Supplementary Material (ESI) for Chemical Communications

Supplementary Information for:

What Makes for a Good Catalytic Cycle? A Theoretical Study of the SPhos Ligand in the Suzuki-Miyaura Reaction.

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The Energetic Span Model

In the energetic span model,[1-4] the TOF of a catalytic cycle can be measured as

$$TOF = \frac{k_B T}{h} e^{-\delta E/RT} \qquad 1$$

$$\delta E = \begin{cases} G_{TDTS} - G_{TDI} & \text{if the } TDTS \text{ appears after the } TDI \\ G_{TDTS} - G_{TDI} + \Delta G_r & \text{if the } TDTS \text{ appears before the } TDI \end{cases} \qquad 2$$

where **δE**, the energetic span, is the difference in Gibbs energy between the **TDTS** (TOF Determining Transition State) to the **TDI** (TOF Determining Intermediate), with the addition of the global Gibbs energy of reaction (ΔG_r) when the TDTS appears before the TDI. δE is the effective activation barrier of the global reaction. The TDTS and TDI are the intermediate and transition state that maximize δE, according to eq 2.

The influence of reactants and products can be easily estimated in the energetic span model as:

$$TOF = \frac{k_B T}{h} e^{-\boldsymbol{\delta} E/RT} \prod \left.\frac{[R]}{[P]}\right|_{\substack{\text{From TDI} \\ \text{to TDTS}}} \qquad 3$$

In this expression, the TOF is dependent only on the concentration of reactants and products ([*R*] and [*P*]) that are consumed or produced in the section of the cycle that goes from the TDI to the TDTS.

Theoretical Method

As can be seen in eq 1, small errors in the Gibbs energies grow to exponential errors on the TOF. Therefore, accurate energy values are critical to obtain quantitative kinetic results. Previously we tested several DFT methods on a Pd based oxidative addition reaction,[5] and found the best speed/accuracy compromise by using the pure GGA B97D functional[6] with density fitting approximation and the Def2-SV(P) basis set[7,8] for geometry optimization and frequencies, and the hybrid PBE0[9] plus the D3 dispersion correction[10] with the Def2-TZVPP basis set[7,8] for single point energies in a continuum THF

solvent model (with the SMD solvation method[11]). The dispersion correction is critical for large and medium size systems, since most DFT methods are unable to asses long range interactions.[12,13]

In summary, all QM calculations were carried out with the PBE0+D3/Def2-TZVPP(THF)//B97D/Def2-SV(P) method, using Gaussian09.[14] The solvent model was the default IEFPCM. Unless specified, Gibbs thermal corrections were estimated at 298.15 K and 24.45 atmospheres, equivalent to a 1 M concentration in solvent (alternatively a correction of 1.89 kcal/mol can be added to a 1 atmosphere calculation).[5,15-17]

In these large systems several conformers can appear. Unless specified, we show only the lowest energy conformations found.

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Detailed Energies

Absolute energies in E_h. Relative Gibbs energies in kcal/mol.

		E (sv)	D3	G corr	abs G	Rel G
	PhBr	-2805.31554	-0.00465	0.06074	-2805.25945	
	$PhB(OH)_3$	-483.86588	-0.00868	0.10046	-483.77410	
	$B(OH)_3$	-252.34278	-0.00143	0.02363	-252.32058	
	Br	-2574.01084	0.00000	-0.01316	-2574.02400	
	Ph_2	-462.91789	-0.00963	0.14556	-462.78196	-58.3
SPhos	L	-1502.58654	-0.05300	0.48817	-1502.15137	
	A_2	-3133.13784	-0.15580	1.00184	-3132.29180	0.0
	A_1	-1630.52870	-0.06138	0.48706	-1630.10302	23.5
	B_1	-4435.85732	-0.08387	0.56381	-4435.37738	14.1
	T_1^{OA}	-4435.84599	-0.08320	0.56267	-4435.36652	20.9
	C_1	-4435.89970	-0.08333	0.56773	-4435.41530	-9.7
	D_1	-4919.76589	-0.11249	0.69382	-4919.18456	-6.6
	E_1	-2345.75332	-0.10399	0.69710	-2345.16021	-6.4
	T_1^{TM}	-2345.72802	-0.10754	0.69545	-2345.14011	6.2
	G_1	-2093.41836	-0.09312	0.64845	-2092.86303	-21.1
	T_1^{RE}	-2093.40271	-0.09343	0.64962	-2092.84653	-10.7
Conformers SPhos[a]	L Away	-1502.57327	-0.05595	0.48887	-1502.14036	6.9
	A_1 Away	-1630.51613	-0.06417	0.48889	-1630.09141	7.3
	A_2 In Away	-3133.14136	-0.15075	1.00177	-3132.29035	0.9
InPhos	L	-1581.12049	-0.06286	0.54382	-1580.63954	
	A_2	-3290.18045	-0.17557	1.11369	-3289.24233	0.0
	A_1	-1709.06195	-0.07280	0.54176	-1708.59298	6.2
	B_1	-4514.38996	-0.09516	0.61896	-4513.86616	-2.5
	T_1^{OA}	-4514.37753	-0.09428	0.61851	-4513.85330	5.6
	D_1	-4998.28113	-0.1244888	0.750477	-4997.65514	-11.8
	E_1	-2424.27050	-0.1147956	0.752133	-2423.63316	-13.1
	T_1^{TM}	-2424.24652	-0.11936	0.75262	-2423.61326	-0.6
	G_1	-2171.94307	-0.10588	0.70673	-2171.34222	-31.7
	T_1^{RE}	-2171.93452	-0.10497	0.70498	-2171.33451	-26.8

[a] Gibbs energies relative to the most stable conformers.

