	-1.657308
32	1	0	1.402630	-3.832182	0.760681
33	1	0	0.289642	-2.692313	1.524086
34	1	0	0.002155	-3.237685	-0.134549
35	1	0	-3.265021	2.749314	-0.747413
36	1	0	-1.737886	2.387426	0.060651
37	1	0	-2.038410	1.792458	-1.580888
38	1	0	-4.984256	0.946606	-1.179337
39	1	0	-3.784351	-0.080477	-1.977899
40	1	0	-4.720926	-0.713101	-0.611919
41	1	0	-4.564231	1.817955	1.203981
42	1	0	-4.301993	0.153714	1.759087
43	1	0	-3.072828	1.395826	2.057586
44	1	0	3.957842	1.102975	-0.520112

Transition state of propyl + 4:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.665132	-1.092302	0.544948
2	15	0	2.299526	-0.118275	0.626517
3	6	0	3.549843	-1.151686	-0.301593
4	15	0	-0.274147	0.369228	-0.226689
5	6	0	-0.564938	1.449783	1.273683
6	6	0	1.526456	0.967523	-0.701848
7	6	0	-2.541997	-0.724750	-0.042946
8	6	0	-3.613935	0.306701	-0.274928
9	6	0	-5.045371	-0.263262	-0.175932
10	1	0	3.875169	-1.990368	0.324259
11	1	0	4.429384	-0.526949	-0.494450
12	1	0	3.185660	-1.544683	-1.256539
13	1	0	-0.846710	2.455483	0.944103
14	1	0	0.311506	1.531000	1.923355
15	1	0	-1.396002	1.041834	1.855521
16	6	0	1.842257	2.458767	-0.718797
17	1	0	1.714513	0.540136	-1.695967
18	1	0	0.300289	-1.320764	1.552355
19	6	0	0.614149	-2.361049	-0.312603
20	1	0	-2.445513	-1.493481	-0.809057
21	1	0	-2.445397	-1.115831	0.972601
22	1	0	-3.513958	1.125932	0.450574
23	1	0	-3.478597	0.757269	-1.267306
24	1	0	-5.793202	0.519284	-0.356564
25	1	0	-5.205430	-1.058780	-0.913134
26	1	0	-5.235309	-0.687439	0.817161
27	1	0	1.291736	-3.131518	0.075243
28	1	0	-0.397398	-2.783164	-0.318744
29	1	0	0.893609	-2.170078	-1.354863
30	1	0	2.883101	2.641087	-1.017573
31	1	0	1.201088	2.991148	-1.433897
32	1	0	1.701203	2.917252	0.265617

Transition state of propyl + 5:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.570988	-1.229513	0.200288
2	15	0	2.202441	-0.293221	0.534476
3	6	0	3.432397	-0.908721	-0.732329
4	15	0	-0.413508	0.412512	0.037700
5	6	0	-0.753846	0.884517	1.815516
6	6	0	1.366714	1.236468	-0.211280
7	6	0	-2.708622	-0.592823	-0.268940
8	6	0	-3.700859	0.539310	-0.335569
9	6	0	-5.154889	0.072369	-0.559626
10	1	0	3.764783	-1.911001	-0.439163
11	1	0	4.311062	-0.254566	-0.703293
12	1	0	3.060842	-0.949673	-1.760126
13	1	0	-1.049684	1.938369	1.846518
14	1	0	0.106095	0.748971	2.477272
15	1	0	-1.587815	0.290340	2.197483
16	6	0	1.638572	2.525275	0.569873
17	6	0	1.588674	1.498122	-1.706692
18	6	0	0.186575	-2.148585	1.366748
19	6	0	0.495530	-2.025607	-1.112727
20	1	0	-2.556824	-1.144719	-1.196488
21	1	0	-2.768148	-1.241298	0.607967
22	1	0	-3.661753	1.129172	0.591020
23	1	0	-3.418768	1.224156	-1.146383
24	1	0	-5.839608	0.928583	-0.609399
25	1	0	-5.249234	-0.488807	-1.496817
26	1	0	-5.492153	-0.580984	0.253854
27	1	0	2.655386	2.890075	0.365376
28	1	0	0.945204	3.322897	0.268102
29	1	0	1.554298	2.391403	1.651744
30	1	0	2.629494	1.786937	-1.907110
31	1	0	1.356603	0.634973	-2.337639
32	1	0	0.946991	2.323618	-2.042928
33	1	0	0.874787	-3.003835	1.414532
34	1	0	0.234012	-1.641438	2.334462
35	1	0	-0.825611	-2.553569	1.239825
36	1	0	1.207326	-2.861392	-1.101997
37	1	0	-0.507022	-2.451922	-1.242241
38	1	0	0.708322	-1.420526	-1.998794

1.3 Optimised geometries at B3LYP/6-31G(d) level for the products of studied reactions presented as Gaussian Archives:

Product of 2′ + 2:

1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C7H18P3(2)\MXN501\24-Mar-2007\0\\#
UB3LYP/6-31G* FOPT SCF=TIGHT INT=ULTRAFINE FREQ=NORAMAN MAXDISK=134217
728\\Untitled-1\\0,2\C,4.2589333422,-0.7338284715,-1.114032817\P,3.132
0297437,-0.0341999597,0.2003239158\C,1.4424026276,-0.4223703627,-0.518
7979684\P,0.0260122762,0.2279096934,0.530476305\C,-1.4016154159,-0.452
9581282,-0.4823798257\P,-3.0797463329,-0.0727157284,0.2737225192\C,-4.
1670906704,-0.8404159998,-1.0368727048\C,-3.2444428456,1.7226049461,-0
.2049169025\C,0.0573914827,-1.0144585391,1.9191040048\C,3.2831007034,1
.7182556882,-0.034182828\H,5.2886594366,-0.4281858452,-0.9004085114\H,
3.9893531967,-0.3906314188,-2.1183473672\H,4.2199466996,-1.8275708076,
-1.0826257017\H,1.3711599059,-1.5139270092,-0.6219189685\H,1.357749676
9,0.0195063574,-1.5192725747\H,0.9469572277,-0.8487060443,2.5347651308
\H,-0.8274432009,-0.8737239748,2.5475231061\H,0.0693694736,-2.04974019
77,1.5555375501\H,-1.3128090399,-1.5443231225,-0.5767416596\H,-1.33623
37314,-0.0262815798,-1.4930360473\H,-3.0836037383,1.8889931706,-1.2775
614976\H,-4.24596071,2.0788560436,0.0595550304\H,-2.5160108184,2.31730
1056,0.3549526451\H,-4.0817710974,-1.9315593966,-0.994914959\H,-3.9108
415329,-0.5053156633,-2.049642831\H,-5.2127585075,-0.5815127963,-0.836
839771\H,4.2723544304,2.1686076094,-0.0733127628\H,2.4653716807,2.3723
287406,0.2569223414\\Version=IA64L-G03RevC.02\State=2-A\HF=-1301.59211
56\S2=0.756267\S2-1=0.\S2A=0.750024\RMSD=9.368e-09\RMSF=7.004e-06\Dipo
le=-0.0570377,-0.3745135,-0.9243519\PG=C01 [X(C7H18P3)]\\@

Product of 3′ + 3:

1\1\GINC-AC23\FOpt\UB3LYP\6-31G(d)\C16H36P3(2)\MXN501\12-Oct-2007\0\\#
B3LYP/6-31G* Fopt Scf=tight Int=UltraFine Freq=Noraman maxdisk=536870
912\\Untitled-1\\0,2\C,0.1313545366,0.0889280524,-0.1699651962\P,0.244
0974895,0.1280580365,1.7431037154\C,1.8857954641,0.6935688427,2.092457
8804\C,-0.8069420568,1.6054702798,2.2388018069\P,-0.7759325493,1.96189
93107,4.096162685\C,-2.3871189046,1.1323504566,4.7214711726\C,-1.20342
96775,3.7947362699,3.9642735518\P,-1.3795206567,4.8114077621,5.5423153
13\C,0.4146034542,5.0829115734,6.1556665163\C,-1.7650669896,6.44109373
51,4.706908989\C,1.1188878347,-0.9900281564,-0.6548276441\C,0.47339647
66,1.4378969132,-0.8229304044\C,-1.3006655771,-0.3352175169,-0.5469363
039\H,-1.8311757246,1.4364164335,1.8875262851\H,-0.4335153332,2.504169
1356,1.7369489991\C,-2.3080041984,-0.3648292569,4.3616791962\C,-2.4008
479389,1.2629373262,6.2592024583\C,-3.6787949338,1.7350729735,4.145904
3142\H,-2.1503888077,3.925620418,3.4249930453\H,-0.4221930441,4.230353
4287,3.3285843495\C,1.4461318296,5.3136649367,5.039825145\C,0.38490020
96,6.3086247866,7.0924726032\C,0.8173410425,3.8440975715,6.9819791622\
H,-2.7183132416,6.3367207369,4.1772627143\H,-1.004719525,6.7614798207,
3.9845367898\H,-1.892651398,7.227078864,5.457103425\H,2.7413529771,0.1
742167299,1.6689248505\H,2.0697915204,1.241661413,3.0127792996\H,2.426
1765151,5.5457548956,5.4790766481\H,1.5761880497,4.4241715815,4.414224
6207\H,1.1758905201,6.154402549,4.3900096051\H,1.8195955288,3.98974929
62,7.4082726433\H,0.1218742914,3.6751273436,7.8120398602\H,0.84304694,
2.9363690499,6.3701897048\H,1.350223548,6.4048253804,7.6069391627\H,0.
2100736328,7.2423458839,6.5470600051\H,-0.3911272205,6.2126641097,7.86
18297685\H,-4.5454173067,1.154595105,4.4908188876\H,-3.8297204955,2.76
81568634,4.4763062738\H,-3.6966786272,1.7190427469,3.0493907872\H,-3.1
44442621,-0.8985516577,4.8329141151\H,-2.3689480667,-0.540864666,3.282
945794\H,-1.3775606086,-0.8204500581,4.7190075579\H,-3.2777219339,0.74
10930499,6.6666899298\H,-1.5068646821,0.8122310654,6.704837278\H,-2.45

41816182,2.3076684118,6.5818406811\H,-1.3845347042,-0.4443494636,-1.63
65220356\H,-1.5701365478,-1.2954595434,-0.0923790067\H,-2.0445241698,0
.407742953,-0.2365054019\H,0.4426846026,1.3466358188,-1.9178201787\H,-
0.2408123158,2.2203154911,-0.5427749519\H,1.4749923745,1.7754033028,-0
.5369283787\H,1.026403531,-1.1181310453,-1.7417338624\H,2.1584585306,-
0.7158261331,-0.4452909816\H,0.9206150223,-1.9607293492,-0.1856457964\
\Version=IA64L-G03RevD.01\State=2-A\HF=-1655.3921308\S2=0.756698\S2-1=
0.\S2A=0.750027\RMSD=4.709e-09\RMSF=9.892e-07\Thermal=0.\Dipole=-0.175
9148,0.5417374,-0.6576211\PG=C01 [X(C16H36P3)]\\@

Product of 4′ + 4:

1\1\GINC-AC56\FOpt\UB3LYP\6-31G(d)\C10H24P3(2)\MXN501\16-Mar-2007\0\\#
UB3LYP/6-31G* FOPT SCF=TIGHT INT=ULTRAFINE MAXDISK=134217728\\Untitle
d-1\\0,2\C,-4.2784797952,0.0491326652,1.9597580271\P,-2.4360094255,0.1
906629002,2.2374693127\C,-2.2898261744,2.0343557997,2.4803194685\C,-1.
7912816126,-0.0334777426,0.4659797441\C,-2.2314123701,1.0312782937,-0.
5499215858\P,0.0968819683,-0.1503192149,0.5866173049\C,0.5920667062,-0
.490706314,-1.2135966135\P,2.48225326,-0.6018387905,-1.3024403022\C,2.
7651986542,-0.7275879436,-3.1514195134\C,2.9757973187,1.0845296462,-0.
9494407239\C,4.3611474651,1.6045542529,-1.1941884246\C,-0.0526371322,-
1.7220318582,-1.8693618779\H,-4.7900329598,0.2631300207,2.9047777307\H
,-4.5289597506,-0.9783481749,1.6746520171\H,-4.6680432286,0.7324919731
,1.1963923232\H,-2.6840599211,2.2860045859,3.4708783279\H,-1.233131196
7,2.3193121878,2.4590854109\H,-2.8316820838,2.6222483432,1.7312542891\
H,-2.1896410449,-1.0118735509,0.1602276403\H,-3.3128800705,1.204971564
9,-0.5118416039\H,-1.7343158242,1.9909670394,-0.3690364207\H,-1.992645
3089,0.7260559604,-1.5752766845\H,-1.1421999337,-1.7163234187,-1.74922
42025\H,0.3241108547,-2.6551817843,-1.4365212901\H,0.1510857807,-1.752
1349835,-2.9459859326\H,-0.3211160865,-2.6118973623,0.8590241965\H,0.0
059922812,-1.7892476539,2.3991607027\H,1.3421563856,-2.1396313366,1.28
47459403\H,4.3391278487,2.6754149984,-1.4392756237\H,4.8706694363,1.08
94813506,-2.016736438\H,5.0051842299,1.5031201876,-0.3045938765\H,2.17
42367854,0.0021120568,-3.7161525085\H,3.8260534426,-0.5542301189,-3.35
81679676\H,2.5240273821,-1.7372460657,-3.4966280868\H,0.300690579,0.41
08888547,-1.7672870723\H,2.3749419721,1.6198694088,-0.2158431974\C,0.2
900175052,-1.84296805,1.3448177651\\Version=IA64L-G03RevC.02\State=2-A
\HF=-1419.5254855\S2=0.755871\S2-1=0.\S2A=0.750024\RMSD=6.499e-09\RMSF
=1.251e-06\Dipole=-0.6119941,0.1924655,-0.7346989\PG=C01 [X(C10H24P3)]
\\@

Product of 5′ + 5:

1\1\GINC-AC21\FOpt\UB3LYP\6-31G(d)\C13H30P3(2)\MXN501\11-Oct-2007\0\\#
UB3LYP/6-31G* Fopt Scf=tight Int=UltraFine freq=Noraman maxdisk=26843
5456\\Untitled-1\\0,2\C,4.867533,0.078139,0.348917\P,3.316656,0.374337
,-0.653336\C,3.156238,2.215806,-0.386136\C,1.937481,-0.347409,0.491012
\C,1.852408,0.407362,1.831566\C,2.282706,-1.825454,0.752114\P,0.332144
,-0.023396,-0.530552\C,-1.166246,-0.955377,0.242336\C,-1.324914,-0.659
914,1.740479\C,-1.19327,-2.478095,0.010108\P,-2.629951,-0.178963,-0.79
4749\C,-4.061923,-1.25865,-0.262526\C,-3.013337,1.406323,-0.008344\C,-
2.299138,2.641375,-0.483717\C,-4.080745,1.638398,1.02397\C,0.609071,-1
.053576,-2.062035\H,5.674193,0.645036,-0.129699\H,4.800265,0.40007,1.3
94721\H,5.149065,-0.978346,0.319092\H,3.920799,2.713905,-0.992755\H,3.
287049,2.523458,0.657098\H,2.176226,2.553749,-0.735302\H,1.455513,1.42
0098,1.710603\H,2.839652,0.487329,2.303343\H,1.207927,-0.116536,2.5441
3\H,3.224733,-1.916945,1.307786\H,1.510704,-2.304674,1.363921\H,2.3892
02,-2.402188,-0.172873\H,-0.593125,-1.221181,2.334384\H,-1.206999,0.40
3738,1.968764\H,-2.317273,-0.967679,2.093627\H,0.875432,-2.096914,-1.8