XYZ Geometries

```
7
B(OH)3
B -0.00001 -0.00004 -0.00004
O 0.79937 -1.12464 0.00001
O 0.57436 1.25452 0.00001
O -1.37368 -0.12987 0.00001
H 1.74277 -0.88341 0.00000
H -0.10619 1.95095 0.00002
H -1.63689 -1.06741 0.00001
```

```
18
PhB(OH)3
C -2.24049 -1.21407 0.02323
C -0.83345 -1.21378 -0.01272
C -0.07543 -0.01560 -0.04074
C -0.81890 1.19053 -0.03868
C -2.22766 1.21311 0.00061
C -2.94957 0.00483 0.03320
H -2.79615 -2.16875 0.04146
H -0.28302 -2.16795 -0.03140
B 1.59929 -0.02719 -0.00014
H -0.25492 2.13834 -0.07734
H -2.76953 2.17594 0.00193
H -4.05260 0.01132 0.06241
O 2.12475 1.27807 -0.54324
O 2.11520 -0.14510 1.39135
O 2.03857 -1.20021 -0.78728
H 1.68821 1.37665 -1.40802
H 2.12228 0.76647 1.73326
H 2.99403 -1.24829 -0.59765
```

```
12
PhBr
C 0.00000 0.00000 -0.09919
C 0.00000 1.22542 -0.78925
C 0.00000 1.21634 -2.19570
C 0.00000 0.00000 -2.90154
C 0.00000 -1.21634 -2.19570
C 0.00000 -1.22542 -0.78925
Br 0.00000 0.00000 1.82211
H 0.00000 2.17307 -0.23452
H 0.00000 2.17220 -2.73999
H 0.00000 0.00000 -4.00106
H 0.00000 -2.17220 -2.73999
H 0.00000 -2.17307 -0.23452
```

```
22
Ph2
C -2.87723 1.15875 -0.36416
C -3.58655 0.00001 -0.00001
C -2.87725 -1.15874 0.36416
C -1.47346 -1.15783 0.36368
C -0.74408 -0.00001 0.00000
C -1.47344 1.15782 -0.36367
H -3.42104 2.06836 -0.65949
H -4.68652 0.00001 -0.00001
H -3.42107 -2.06835 0.65948
H -0.92939 -2.06087 0.67422
H -0.92936 2.06086 -0.67421
C 3.58655 0.00001 -0.00000
C 2.87723 1.15874 0.36416
C 1.47345 1.15782 0.36368
C 0.74408 -0.00001 0.00001
C 1.47346 -1.15783 -0.36367
C 2.87724 -1.15874 -0.36416
H 4.68652 0.00001 -0.00001
H 3.42104 2.06836 0.65948
H 0.92936 2.06086 0.67422
H 0.92938 -2.06087 -0.67422
H 3.42106 -2.06835 -0.65949
```

SPhos

64
L(SPhos)
H -3.79319 -2.63590 -3.04671
H 0.63616 -3.57505 -1.82605
H -1.72675 -3.78188 -2.26691
H 5.24993 -1.68399 -1.47337
H -0.23303 -4.90285 -0.94341
C -3.27454 -2.26759 -2.14924
C -2.10912 -2.91617 -1.71464
C 0.37195 -3.97425 -0.82047
H 6.52735 -0.96597 -0.44709
H 5.53984 0.74142 -2.03508
H 1.29753 -4.20886 -0.25978
C 5.43492 -0.95550 -0.65160
H 3.21524 -0.17411 -2.22312
H -4.71090 -0.67710 -1.81905
H 2.86611 -2.09006 -0.45049
H 4.95114 -2.42478 0.90257
C 4.98986 0.44498 -1.11572
C -3.79624 -1.16233 -1.46044
C -1.44600 -2.43999 -0.56275
O -0.31594 -3.00413 -0.05285
C 3.46882 0.49748 -1.37183
C 4.64765 -1.39996 0.59680
H 3.17342 1.52562 -1.66976
C 3.12769 -1.35262 0.34118
H 5.24921 1.18784 -0.32792
H -4.37350 1.57724 -1.08032
C -3.12735 -0.69271 -0.30774
C -1.93419 -1.30995 0.14237
H 4.89524 -0.72172 1.44451
C 2.67494 0.05164 -0.12182
H 2.56977 -1.64969 1.25351
P 0.82370 0.02253 -0.50115
H 0.95322 2.06438 -1.79977
H -5.56639 0.59920 -0.12580
H -1.44103 1.33147 -1.79068
C -4.61278 1.17389 -0.06954
O -3.55399 0.37741 0.42772
H -0.96551 3.71495 -2.42189
H 2.90867 0.77474 0.68759
C 0.45511 1.86097 -0.82486
H -4.72974 2.01128 0.64602
C -1.19597 -0.78635 1.33360
C -1.06722 2.04474 -1.02631
C 0.08503 -0.17891 1.20961
C -1.41399 3.49287 -1.42702
H -2.51543 3.60269 -1.53548
H 1.16558 4.56783 -1.15208
H -2.78614 -1.37013 2.68007
H -1.58630 1.79516 -0.07806
H 2.08815 2.77000 0.32390
C -1.79196 -0.90818 2.60688
C 0.98923 2.87383 0.20744
C 0.64451 4.32340 -0.19867
C 0.73335 0.26158 2.38536
C -0.87348 4.50195 -0.39551
H -1.10356 5.54278 -0.71095
H 1.72136 0.73427 2.32242
H 0.53126 2.65701 1.19616
C -1.13485 -0.46035 3.76197
H 1.02192 5.03306 0.56954
H -1.38634 4.33359 0.57847
C 0.13864 0.12215 3.65027
H -1.61314 -0.57017 4.74667
H 0.66980 0.47581 4.54683