6508\H,1.406221,-0.600341,-2.655083\H,-0.313908,-1.030286,-2.649616\H,
-1.26908,-2.741509,-1.049648\H,-2.049071,-2.931045,0.525535\H,-0.29183
,-2.957557,0.405215\H,-3.978088,-2.23001,-0.757829\H,-4.987866,-0.7905
47,-0.61198\H,-4.144371,-1.42593,0.817395\H,-3.655568,2.123838,1.91806
4\H,-4.584447,0.727227,1.355305\H,-4.854664,2.328475,0.649138\H,-1.762
825,3.135464,0.342666\H,-3.016936,3.384908,-0.869346\H,-1.568862,2.431
154,-1.268469\\Version=IA64L-G03RevD.01\State=2-A\HF=-1537.4486607\S2=
0.75618\S2-1=0.\S2A=0.750028\RMSD=5.853e-09\RMSF=4.354e-06\Thermal=0.\
Dipole=-0.0090868,-0.235269,0.9233962\PG=C01 [X(C13H30P3)]\\@

Product of propyl + 2:

1\1\GINC-AC22\FOpt\UB3LYP\6-31G(d)\C7H17P2(2)\MXN501\03-Sep-2007\0\\#
B3LYP/6-31G* Fopt Scf=tight Int=UltraFine Freq=Noraman maxdisk=2684354
56\\Untitled-1\\0,2\C,0.0333173078,-0.1148377191,-0.0075129562\P,0.083
1202256,-0.0535117369,1.8581389988\C,1.8167689491,0.0911898684,2.20782
1014\C,-0.5711344487,1.6730341362,2.1893506589\P,-0.5793853949,2.12439
60189,4.0130707686\C,-2.0689286414,1.1452812805,4.5670026816\C,-1.3375
525367,3.8358376576,3.8677842817\C,-1.5870376686,4.5111468528,5.225237
7722\H,-0.6497174811,4.5352912831,5.7965903706\C,-2.1397894617,5.93444
18685,5.0853540511\H,0.547006545,-1.0198198226,-0.34886667\H,0.5121763
901,0.7573692683,-0.4647687437\H,-1.0075298947,-0.1730359776,-0.342318
2539\H,-1.588109138,1.7246162138,1.7765712217\H,0.0465844527,2.4085237
329,1.6591863673\H,-1.8478144807,0.0762510585,4.4862759676\H,-2.285654
7625,1.3633818099,5.6177848449\H,-2.9629151932,1.3640977838,3.96920750
49\H,-2.2723210019,3.7879528559,3.2897008497\H,-0.6338698981,4.4441841
963,3.2827325948\H,-3.0943879433,5.9384568574,4.5450134111\H,-1.443420
0921,6.5765665595,4.5322548434\H,-2.309638187,6.3932148151,6.066300284
3\H,2.5140017785,-0.6096182408,1.7542861593\H,2.1411903049,0.569448029
9,3.1282602573\H,-2.2900379698,3.9082812675,5.8155532772\\Version=IA64
L-G03RevD.01\State=2-A\HF=-959.6380323\S2=0.756252\S2-1=0.\S2A=0.75002
4\RMSD=4.453e-09\RMSF=1.832e-06\Thermal=0.\Dipole=-0.42492,0.3981804,-
0.4328442\PG=C01 [X(C7H17P2)]\\@

Product of propyl + 3:

1\1\GINC-AC28\FOpt\UB3LYP\6-31G(d)\C13H29P2(2)\MXN501\12-Oct-2007\0\\#
B3LYP/6-31G* Fopt Scf=tight Int=UltraFine Freq=Noraman maxdisk=268435
456\\Untitled-1\\0,2\C,0.0828407043,0.08874828,-0.1752553578\P,-0.0281
681858,0.0207407188,1.738016458\C,1.645048781,0.1351729564,2.305746699
6\C,-0.7330158172,1.6913198136,2.2205297512\P,-0.8257627834,2.03053645
97,4.0757083859\C,-2.3481666096,1.02299951,4.6683764552\C,-1.494925107
1,3.7933877935,3.9597666129\C,-1.1206888868,4.6785003188,5.1602208832\
H,-0.0290553649,4.6825346379,5.2748271657\C,-1.6295932908,6.1171721785
,5.0122374933\C,0.8343963381,-1.1796027621,-0.6228098227\C,0.815752949
5,1.3371986698,-0.6914122648\C,-1.3528903741,0.0466566488,-0.730696943
4\H,-1.7170028828,1.7965820227,1.7502044752\H,-0.0902833594,2.48356224
9,1.8196821293\C,-1.868225465,-0.4140250693,4.9601735729\C,-2.82999981
73,1.652138899,5.9912142332\C,-3.5142155674,0.9810196527,3.6675938781\
H,-2.5828526368,3.7959262048,3.807029874\H,-1.0600976379,4.2313420271,
3.0516336707\H,-2.7234916734,6.146629583,4.932992837\H,-1.2207419033,6
.5919869833,4.1116096869\H,-1.3414407143,6.7317325526,5.8730291965\H,2
.3826077897,-0.5935127343,1.9805233251\H,1.8577435604,0.6525372915,3.2
374240802\H,-1.5183747683,4.2460124207,6.0865245245\H,-4.3716679372,0.
4584956765,4.1139240905\H,-3.8574263868,1.9834328904,3.3847706488\H,-3
.2469951405,0.4399544013,2.7537030433\H,-3.6025433977,1.0152686534,6.4
42523411\H,-2.0138434445,1.7456987775,6.7177321701\H,-3.2704868027,2.6
440699224,5.8429389965\H,-2.697873007,-1.0083260499,5.3679146338\H,-1.

5099862506,-0.9169335221,4.05602804\H,-1.0563316692,-0.4213708261,5.69
60875513\H,-1.3287805365,0.0081662158,-1.8280016649\H,-1.8970472417,-0
.8362394468,-0.3762339705\H,-1.9285181807,0.9359216838,-0.4488419642\H
,0.8470802498,-1.2371482055,-1.7195219335\H,1.8757293444,-1.1774493791
,-0.2830886665\H,0.3535131244,-2.089821691,-0.2459323397\H,0.898563469
1,1.3006063432,-1.7867419486\H,0.2812732777,2.2593940668,-0.4374842743
\H,1.8262337356,1.4051638828,-0.2751957909\\Version=IA64L-G03RevD.01\S
tate=2-A\HF=-1195.5055944\S2=0.756765\S2-1=0.\S2A=0.750027\RMSD=4.921e
-09\RMSF=3.344e-06\Thermal=0.\Dipole=-0.3850342,0.3454426,-0.4218515\P
G=C01 [X(C13H29P2)]\\@

Product of propyl + 4:

1\1\GINC-AC44\FOpt\UB3LYP\6-31G(d)\C9H21P2(2)\MXN501\03-Sep-2007\0\\#
B3LYP/6-31G* Fopt Scf=tight Int=UltraFine Freq=Noraman maxdisk=2684354
56\\Untitled-1\\0,2\C,-0.2099048651,-0.2923016866,0.2556049577\P,0.090
0943461,-0.0031090292,2.0753395662\C,1.8776701691,-0.0417072743,2.1417
480588\C,-0.4054114952,1.8317414932,2.2355868071\P,-0.6263384663,2.263
7588029,4.0657792136\C,-2.173631709,1.2876618743,4.4389492088\C,-1.372
2861825,3.9825684268,3.9147690381\C,-1.8460743796,4.5579591251,5.25914
61124\H,-1.0185951781,4.525129149,5.9804400987\C,-2.3611954666,5.99706
65136,5.1365485042\H,0.1431311766,-1.2963917866,-0.0019304816\H,0.2979
142728,0.4317884208,-0.3902547936\H,-1.2852739363,-0.255808475,0.05429
83811\H,-1.3964084434,1.8723793435,1.7573034345\C,0.5445654155,2.80789
98977,1.5250479698\H,-1.9552550869,0.2188931381,4.3598379275\H,-2.4964
110619,1.4909077673,5.4650752802\H,-2.9988138543,1.5293283713,3.756530
9713\H,-2.2026380717,3.9737709519,3.1924636226\H,-0.5968394335,4.64004
06423,3.5016768716\H,-3.209750561,6.0574033056,4.4440212961\H,-1.57833
33621,6.6669632249,4.7603090133\H,-2.694059191,6.384184712,6.106628364
9\H,2.3787481241,-0.6125384934,1.3592425261\C,2.6815373645,0.271419013
5,3.368236252\H,-2.6411284965,3.9259766709,5.6757133521\H,0.1210844844
,3.8181993184,1.4829501474\H,1.5102830523,2.8662733583,2.0379853895\H,
0.7400339342,2.4948670021,0.493465228\H,3.6216445341,0.7759144369,3.10
26666043\H,2.1403362683,0.9152027904,4.0692752841\H,2.9657130715,-0.64
21371599,3.9170689853\\Version=IA64L-G03RevD.01\State=2-A\HF=-1038.263
5662\S2=0.756141\S2-1=0.\S2A=0.750026\RMSD=9.250e-09\RMSF=1.098e-06\Th
ermal=0.\Dipole=-0.2644358,0.3395446,-0.5092683\PG=C01 [X(C9H21P2)]\\@