64
L_Away(SPhos)
C -3.65910 0.43975 0.94188
C -2.87390 -0.42632 0.14813
C -1.63864 -0.93151 0.62275
C -1.24992 -0.61787 1.94887
C -2.01673 0.26457 2.74293
C -3.21137 0.78484 2.22443
O -3.22872 -0.82740 -1.10720
C -0.84196 -1.88751 -0.21622
O -0.10780 -1.21904 2.38660
H -1.70168 0.52923 3.75839
H -3.81361 1.46908 2.83988
H -4.60136 0.85210 0.56584
C -1.19841 -3.24841 -0.06003
C -0.56630 -4.27283 -0.77496
C 0.44195 -3.93823 -1.69374
C 0.79227 -2.59391 -1.87149
C 0.18998 -1.53795 -1.13503
H -1.99791 -3.49370 0.65409
H -0.86591 -5.32048 -0.62394
H 0.94620 -4.71850 -2.28323
H 1.56402 -2.34919 -2.61890
P 0.96510 0.11054 -1.61225
C 0.03350 1.47999 -0.69472
C -4.40391 -0.29225 -1.69032
C 2.61933 -0.11961 -0.69284
H 2.93377 -1.12437 -1.05236
C 0.45026 -0.82559 3.62670
H -0.22363 -1.08415 4.47581
H 0.65732 0.26873 3.64735
H 1.40214 -1.38229 3.72499
H -4.34459 0.81756 -1.76896
H -5.30991 -0.56709 -1.10233
H -4.47157 -0.73403 -2.70331
C 2.54193 -0.20569 0.84314
C 3.70765 0.87088 -1.17258
C 5.07538 0.52710 -0.54606
H 3.43896 1.90867 -0.88885
H 3.77180 0.84800 -2.28133
C 3.92251 -0.51417 1.46020
H 1.81148 -0.98521 1.12463
H 2.16445 0.75290 1.25892
H 3.85095 -0.51792 2.57044
C 4.99200 0.49217 0.99292
H 4.23297 -1.53843 1.15300
H 5.84067 1.26232 -0.87698
H 5.40271 -0.47220 -0.91281
H -0.32305 1.12352 0.28861
H 5.98224 0.23658 1.42831
H 4.72501 1.50788 1.36483
C -1.18623 1.86398 -1.57081
C 0.89894 2.73839 -0.44697
C -2.02525 2.98821 -0.93315
H -1.81162 0.97393 -1.76897
H -0.80674 2.21232 -2.55769
C 0.06214 3.86489 0.19830
H 1.32191 3.09852 -1.41176
H 1.75358 2.50251 0.21443
H -2.87920 3.24617 -1.59793
C -1.16011 4.23309 -0.66214
H -2.45340 2.62116 0.02339
H 0.70196 4.75813 0.36802
H -0.29002 3.51803 1.19603
H -1.75981 5.02471 -0.16251
H -0.80837 4.65284 -1.63167

65
A1(SPhos)
Pd -0.09933 -1.33866 -1.41647
P 0.86913 0.30312 -0.22187
C -1.92182 -2.83491 -1.00136
C -1.37879 -2.24302 0.19350
C -1.92778 -1.00737 0.69636
C -3.07343 -0.46776 0.08534
C -3.65538 -1.08637 -1.05722
C -3.06487 -2.23269 -1.59545
O -0.57627 -2.91327 1.08605
C -1.17173 -0.27249 1.75255
O -3.54108 0.70174 0.62295
H -4.54568 -0.66201 -1.53418
H -3.50936 -2.70304 -2.48475
H -1.59972 -3.82999 -1.32980
C -1.73423 -0.15820 3.04106
C -1.05933 0.49585 4.08195
C 0.20746 1.05086 3.84193
C 0.77341 0.96136 2.55966
C 0.10604 0.31511 1.49465
H -2.72135 -0.60599 3.21900
H -1.51851 0.56446 5.07930
H 0.75670 1.56061 4.64747
H 1.75716 1.41746 2.39337
C 0.47512 2.04012 -0.84089
C 0.19705 -3.99885 0.60649
C 2.71324 0.32758 0.11045
H 2.96923 1.17960 0.77463
C -4.55003 1.41908 -0.06255
H -5.50660 0.84790 -0.09821
H -4.23665 1.66523 -1.10293
H -4.70389 2.35532 0.50942
H 0.83607 -3.67215 -0.24830
H -0.44677 -4.85020 0.28475
H 0.83561 -4.32292 1.45188
C 3.48250 0.52114 -1.21558
C 3.13316 -0.98819 0.80279
C 4.65723 -1.04376 1.02661
H 2.82110 -1.83679 0.15420
H 2.59317 -1.10101 1.76555
C 5.00750 0.46079 -0.98945
H 3.20767 1.49069 -1.68143
H 3.17576 -0.28074 -1.92374
H 5.53649 0.57176 -1.96052
C 5.42179 -0.85301 -0.29800
H 5.31480 1.32001 -0.35141
H 4.93510 -2.01079 1.49874
H 4.95236 -0.23898 1.73741
H 0.97437 2.08763 -1.83352
H 6.51860 -0.86618 -0.11939
H 5.19001 -1.70600 -0.97484
C 0.99319 3.20483 0.02629
C -1.04941 2.15442 -1.06474
C 0.61616 4.56715 -0.59583
H 2.09462 3.13785 0.15250
H 0.53896 3.13263 1.03713
C -1.42618 3.51687 -1.67808
H -1.56459 2.03886 -0.08875
H -1.39492 1.31677 -1.70836
H 0.97848 5.39296 0.05409
C -0.90596 4.67984 -0.81051
H 1.13054 4.67458 -1.57747
H -2.52966 3.58580 -1.79548
H -0.98491 3.59651 -2.69736
H -1.15930 5.65701 -1.27560
H -1.41331 4.64651 0.18016

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65
A1_Away(SPhos)
H 4.17318 1.26827 -3.07968
H -0.16989 3.16581 -2.80147
H 2.10870 2.65136 -3.03494
H 0.94608 4.44428 -2.15754
C 3.56778 1.30803 -2.16239
C 2.40031 2.08519 -2.14355
C 0.12026 3.74432 -1.89441
H -0.75315 4.31637 -1.52992
H 4.91282 0.00890 -1.06949
C 3.98742 0.59367 -1.03135
C 1.62331 2.12835 -0.96391
O 0.49634 2.88524 -0.83307
H 4.67419 -1.62356 0.58378
C 3.19834 0.63395 0.13982
C 1.98245 1.36266 0.17170
P -0.87366 -0.55841 0.30901
H 5.60670 -0.17243 1.14956
C 4.70502 -0.80124 1.33241
O 3.52029 -0.02366 1.28912
H 4.75150 -1.22894 2.35257
C 1.13344 1.34843 1.40404
C -0.04132 0.55836 1.56194
H 2.48453 2.75131 2.34187
C 1.56686 2.16102 2.47530
C -0.73056 0.62663 2.79700
H -1.62423 -0.00344 2.92823
C 0.85991 2.22825 3.68361
C -0.30145 1.45532 3.84344
H 1.21984 2.87523 4.49746
H -0.86818 1.48504 4.78580
C 0.47356 -1.25241 -0.79892
C 1.33934 -2.22365 0.03417
C -0.11372 -1.96354 -2.03607
H 1.10509 -0.42326 -1.16429
C 2.45074 -2.86232 -0.82088
H 0.67108 -3.01884 0.43531
H 1.77521 -1.69552 0.90371
C 1.00212 -2.61310 -2.88223
H -0.84009 -2.73701 -1.69971
H -0.66680 -1.23703 -2.66454
C 1.85891 -3.58239 -2.04699
H 3.04244 -3.57148 -0.20156
H 3.14534 -2.06577 -1.16722
H 0.55350 -3.14038 -3.75193
H 1.65739 -1.80971 -3.28813
H 2.66729 -4.02014 -2.67209
H 1.21971 -4.42456 -1.69872
C -1.86887 0.63030 -0.78179
C -3.02733 -0.13184 -1.47150
C -2.43888 1.80912 0.03958
H -1.17337 1.03116 -1.55037
C -3.87916 0.80160 -2.35485
H -3.66211 -0.57352 -0.67159
H -2.64909 -0.98345 -2.06769
C -3.31516 2.73583 -0.82917
H -3.05646 1.39343 0.86684
H -1.61620 2.38713 0.49975
C -4.45132 1.96769 -1.52867
H -4.69873 0.22124 -2.83107
H -3.24865 1.21010 -3.17794
H -3.72653 3.55586 -0.20119
H -2.67894 3.21078 -1.60750
H -5.04418 2.65269 -2.17303
H -5.14386 1.55935 -0.75899
Pd -2.10292 -2.14054 1.19509
129
A2_In_In(SPhos)
Pd -0.00006 -0.00000 -0.19614
P 2.21380 0.42609 0.20207
P -2.21386 -0.42618 0.20192
C 1.33898 -3.58251 0.17157
C 0.20534 -4.30925 -0.25045
C -0.26503 -4.13031 -1.55831
O 2.19440 -1.66678 -2.80834
C 3.34757 -2.15915 -0.31463
O 1.86954 -3.66988 1.42748
H -0.30842 -5.00113 0.42547
H -1.14436 -4.69723 -1.89393
H -0.05685 -3.09617 -3.44906
C 4.41932 -3.08199 -0.34683
C 5.70650 -2.72767 0.07616
C 5.93546 -1.43195 0.56851
C 4.88069 -0.50863 0.60114
C 3.58328 -0.83727 0.13819
H 4.21899 -4.10280 -0.70215
H 6.52252 -3.46477 0.03952
H 6.93172 -1.13951 0.93279
H 5.07441 0.48703 1.01479
C 1.49103 -2.52119 -2.01309
C 2.42193 1.02981 1.97155
C 1.67182 -1.33382 -4.07798
C 2.84294 1.85831 -0.85362
H 2.03763 2.60512 -0.70328
C 1.39509 -4.67893 2.29905
H 1.99500 -4.59260 3.22620
H 1.53314 -5.69194 1.85416
H 0.31974 -4.53546 2.54208
H 2.35641 -0.57597 -4.50506
H 0.64962 -0.90212 -3.98615
H 1.63158 -2.22305 -4.74968
C 2.81423 1.44302 -2.34027
C 4.18511 2.52133 -0.49236
C 4.45388 3.73798 -1.40353
H 5.01048 1.79653 -0.64504
H 4.19694 2.82498 0.57569
C 3.16789 2.61402 -3.28037
H 1.80390 1.05231 -2.57693
H 3.52980 0.60823 -2.49695
H 3.22662 2.24779 -4.32934
C 4.48729 3.30369 -2.88200
H 2.35075 3.36397 -3.24551
H 5.41346 4.22274 -1.12065
H 3.64896 4.49327 -1.25812
H 3.48240 1.31359 2.14110
H 4.68050 4.17725 -3.54187
H 5.33179 2.59247 -3.02610
C 2.06533 -0.12490 2.93537
C 1.54341 2.26710 2.24741
C 2.17708 0.31522 4.40715
H 2.71489 -1.00263 2.73985
H 1.02434 -0.44561 2.71875
C 1.66744 2.70490 3.72201
H 0.48943 2.01232 2.00301
H 1.83083 3.10201 1.57514
H 1.87936 -0.52111 5.07611
C 1.30689 1.55633 4.68365
H 3.23935 0.55507 4.63971
H 1.01913 3.58553 3.91916
H 2.71545 3.02698 3.91851
H 1.42336 1.88514 5.73917
H 0.23828 1.28682 4.54006
C -0.34659 3.22943 -2.43981
C -1.49072 2.52151 -2.01268
C -2.01011 2.70324 -0.71039
C -1.33865 3.58254 0.17211
C -0.20508 4.30941 -0.24986
C 0.26525 4.13068 -1.55776
O -2.19407 1.66719 -2.80803
C -3.34729 2.15930 -0.31431
O -1.86917 3.66974 1.42805
H 0.30868 5.00122 0.42613
H 1.14453 4.69771 -1.89334
H 0.05706 3.09681 -3.44865
C -4.41893 3.08228 -0.34637
C -5.70618 2.72804 0.07645
C -5.93535 1.43223 0.56849
C -4.88070 0.50878 0.60099
C -3.58320 0.83736 0.13821
H -4.21845 4.10314 -0.70146
H -6.52210 3.46525 0.03992
H -6.93167 1.13984 0.93262
H -5.07456 -0.48696 1.01440
C 2.01045 -2.70312 -0.71085
C -2.42225 -1.03034 1.97122
C -1.67152 1.33443 -4.07773
C -2.84304 -1.85810 -0.85416
H -2.03785 -2.60505 -0.70385
C -1.39488 4.67883 2.29966
H -1.99481 4.59241 3.22679
H -1.53303 5.69183 1.85478
H -0.31951 4.53549 2.54274
H -2.35608 0.57660 -4.50489
H -0.64929 0.90278 -3.98598
H -1.63133 2.22376 -4.74931
C -2.81408 -1.44253 -2.34072
C -4.18535 -2.52101 -0.49322
C -4.45412 -3.73748 -1.40464
H -5.01060 -1.79608 -0.64588
H -4.19738 -2.82487 0.57477
C -3.16771 -2.61335 -3.28108
H -1.80370 -1.05182 -2.57717
H -3.52958 -0.60766 -2.49734
H -3.22621 -2.24695 -4.32999
C -4.48725 -3.30294 -2.88304
H -2.35066 -3.36340 -3.24617
H -5.41380 -4.22218 -1.12199
H -3.64931 -4.49287 -1.25924
H -3.48279 -1.31396 2.14058
H -4.68045 -4.17636 -3.54308
H -5.33164 -2.59159 -3.02715
C -2.06553 0.12404 2.93540
C -1.54398 -2.26787 2.24683
C -2.17752 -0.31648 4.40705
H -2.71490 1.00194 2.74003
H -1.02445 0.44459 2.71900
C -1.66824 -2.70604 3.72129
H -0.48994 -2.01319 2.00258
H -1.83148 -3.10255 1.57431
H -1.87973 0.51962 5.07628
C -1.30756 -1.55781 4.68327
H -3.23985 -0.55622 4.63943
H -1.02014 -3.58687 3.91827
H -2.71634 -3.02795 3.91759
H -1.42416 -1.88688 5.73869
H -0.23889 -1.28843 4.53984
C 0.34684 -3.22899 -2.44027
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129
A2_In_Away(SPhos)
Pd -0.695287 0.238132 -0.168927
P 1.524922 0.716269 -0.032009
P -2.910717 0.211034 0.399679
O -1.934822 -3.742881 0.248354
O 4.393224 -2.596903 -1.202197
O 5.114955 1.954997 -0.268357
C 4.998826 -1.689252 -0.381018
O -2.686915 -0.686859 -3.240604
C -2.284293 -2.253801 -1.536626
C -3.698880 -2.105913 -1.069480
C -4.118623 -1.074920 -0.187014