Product of propyl + 5:

1\1\GINC-AC18\FOpt\UB3LYP\6-31G(d)\C11H25P2(2)\MXN501\03-Sep-2007\0\\#
B3LYP/6-31G* Fopt Scf=tight Int=UltraFine Freq=Noraman maxdisk=268435
456\\Untitled-1\\0,2\C,-0.1461938141,-0.5834435279,0.314809663\P,-0.03
70023761,-0.1380153141,2.1270934372\C,1.7482863731,-0.0849837364,2.423
280278\C,-0.6270736569,1.7125887235,2.0953249104\P,-0.7277074311,2.193
9516769,3.9432839762\C,-2.3147795465,1.3689186754,4.4817950694\C,-1.30
61125726,3.982111209,3.8662766438\C,-1.5521238048,4.5796313681,5.26223
19086\H,-0.652060442,4.4496387692,5.8776474074\C,-1.927225987,6.065550
6916,5.2099599529\H,0.3579490647,-1.5440692203,0.1679927916\H,0.295308
869,0.1486322212,-0.3706113504\H,-1.1973204003,-0.7201348152,0.0453115
102\C,-1.9753057697,1.7676598166,1.355213433\C,0.389516571,2.637499989
1,1.4048017996\H,-2.2264863925,0.2887074446,4.331603649\H,-2.457607338
3,1.5458781258,5.5527566203\H,-3.2012236671,1.7309939364,3.948601585\H
,-2.2140792661,4.0845161763,3.2555134635\H,-0.51796576,4.5605620872,3.
3679028302\H,-2.8427322242,6.2239540684,4.626756036\H,-1.1308917389,6.
6586069177,4.743686935\H,-2.0982979969,6.468108563,6.2152029594\C,2.81
71906019,-0.1333025184,1.3682267053\C,2.2422810209,-0.0835728702,3.843
6102619\H,-2.3524885342,4.0246879079,5.7689119813\H,-0.0093105184,3.65
48486874,1.299710926\H,1.3296451647,2.699150544,1.963235465\H,0.623908
2977,2.2824713082,0.3936380673\H,2.8330638314,0.8206474984,4.061324823

3\H,1.4306451468,-0.1244305922,4.5743795265\H,2.9124245749,-0.9401446737,4.0268081275\H,-2.4446017532,2.7530267839,1.4661428715\H,-1.8404324317,1.6000860885,0.2796781239\H,-2.68485553,1.0178657829,1.7214740989\H,3.49294243,0.7332190204,1.460900315\H,3.4554847662,-1.024138379,1.4880909464\H,2.4317893179,-0.1386218653,0.3457807801\\Version=IA64L-G03RevD.01\State=2-A\HF=-1116.8868936\S2=0.756057\S2-1=0.\S2A=0.750027\RMSD=9.405e-09\RMSF=1.156e-06\Thermal=0.\Dipole=-0.1021108,0.3704627,-0.5121349\PG=C01 [X(C11H25P2)]\\@

Product of 2′ + 5a:

1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C10H24P3(2)\MXN501\12-Oct-2007\0\\# B3LYP/6-31G* Fopt Scf=tight Int=UltraFine Freq=Noraman maxdisk=268435456\\Untitled-1\\0,2\C,0.0909811647,-0.1073208819,0.0264550591\P,0.0222966802,-0.0211559682,1.8905863708\C,1.8507445684,-0.0233859999,2.3140403721\P,2.2826575116,-0.2281632065,4.1394831426\C,4.159078993,-0.2798309989,3.9277247759\P,5.0380410976,-1.2079867318,5.3068563383\C,6.7763816957,-1.1519316637,4.6216159361\C,-0.5108343355,-1.6501205395,2.3470174278\C,1.978402575,1.5045489455,4.9003063613\C,2.3908202546,2.6796226677,3.9993142467\C,0.4716725084,1.6051335068,5.2181469453\C,2.7614092573,1.569371292,6.2270603427\C,4.5877558759,-2.95704868,4.8407659337\H,2.2869639329,0.8920013355,1.8961726349\H,2.3200815729,-0.873972108,1.8041412746\H,4.5837149408,0.7301500949,3.8684907913\H,4.3696972466,-0.7697547581,2.9676270521\H,7.1659731234,-0.1299794788,4.6838041591\H,6.8327896978,-1.4866202377,3.5780102823\H,7.4266010083,-1.7914810087,5.2288671423\H,-1.3944305798,-2.07367607,1.8750750102\H,-0.2392559131,-2.0536754913,3.3186692527\H,2.2605855862,3.6268946041,4.5402759592\H,3.4427694266,2.6245221367,3.6944825802\H,1.7752469655,2.7375805132,3.0952427503\H,2.4931756382,2.4884373892,6.7653782443\H,2.5289465777,0.7199091605,6.879081722\H,3.8452483799,1.5803961605,6.0736493199\H,0.2622828547,2.5576146823,5.7242019827\H,-0.1434399797,1.5674419157,4.3128666613\H,0.1493720235,0.7953515929,5.8823237007\H,0.4448996871,0.849972759,-0.3700487784\H,0.7460416688,-0.9100225533,-0.3286942804\H,-0.9192949281,-0.2779837822,-0.3603198947\H,5.1322332112,-3.6557441907,5.4851720576\H,3.5167592519,-3.1113429777,5.0049162077\H,4.8218357969,-3.1898549298,3.7939794449\\Version=IA64L-G03RevD.01\State=2-A\HF=-1419.5228296\S2=0.756296\S2-1=0.\S2A=0.750025\RMSD=8.947e-09\RMSF=4.828e-06\Thermal=0.\Dipole=0.5145877,0.0867661,-0.8340032\PG=C01 [X(C10H24P3)]\\@

Product of 4a′ + 5:

1\1\GINC-AC15\FOpt\UB3LYP\6-31G(d)\C11H26P3(2)\MXN501\24-Mar-2007\0\\# UB3LYP/6-31G* FOPT SCF=TIGHT INT=ULTRAFINE FREQ=NORAMAN MAXDISK=134217728\\Untitled-1\\0,2\P,4.048885001,-0.1935899782,-0.747451\C,2.5957919987,0.237247014,0.422427\C,2.7205210038,-0.7067649853,1.633783\C,2.7110889908,1.7037750146,0.884956\P,1.0249869997,0.0542700055,-0.676283\C,1.1726540092,-1.7033179937,-1.289033\C,-0.5341969995,-0.0898500029,0.442708\C,-0.7040279923,-1.4284180038,1.182961\C,-0.6221880057,1.0613569966,1.45676\P,-1.9478230001,0.0261409895,-0.901586\C,-1.9487670099,1.8399609895,-1.325395\C,-3.4933639989,-0.1958920188,0.014955\C,-4.0005699914,-1.5972320216,0.22617\C,-4.4423190048,0.896162976,0.421282\H,5.0496479975,0.4648070272,0.028913\H,3.8996229951,0.907264021,-1.640438\H,2.6116690095,-1.7603869859,1.35815\H,3.7026540032,-0.59239898,2.113762\H,1.9679660025,-0.4723569894,2.394198\H,3.6744639899,1.8728550198,1.382485\H,2.6406009871,2.3986350142,0.041841\H,1.9260159894,1.9654300104,1.602523\H,1.4057060131,-2.4376399924,-0.511117\H,1.9507670095,-1.7562619895,-2.055204\H,0.2215690106,-1.9727249988,-1.75849\H,-0.7731629877,-2.2815290042,0.501454\H,0.1303050087,-1.6145269993,1.866397\H,-1.6203149924,-1.4125090087,1.785451\H,0.0785859951,0.9108910004,2.287474\