C 3.829919 0.035518 -1.804047
C -6.368929 -2.063206 -0.130009
H -7.400809 -2.046090 0.251889
C 4.743069 -0.329132 -0.679670
C -5.958185 -3.062491 -1.028644
H -6.666606 -3.834820 -1.363724
C -4.631251 -3.082518 -1.481824
H -4.292035 -3.876495 -2.162106
C 2.172091 3.419303 -0.728585
H 3.039850 3.052273 -1.307699
H 1.285158 3.373301 -1.399057
C 2.278179 -0.358515 1.316442
H 3.374314 -0.235748 1.367124
C 2.247895 0.693243 -4.054901
H 1.619876 0.952412 -4.920679
C -1.794198 -1.536339 -2.652185
C 5.368898 0.668811 0.106122
C 4.337554 -0.092210 -3.116480
H 5.366597 -0.456659 -3.244954
C 1.698305 0.030076 2.695043
H 2.013706 1.058348 2.964590
H 0.588598 0.028104 2.629134
C -1.406462 -3.127153 -0.852625
C -0.460127 -1.697981 -3.085400
H -0.066616 -1.129269 -3.932468
C 0.746955 3.054757 1.332843
H -0.177882 2.976582 0.720531
H 0.569646 2.423600 2.222835
C 2.493123 0.477012 -1.611550
C 3.564937 0.238888 -4.238219
H 3.987660 0.137543 -5.248847
C -2.410879 1.255843 2.965233
H -2.929479 2.203627 2.709460
H -1.376836 1.333795 2.564439
C 0.382335 -2.579205 -2.394964
H 1.430372 -2.677414 -2.711144
C 1.934900 -1.826260 0.984952
H 2.361740 -2.107791 0.005370
H 0.831534 -1.898386 0.871434
C -0.074414 -3.301239 -1.284559
H 0.610336 -3.963350 -0.744613
C 1.919977 2.500533 0.487654
H 2.843923 2.473801 1.104435
C -5.112191 2.200826 0.371720
H -5.808478 1.530476 -0.173832
H -5.257695 2.021494 1.458299
C -2.373679 1.080823 4.497203
H -1.836525 1.937843 4.959019
H -3.414420 1.098200 4.893497
C 1.724297 0.788763 -2.758839
H 0.675345 1.087802 -2.614450
C -3.664018 1.878069 -0.046122
H -2.987659 2.574052 0.496696
C 4.467561 -3.974759 -0.878644
H 5.518475 -4.343997 -0.913284
H 3.865930 -4.501224 -1.645043
H 4.043864 -4.172495 0.131494
C 6.177661 0.319377 1.210443
H 6.647412 1.087867 1.834056
C -1.076179 -4.483449 1.093905
H -0.657175 -5.375804 0.572335
H -1.696960 -4.815477 1.949070
H -0.236121 -3.855507 1.465240
C -5.451162 -1.086617 0.286320
H -5.776458 -0.326056 1.006752
C 5.682737 3.015134 0.478859
H 5.318437 3.009413 1.531701
H 5.354736 3.947734 -0.017302
H 6.795629 2.959098 0.479036
C 2.397798 4.883766 -0.300221
H 3.328484 4.946780 0.307342
H 2.554925 5.516809 -1.200585
C -3.097756 0.063786 2.265850
H -4.173755 0.045846 2.543620
C 1.223778 5.419982 0.539221
H 1.418132 6.467461 0.856920
H 0.304585 5.432391 -0.089124
C -3.829307 3.585906 -1.924908
H -3.114945 4.275905 -1.420876
H -3.713974 3.742161 -3.019967
C -3.460337 2.136266 -1.555832
H -2.402164 1.923565 -1.817638
H -4.089447 1.424709 -2.132592
C -5.462282 3.664216 0.021656
H -6.509555 3.887327 0.320485
H -4.803129 4.345259 0.605985
C 0.981112 4.516155 1.761488
H 0.108258 4.877992 2.347299
H 1.867360 4.567157 2.435177
C -1.708420 -0.249526 4.899082
H -0.644430 -0.235763 4.576046
H -1.714138 -0.366379 6.004519
C 5.807339 -2.048916 0.719968
H 5.987876 -3.100250 0.968411
C -2.418175 -1.439725 4.225928
H -3.460141 -1.511234 4.612597
H -1.908111 -2.392367 4.489139
C -2.448170 -1.273892 2.694675
H -1.407840 -1.285463 2.299786
H -2.978559 -2.123613 2.219304
C 2.403309 -2.794093 2.085388
H 2.116799 -3.835451 1.817357
H 3.513080 -2.765924 2.153906
C -2.211279 0.215993 -4.220059
H -1.380057 0.838288 -3.818765
H -3.067145 0.867943 -4.481537
H -1.857859 -0.319833 -5.131931
C 6.378842 -1.037652 1.505375
H 7.004041 -1.313962 2.366906
C 2.158612 -0.947198 3.795546
H 3.262479 -0.866911 3.914886
H 1.700969 -0.658093 4.766243
C -5.264002 3.935796 -1.483246
H -5.982371 3.309118 -2.058716
H -5.495882 4.997218 -1.718338
C 1.798692 -2.403184 3.447005
H 0.690729 -2.498962 3.392960
H 2.149994 -3.091133 4.246460
77
B1(SPhos)
Pd -0.728941 -0.857676 -0.392616
Br -4.134843 -0.773933 -0.125936
P 0.308509 1.098536 0.189329
C 0.716238 -2.247272 -2.837453
C 1.190638 -0.937052 -2.580819
C 2.215575 -0.715706 -1.622926
C 2.770406 -1.828386 -0.947238
C 2.307774 -3.137709 -1.208037
C 1.288349 -3.327494 -2.150875
O 0.737053 0.168982 -3.231930
C 2.688629 0.673950 -1.338781
O 3.741450 -1.538642 -0.031925
H 2.729688 -3.999778 -0.680060
H 0.923065 -4.345074 -2.351319
H -0.078799 -2.419430 -3.570756
C 3.938166 1.068483 -1.861838
C 4.432598 2.366551 -1.669006
C 3.670814 3.295870 -0.941564
C 2.432699 2.910381 -0.404199
C 1.923198 1.604005 -0.583060
H 4.521112 0.334799 -2.435770
H 5.407399 2.653247 -2.090497
H 4.040128 4.320472 -0.785955
H 1.858673 3.646998 0.171682
C 0.725020 0.945007 2.019027
C -0.539993 0.107020 -3.848425
C -0.750702 2.638017 0.069346
H -0.182145 3.526174 0.416507
C 4.161494 -2.554293 0.861652
H 4.686585 -3.378579 0.325716
H 3.296612 -2.976865 1.421824
H 4.862772 -2.070461 1.569222
H -1.299001 -0.255354 -3.116196
H -0.530958 -0.554943 -4.744916
H -0.782892 1.141627 -4.157569
C -2.003280 2.489188 0.960646
C -1.146770 2.847834 -1.410201
C -2.103237 4.044006 -1.577532
H -1.649914 1.922465 -1.765272
H -0.236498 2.983551 -2.031030
C -2.965066 3.681770 0.781021
H -1.707335 2.405977 2.027002
H -2.523777 1.546648 0.687849
H -3.871843 3.525718 1.404081
C -3.356263 3.874068 -0.696845
H -2.470544 4.609221 1.149690
H -2.390732 4.149925 -2.646115
H -1.575665 4.981409 -1.289032
H -0.267185 0.752065 2.480703
H -4.031227 4.750147 -0.806954
H -3.920278 2.977949 -1.039182
C 1.354407 2.179726 2.690980
C 1.587716 -0.315715 2.245336
C 1.581098 1.927149 4.197394
H 0.711125 3.073540 2.546222
H 2.332421 2.394642 2.211164
C 1.832849 -0.559103 3.747123
H 2.559550 -0.189060 1.723777
H 1.080306 -1.191422 1.788536
H 2.050085 2.819277 4.666160
C 2.454659 0.677616 4.425075
H 0.595321 1.777807 4.693073
H 2.488316 -1.447002 3.884096
H 0.861285 -0.794174 4.236659
H 2.594620 0.496744 5.512825
H 3.463703 0.859593 3.990612
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C -1.490711 -2.437631 2.683626
C -2.332428 -1.534450 2.035761
C -2.516419 -1.634645 0.617429
C -1.918015 -2.721312 -0.118205
C -1.059645 -3.621904 0.593266
H -0.180957 -4.178019 2.493329