H,-0.404784011,2.0372499978,1.012388\H,-1.628968006,1.1044579912,1.891
301\H,-0.9959130112,2.0775869946,-1.806102\H,-2.0875690136,2.512981988
7,-0.47363\H,-2.7499710109,2.0233269852,-2.048836\H,-4.7439620042,0.77
57589744,1.47449\H,-4.0319150103,1.9023519783,0.308673\H,-5.3766930046
,0.853160971,-0.163621\H,-4.1918509903,-1.8018930226,1.291823\H,-4.963
7409906,-1.7489440268,-0.289464\H,-3.3091949873,-2.3600680178,-0.14406
4\\Version=IA64L-G03RevC.02\State=2-A\HF=-1458.8144248\S2=0.756428\S2-
1=0.\S2A=0.75003\RMSD=5.637e-09\RMSF=1.949e-06\Dipole=-0.4156278,0.283
1068,0.8767966\PG=C01 [X(C11H26P3)]\\@

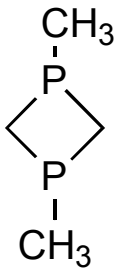
Table 1s. G3MP2-Rad and ONIOM (at MP2/6-311+G(3df,2p) level of theory) calculations of studies species.

Species[a]	Energy / Hartree					ZPE[b]	TC[b]	S[b]	G3MP2-RAD /kJ.mol^{-1}		
	B3LYP 6-31G(d)	MP2 6-31G(d)	CCSD(T) 6-31G(d)	MP2 GTMP2Large	MP2 6-311+G(3df,2p)	kJ.mol^{-1}	kJ.mol^{-1}	J.mol^{-1}K^{-1}	E(ZPE, 0 K)	H(298 K)	G(298 K)
2	-841.13923	-839.45392	-839.55667	-839.82138	-839.82343	340.0	24.7	372.1	-2205325.6	-2205301.0	-2205411.9
3	-1077.01114	-1074.45624	-1074.65197	-1075.13839	-1075.15055	779.2	45.4	526.7	-2823400.2	-2823354.8	-2823511.8
4	-919.76333	-917.78700	-917.92051	-918.25919	-918.26465	486.9	32.4	426.2	-2411346.2	-2411313.8	-2411440.9
5	-998.38520	-996.12271	-996.28610	-996.70149	-996.71055	632.0	39.5	467.8	-2617378.2	-2617338.7	-2617478.1
5a	-959.07539	-956.95507	-957.10423	-957.47964	-957.48675	559.6	35.2	451.9	-2514362.1	-2514327.0	-2514461.7
2’	-460.43285	-459.41321	-459.48887	-459.65983	-459.66177	256.2	20.4	332.5	-1207090.2	-1207069.8	-1207168.9
3’	-578.36954	-	-	-	-577.32431	475.8	30.7	412.6	-	-	-
4’	-499.74987	-498.58149	-498.67317	-498.87935	-498.88298	329.9	24.7	374.9	-1310103.5	-1310078.8	-1310190.6
5’	-539.06659	-537.75139	-537.85870	-538.10112	-538.10652	403.7	28.4	406.2	-1413404.0	-1413375.6	-1413496.8
4a’	-460.42715	-459.40545	-459.48192	-459.64820	-459.65042	251.8	20.2	338.1	-1207066.2	-1207046.0	-1207146.8
Propyl	-118.47111	-118.00008	-118.05556	-118.16493	-118.16945	229.0	15.6	290.2	-310391.5	-310375.9	-310462.5
2’+2 (TS)	-1301.56446	-1298.86170	-1299.04021	-1299.48067	-1299.48486	600.2	44.4	543.0	-3412410.6	-3412366.2	-3412528.1
4’+4 (TS)	-1419.50205	-1416.36510	-1416.58958	-1417.14249	-1417.15202	821.5	55.8	614.9	-3721453.6	-3721397.8	-3721581.1
5’+5 (TS)	-1532.06172	-	-	-	-1534.82048	1040.4	66.2	674.4	-	-	-
4a’+5 (TS)	-1458.79314	-1455.52753	-1455.75870	-1456.36224	-1456.36418	889.3	57.9	613.7	-3824448.0	-3824390.1	-3824573.1
3’+3 (TS)	-1655.36494	-	-	-	-1652.47335	1259.8	72.8	735.6	-	-	-
2’+5a (TS)	-1419.49605	-1416.36056	-1416.58521	-1417.13839	-1417.14774	821.1	54.0	607.7	-3721443.7	-3721389.7	-3721570.9
2’+2 (P)	-1301.59212	-1298.89458	-1299.07171	-1299.51229	-1299.51589	600.4	46.8	559.0	-3412489.9	-3412443.1	-3412609.7
4’+4 (P)	-1419.52549	-1416.39209	-1416.61575	-1417.16703	-1417.17602	821.9	58.3	642.0	-3721515.5	-3721457.1	-3721648.5
5’+5 (P)	-1537.44866	-	-	-	-1534.83419	1041.1	68.7	709.9	-	-	-
4a’+5 (P)	-1458.81442	-1455.54120	-1455.78034	-1456.36831	-1456.37969	890.7	60.0	639.9	-3824484.5	-3824424.4	-3824615.2
3’+3 (P)	-1655.39213	-	-	-	-1652.50055	1260.0	77.8	782.2	-	-	-
2’+5a (P)	-1419.52283	-1416.39128	-1416.61508	-1417.16671	-1417.17551	820.3	57.0	630.2	-3721516.6	-3721459.6	-3721647.5
propyl +2 (TS)	-959.60807	-957.44918	-957.60883	-957.98685	-957.99318	575.6	38.3	493.7	-2515715.8	-2515677.5	-2515824.7

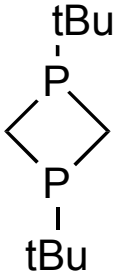
propyl +3 (TS)	-1195.47479	-1192.44858	-1192.70089	-1193.30169	-1193.31818	1015.8	58.5	637.1	-3133782.7	-3133724.2	-3133914.2
propyl +4 (TS)	-1038.23088	-1035.78239	-1035.97264	-1036.42492	-1036.43460	722.4	46.1	544.5	-2721740.6	-2721694.5	-2721856.9
propyl +5 (TS)	-1116.85210	-1114.11800	-1114.33821	-1114.86734	-1114.88063	867.3	53.2	585.9	-2927773.2	-2927720.0	-2927894.7
propyl +2 (P)	-959.63803	-957.48451	-957.64301	-958.02005	-958.02587	576.4	40.6	508.5	-2515799.1	-2515758.5	-2515910.1
propyl +3 (P)	-1195.50559	-1192.48243	-1192.73452	-1193.33261	-1193.34857	1016.3	61.1	657.5	-3133862.9	-3133801.7	-3133997.8
propyl +4 (P)	-1038.26357	-1035.81766	-1036.00766	-1036.45712	-1036.46646	723.6	48.6	569.7	-2721823.3	-2721774.6	-2721944.5
propyl +5 (P)	-1116.88689	-1114.15345	-1114.37378	-1114.89809	-1114.91121	869.7	55.9	**620.8**	-2927851.8	-2927796.0	-2927981.1

[a]For the structure of species see Figure 1s. TS and P stand for transition state and product, respectively. [b]Frequencies calculations are the level of B3LYP/6-31G(d); Zero-point-energies (ZPE), Thermal corrections (TC) and Entropies (S) have been scaled by 0.9806, 0.9989 and 1.0015, respectively.

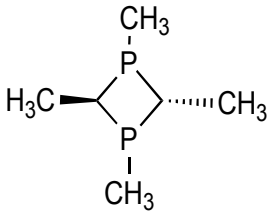
Figure 1s. Structure of studied species.