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H -1.329097 -2.338448 3.767048
H -2.851456 -0.743254 2.592183
H -2.289564 -2.993368 -1.116527
H -0.594830 -4.449782 0.040285
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77

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T1OA(SPhos)
Pd -1.06232 0.73794 -0.19236
H -2.87785 -2.33152 3.73474
P 1.18423 0.53905 0.24674
Br -3.51348 1.78605 -0.48259
C -1.60323 -0.97369 -3.03444
C -0.23966 -0.76269 -2.72729
C 0.48257 -1.70881 -1.95510
C -0.17783 -2.88304 -1.52341
C -1.53463 -3.10993 -1.84381
C -2.22633 -2.15132 -2.59858
O 0.47133 0.31983 -3.14444
C 1.92791 -1.47274 -1.65599
O 0.57644 -3.74884 -0.78169
H -2.04817 -4.01842 -1.50987
H -3.28397 -2.32239 -2.84744
H -2.16911 -0.23481 -3.61107
C 2.87553 -2.27538 -2.32754
C 4.25321 -2.07969 -2.15696
C 4.70568 -1.06098 -1.30256
C 3.77412 -0.26868 -0.61387
C 2.38183 -0.46093 -0.76617
H 2.50958 -3.06011 -3.00387
H 4.97110 -2.71480 -2.69681
H 5.78280 -0.88498 -1.16406
H 4.14804 0.50882 0.06341
C 1.28442 -0.30406 1.93416
C -0.23739 1.45467 -3.61777
C 2.05049 2.18335 0.49706
H 3.06295 2.02564 0.92507
C -0.07465 -4.79415 -0.08306
H -0.50778 -5.54653 -0.78237
H -0.88450 -4.39556 0.56985
H 0.70214 -5.27780 0.54114
H -0.97701 1.79081 -2.85476
H -0.75525 1.23907 -4.58097
H 0.52185 2.24458 -3.77615
C 1.24020 3.04193 1.49399
C 2.18478 2.90528 -0.86303
C 2.80076 4.30840 -0.69920
H 1.16808 2.99767 -1.30489
H 2.78891 2.29154 -1.56300
C 1.85032 4.44999 1.64984
H 1.18987 2.53963 2.48273
H 0.19570 3.12052 1.11543
H 1.22704 5.05375 2.34418
C 1.98096 5.16088 0.28869
H 2.85976 4.36253 2.11181
H 2.86201 4.81160 -1.68838
H 3.84306 4.20988 -0.31955
H 0.66329 0.35010 2.58275
H 2.44658 6.16159 0.41842
H 0.96382 5.32481 -0.13315
C 2.69155 -0.42811 2.55119
C 0.58820 -1.67964 1.85070
C 2.63091 -1.11579 3.93295
H 3.16547 0.57223 2.64280
H 3.33100 -1.03557 1.87662
C 0.54386 -2.36907 3.22699
H 1.14186 -2.32181 1.13464
H -0.43846 -1.55157 1.45253
H 3.65628 -1.21353 4.35100
C 1.95210 -2.49636 3.83762
H 2.05161 -0.47421 4.63487
H 0.06784 -3.36926 3.13128
H -0.09969 -1.77046 3.90844
H 1.90254 -2.97155 4.84135
H 2.57091 -3.15911 3.19109
C -3.22318 -1.01391 0.57731
C -2.89299 0.33016 0.87753
C -2.65465 0.74427 2.21470
C -2.63541 -0.22762 3.22733
C -2.89859 -1.58036 2.93289
C -3.19179 -1.96447 1.61168
H -2.46202 1.80113 2.43533
H -2.40872 0.07832 4.25947
H -3.39935 -3.01845 1.37359
H -3.44359 -1.30763 -0.45411
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94
D1(SPhos)
Pd 0.58733 0.12065 0.59629
H -1.45392 -2.07897 5.71624
P -0.94459 -0.81416 -0.75097
C 0.44508 3.94989 0.49044
C -0.07796 3.21567 -0.59019
C -1.29667 2.50525 -0.48046
C -2.04235 2.64125 0.71855
C -1.54367 3.40080 1.79743
C -0.29434 4.02708 1.67577
O 0.58281 3.09733 -1.79359
C -1.87837 1.78091 -1.65742
O -3.25704 2.02412 0.72544
H -2.11470 3.49736 2.72727
H 0.11574 4.58378 2.53028
H 1.44053 4.39815 0.42641
C -2.54149 2.58409 -2.61318
C -3.14238 2.03506 -3.75338
C -3.08571 0.64765 -3.96438
C -2.42627 -0.16490 -3.03212
C -1.81988 0.37580 -1.87171
H -2.57870 3.66884 -2.44190
H -3.65063 2.68898 -4.47720
H -3.54591 0.19643 -4.85552
H -2.37124 -1.24338 -3.22347
C -2.27283 -1.88709 0.02245
C 1.54120 4.10694 -2.14102
C -0.04998 -1.97295 -1.92555
H -0.81369 -2.50440 -2.53006
C -4.02550 2.02937 1.91561
H -4.32829 3.06478 2.19545
H -3.46443 1.56949 2.75903
H -4.92583 1.42285 1.70062
H 2.46017 3.99706 -1.52763
H 1.10059 5.11829 -1.99845
H 1.77158 3.94080 -3.21174
C 0.73256 -3.02688 -1.10751
C 0.88024 -1.21144 -2.89428
C 1.61811 -2.19604 -3.82346
H 1.61270 -0.62488 -2.30629
H 0.28971 -0.48984 -3.49539
C 1.49930 -3.99461 -2.03380
H 0.04070 -3.60000 -0.45528
H 1.44464 -2.49748 -0.43932
H 2.09214 -4.70462 -1.41812
C 2.41496 -3.23916 -3.01704
H 0.76497 -4.60025 -2.61200
H 2.29565 -1.63277 -4.50006
H 0.87700 -2.72246 -4.46787
H -1.69225 -2.52317 0.71983
H 2.91430 -3.95834 -3.70120
H 3.21632 -2.72197 -2.44744
C -3.05775 -2.82047 -0.92745
C -3.24802 -1.04045 0.86331
C -4.00691 -3.72906 -0.11363
H -2.37149 -3.45042 -1.52926
H -3.65921 -2.20844 -1.63266
C -4.19087 -1.94324 1.67910
H -3.83771 -0.39339 0.18207
H -2.68539 -0.37606 1.54033
H -4.57624 -4.38712 -0.80491
C -4.96987 -2.90534 0.76338
H -3.39568 -4.39197 0.53882
H -4.89325 -1.31582 2.26924
H -3.58614 -2.52639 2.40794
H -5.61573 -3.58217 1.36308
H -5.64231 -2.31308 0.10205
C -0.77903 0.19688 3.22483
C -0.21150 -0.66035 2.25692
C -0.06900 -2.03125 2.56730
C -0.50965 -2.53736 3.80649
C -1.10226 -1.68201 4.75227
C -1.22625 -0.31133 4.45968
H 0.39367 -2.71339 1.83966
H -0.38657 -3.60840 4.03085
H -1.67157 0.37218 5.19987
H -0.86791 1.26944 3.00878
O 2.08680 0.94565 -0.78485
B 3.07954 1.32486 0.31010
H 1.73446 1.72633 -1.26104
O 3.52889 2.69484 0.16237
H 4.47817 2.69708 -0.04711
O 2.15683 1.21098 1.57395
H 2.60163 0.72839 2.29498
C 6.26869 -1.78757 0.76236
C 6.40766 -0.53275 1.38251
C 5.41119 0.44779 1.21400
C 4.25808 0.21008 0.42862
C 4.14524 -1.05985 -0.18264
C 5.13064 -2.04931 -0.02428
H 7.04387 -2.55829 0.89177
H 7.29424 -0.31963 1.99996
H 5.53146 1.42565 1.71047
H 3.26138 -1.26235 -0.80170
H 5.01431 -3.02798 -0.51629