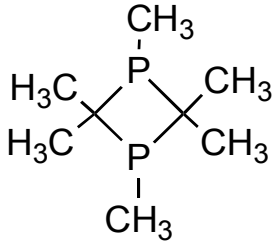
2



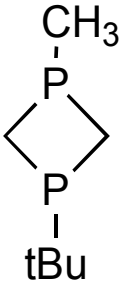
3



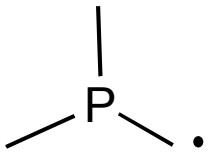
4



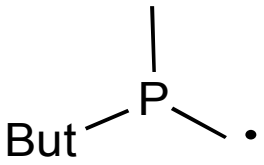
5



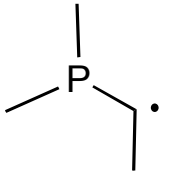
5a



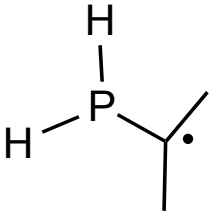
2’



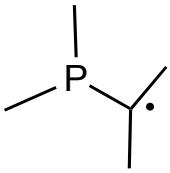
3’



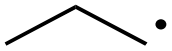
4’



4a’

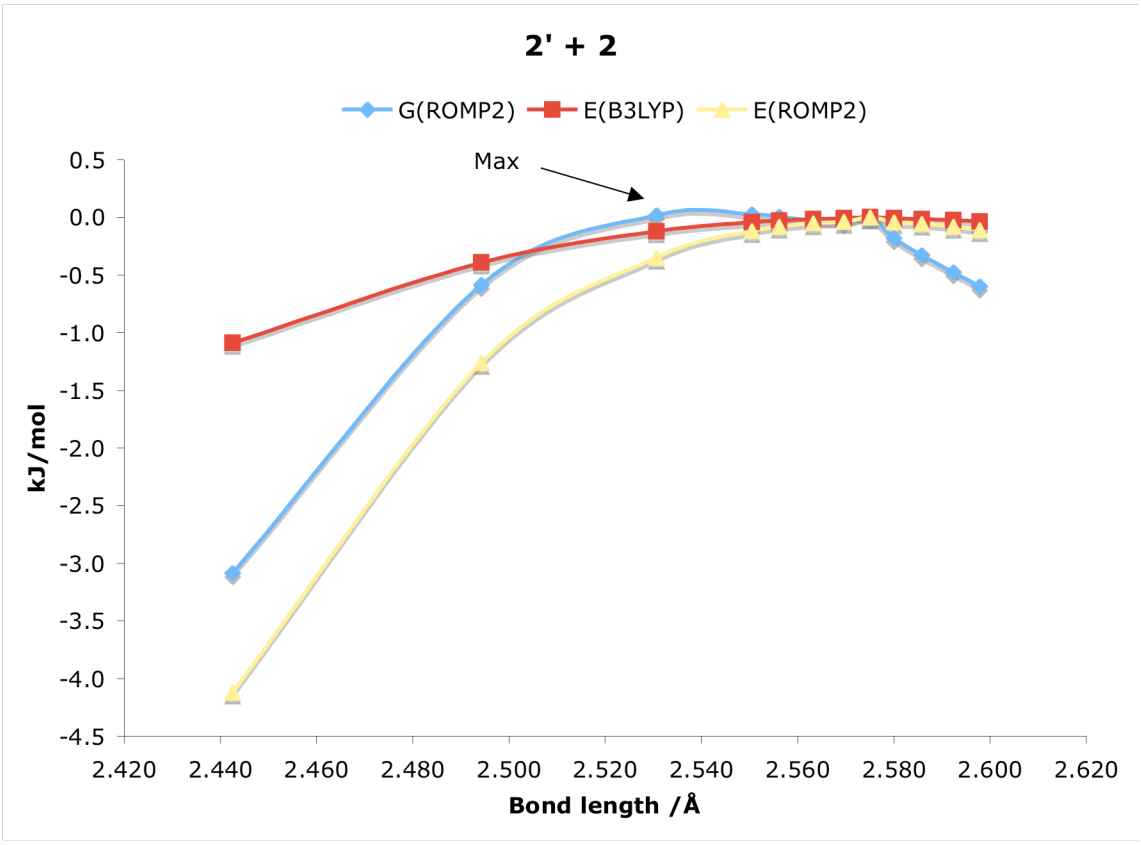


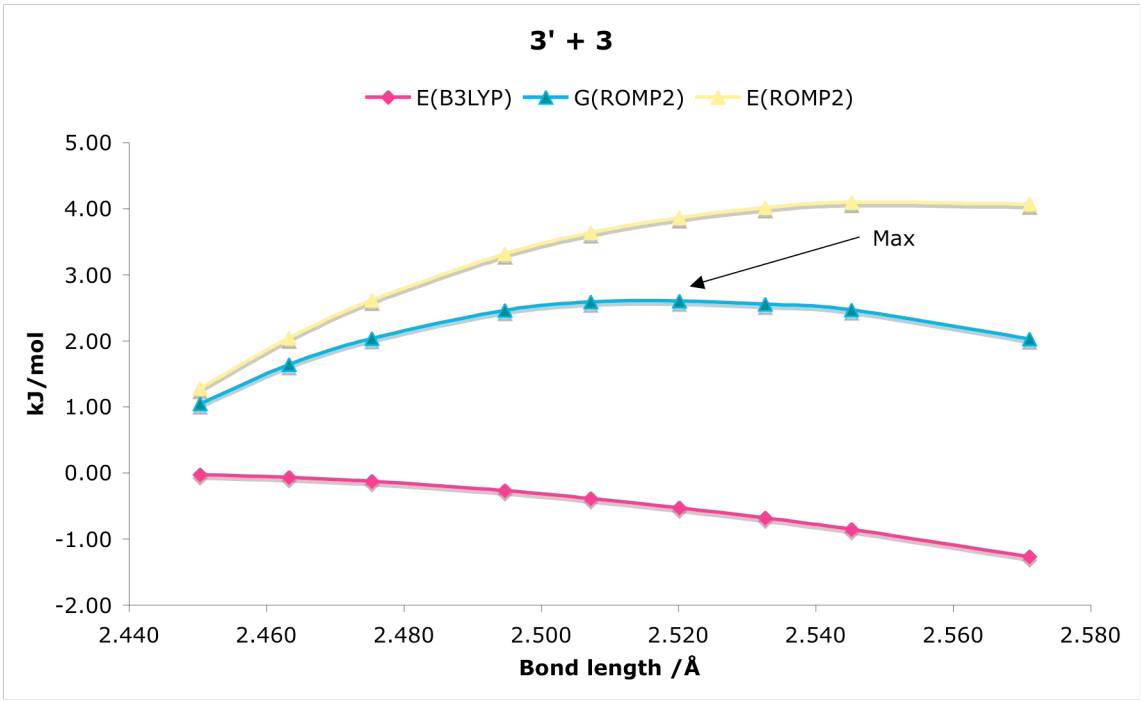
5’