94
T1TM(SPhos)
Pd 0.853211 0.001869 0.532289
H 0.901917 5.923051 -0.095895
P -1.445557 -0.174167 0.510635
C 2.172793 -1.818364 -2.838750
C 0.925827 -2.120734 -2.258751
C -0.178992 -1.246246 -2.380079
C -0.009552 -0.055486 -3.133425
C 1.236568 0.261637 -3.714671
C 2.310970 -0.626276 -3.560864
O 0.705855 -3.259044 -1.514969
C -1.551850 -1.674394 -1.949456
O -1.126371 0.705628 -3.281190
H 1.369221 1.184605 -4.289295
H 3.284720 -0.374746 -4.005071
H 3.031358 -2.477186 -2.684173
C -2.216683 -2.557183 -2.832050
C -3.515364 -3.017135 -2.578610
C -4.183152 -2.597268 -1.416070
C -3.535883 -1.730245 -0.525489
C -2.224726 -1.254624 -0.771766
H -1.688279 -2.880143 -3.739896
H -4.004414 -3.702701 -3.286213
H -5.201938 -2.948904 -1.196861
H -4.057745 -1.430365 0.391155
C -2.422519 1.432110 0.516978
C 1.590092 -4.375364 -1.691473
C -1.938993 -0.991665 2.131454
H -3.043272 -0.932802 2.223388
C -1.025766 1.965794 -3.923914
H -0.726999 1.850356 -4.991266
H -0.296286 2.622977 -3.401728
H -2.033589 2.418431 -3.865187
H 2.582056 -4.159493 -1.244370
H 1.692103 -4.613173 -2.773147
H 1.108876 -5.220315 -1.161533
C -1.317479 -0.198611 3.304610
C -1.541952 -2.482702 2.191404
C -1.931724 -3.094614 3.552190
H -0.448491 -2.572646 2.046472
H -2.033749 -3.037283 1.366314
C -1.688924 -0.827065 4.662856
H -1.645083 0.861791 3.272835
H -0.211877 -0.200199 3.180260
H -1.198977 -0.260737 5.483875
C -1.290495 -2.314289 4.716094
H -2.788228 -0.738210 4.816966
H -1.621223 -4.160856 3.584216
H -3.039823 -3.073397 3.666954
H -1.857473 2.046054 1.246882
H -1.584388 -2.757514 5.691723
H -0.183040 -2.396909 4.637820
C -3.891595 1.366989 0.989525
C -2.336140 2.141417 -0.849062
C -4.488947 2.789547 1.075773
H -3.974548 0.880248 1.982020
H -4.485535 0.766986 0.267827
C -2.926821 3.561157 -0.766319
H -2.892597 1.541240 -1.598538
H -1.286315 2.194677 -1.181204
H -5.548203 2.730114 1.407130
C -4.384026 3.533554 -0.269430
H -3.934992 3.362102 1.853050
H -2.866418 4.050098 -1.762820
H -2.302227 4.164676 -0.072595
H -4.784963 4.565369 -0.170162
H -5.015212 3.008508 -1.021970
C 1.203689 2.590633 -0.896332
C 0.811071 2.002969 0.325378
C 0.486978 2.854481 1.403159
C 0.516561 4.255093 1.253569
C 0.879481 4.829377 0.022593
C 1.230397 3.989241 -1.049822
H 0.208266 2.424217 2.376509