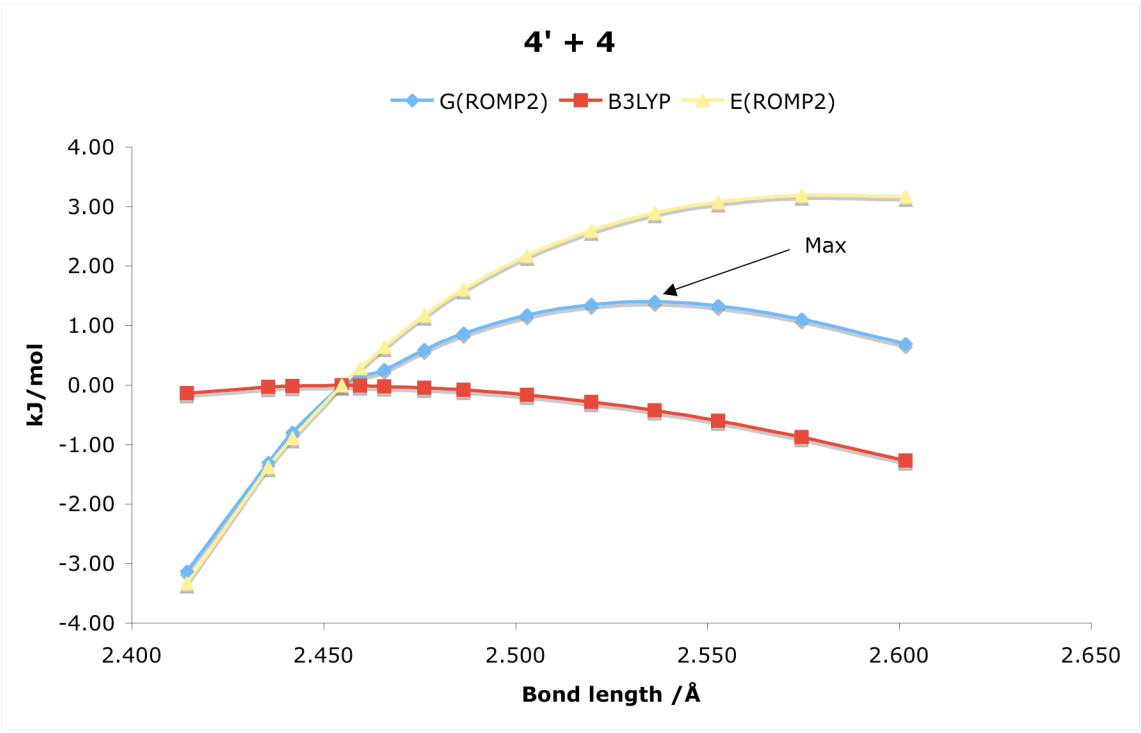


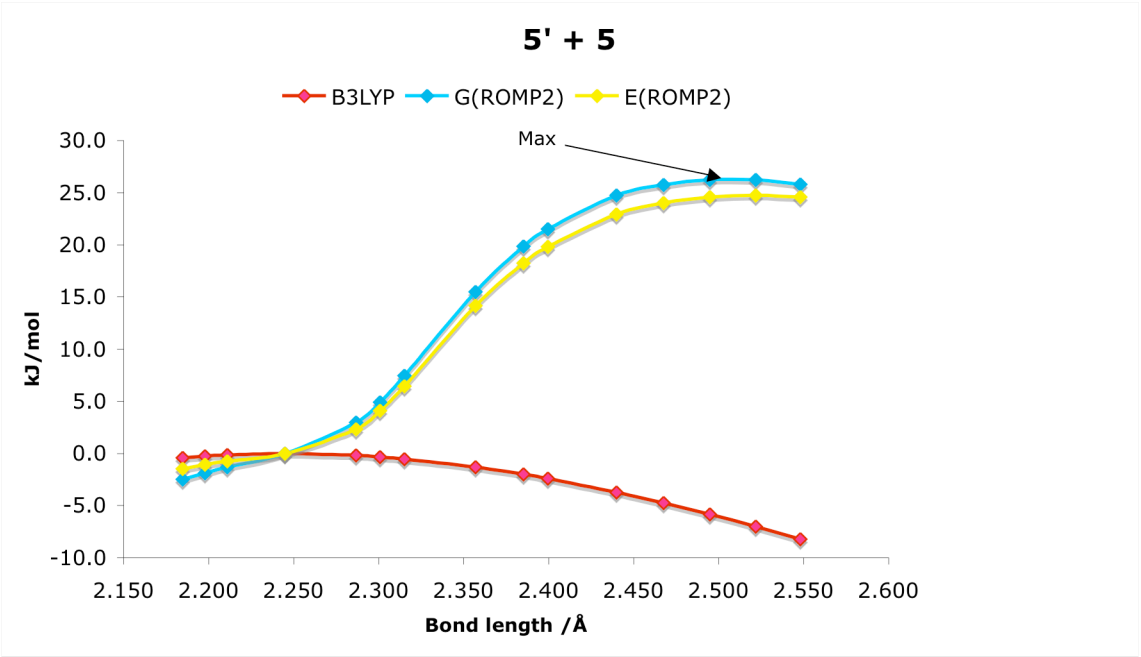
propyl

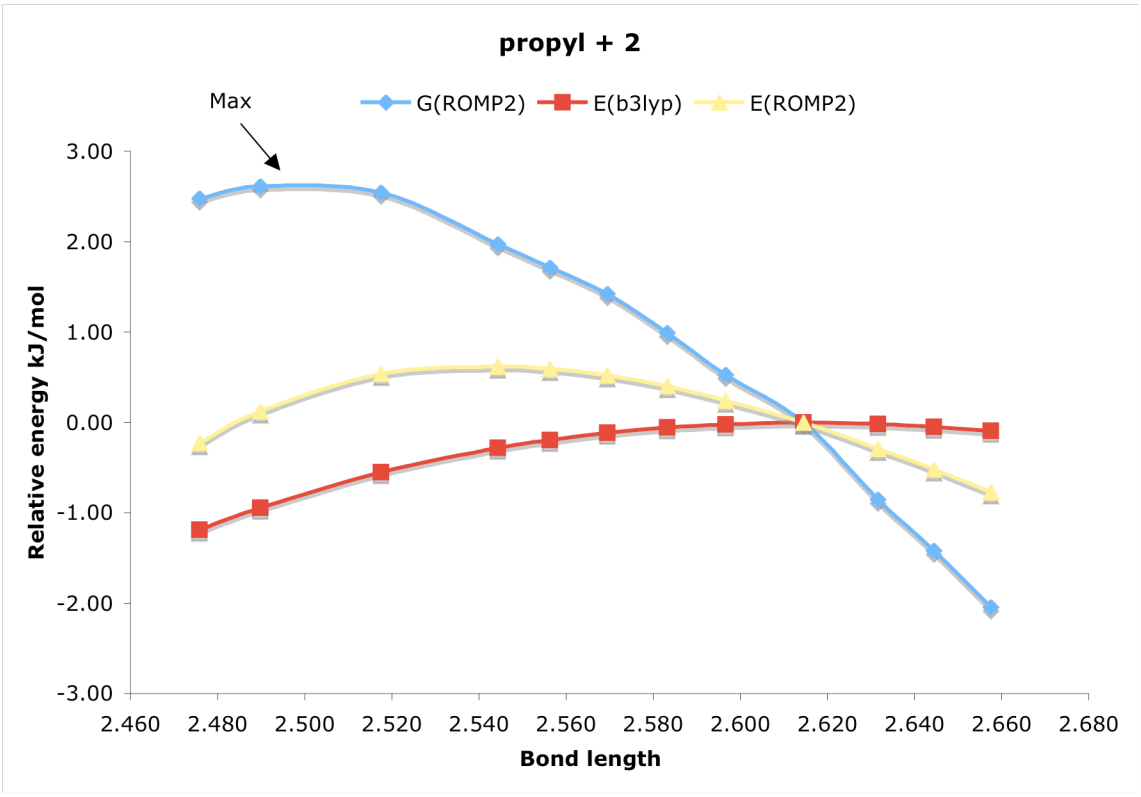
Figure 2s. The results of IRC calculations for the studied transition states.

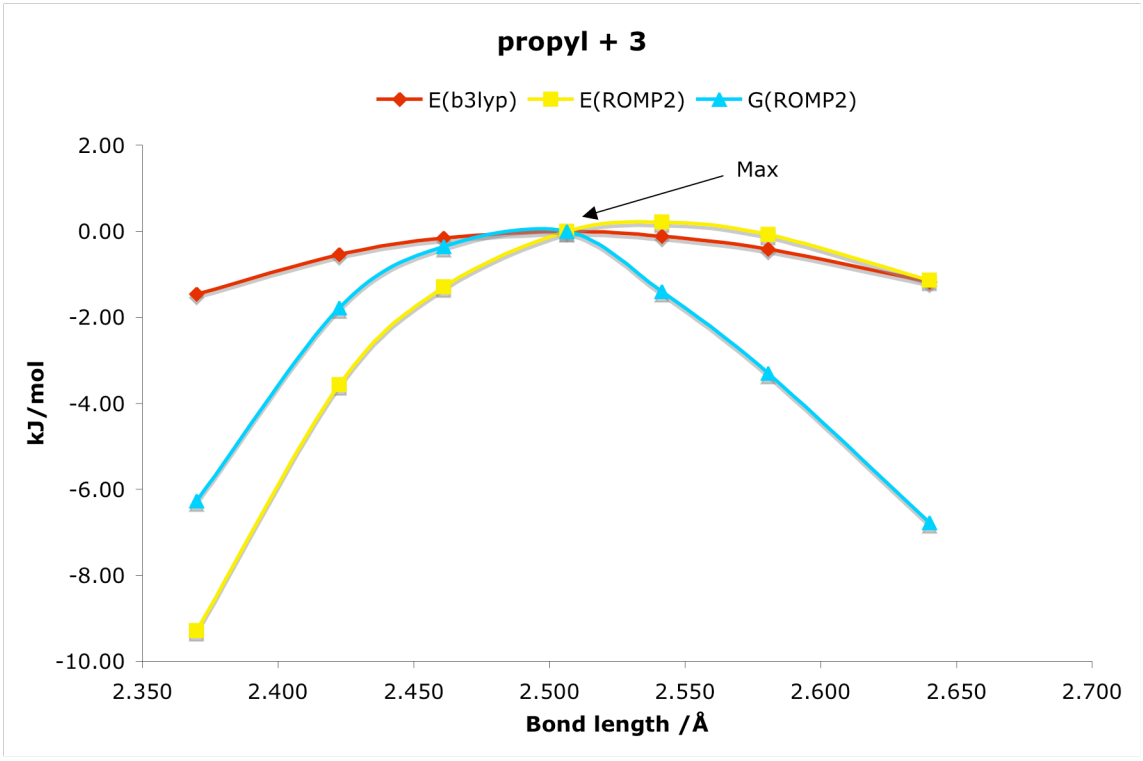


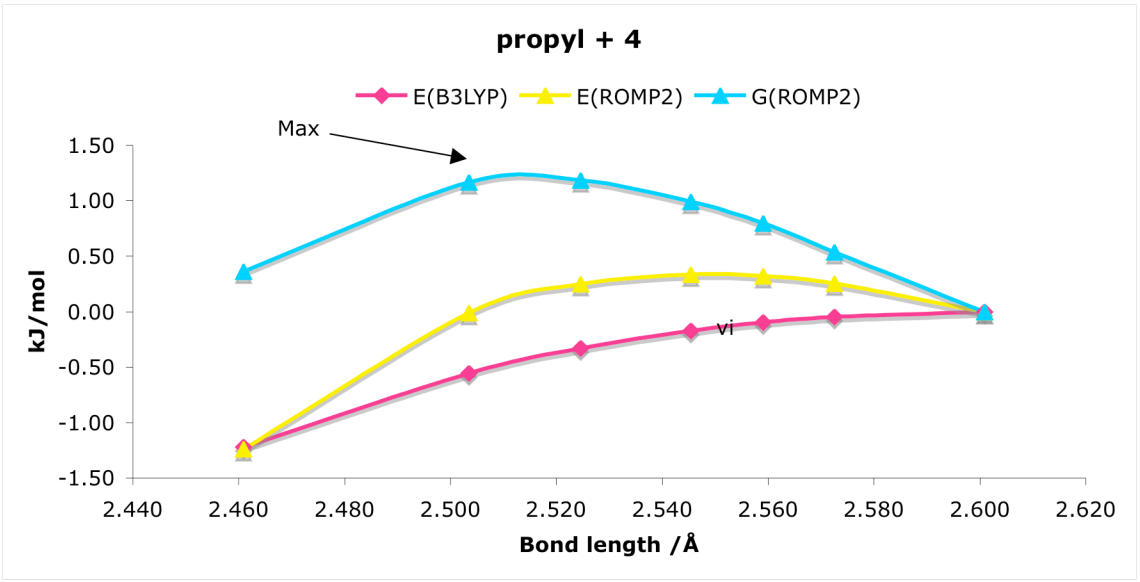


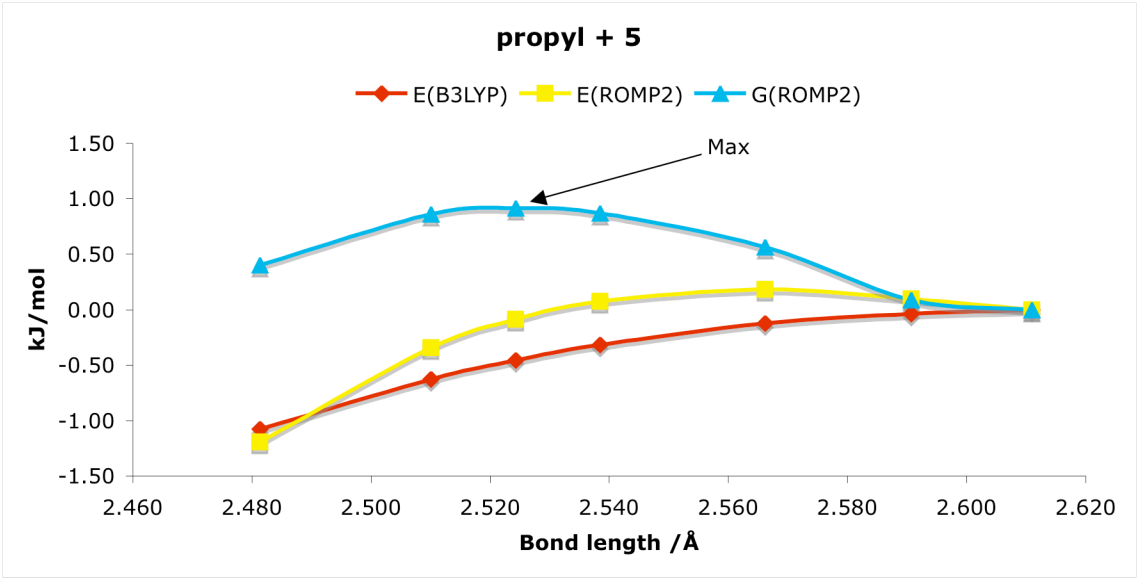

4' + 4
G(ROMP2)
B3LYP
E(ROMP2)
Max
kJ/mol
Bond length /Å
4.00
3.00
2.00
1.00
0.00
-1.00
-2.00
-3.00
-4.00
2.400
2.450
2.500
2.550
2.600
2.650


5' + 5
B3LYP
G(ROMP2)
E(ROMP2)
Max
kJ/mol
Bond length /Å
30.0
25.0
20.0
15.0
10.0
5.0
0.0
-5.0
-10.0
2.150
2.200
2.250
2.300
2.350
2.400
2.450
2.500
2.550
2.600


propyl + 2
Max
G(ROMP2)
E(b3lyp)
E(ROMP2)
3.00
2.00
1.00
0.00
-1.00
-2.00
-3.00
Relative energy kJ/mol
2.460
2.480
2.500
2.520
2.540
2.560
2.580
2.600
2.620
2.640
2.660
2.680
Bond length


propyl + 3
E(b3lyp)
E(ROMP2)
G(ROMP2)
Max
2.00
0.00
-2.00
-4.00
-6.00
-8.00
-10.00
kJ/mol
2.350
2.400
2.450
2.500
2.550
2.600
2.650
2.700
Bond length /Å


propyl + 4
E(B3LYP)
E(ROMP2)
G(ROMP2)
Max
vi
1.50
1.00
0.50
0.00
-0.50
-1.00
-1.50
kJ/mol
2.440
2.460
2.480
2.500
2.520
2.540
2.560
2.580
2.600
2.620
Bond length /Å


propyl + 5
E(B3LYP)
E(ROMP2)
G(ROMP2)
Max
1.50
1.00
0.50
0.00
-0.50
-1.00
-1.50
kJ/mol
2.460
2.480
2.500
2.520
2.540
2.560
2.580
2.600
2.620
Bond length /Å