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H 0.257669 4.899368 2.108496
H 1.536937 4.424978 -2.014235
H 1.491401 1.944993 -1.735863
O 3.589531 -2.436368 0.066176
B 2.834409 -1.819381 1.101880
H 4.532297 -2.380641 0.302117
O 3.327099 -2.029811 2.416232
H 2.762120 -1.567535 3.058345
O 1.386316 -2.071353 0.934853
H 1.177003 -2.625412 0.147841
C 4.917896 2.327345 0.739801
C 4.266405 2.008332 1.946569
C 3.354027 0.944633 1.980179
C 3.053485 0.160459 0.831344
C 3.729769 0.517573 -0.366547
C 4.650947 1.574723 -0.418930
H 5.630054 3.165982 0.703102
H 4.465402 2.598862 2.853828
H 2.846514 0.716345 2.931867
H 3.515462 -0.058331 -1.276316
H 5.154454 1.825705 -1.365695
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87)
G1(SPhos)

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P 1.399259 -0.267497 -0.150917
C -3.126489 -1.003857 -1.925702
C -1.736151 -1.253732 -1.956927
C -1.107169 -2.016227 -0.923531
C -1.923585 -2.507724 0.141176
C -3.306728 -2.250061 0.170220
C -3.889660 -1.511088 -0.870522
O -0.917340 -0.854673 -2.968598
C 0.254804 -2.606962 -1.168265
O -1.259751 -3.230249 1.085049
H -3.927969 -2.596710 1.001972
H -4.962873 -1.282784 -0.827910
H -3.602677 -0.394583 -2.699946
C 0.288968 -3.908216 -1.716478
C 1.503332 -4.518905 -2.061127
C 2.712561 -3.826501 -1.872082
C 2.692528 -2.538439 -1.316746
C 1.474954 -1.925031 -0.946558
H -0.660071 -4.436974 -1.883288
H 1.505303 -5.531719 -2.490361
H 3.669700 -4.290043 -2.153050
H 3.638958 -2.002971 -1.166806
C 2.175939 -0.489222 1.535281
C -1.356866 0.200950 -3.810194
C 2.602214 0.780432 -1.125759
H 3.492066 0.161503 -1.371391
C -1.944848 -3.594061 2.272355
H -2.774346 -4.306887 2.060106
H -2.358754 -2.696320 2.784572
H -1.192984 -4.082048 2.922579
H -1.668433 1.078674 -3.201528
H -2.202242 -0.120637 -4.460359
H -0.488596 0.471751 -4.441032
C 3.081648 2.017896 -0.331403
C 1.909261 1.187957 -2.447925
C 2.811219 2.098891 -3.302129
H 0.970261 1.725723 -2.196241
H 1.618551 0.277799 -3.011829
C 3.976915 2.919691 -1.205188
H 3.641805 1.698392 0.570633
H 2.206517 2.600756 0.015755
H 4.276158 3.816894 -0.622489
C 3.259946 3.338009 -2.503303
H 4.910725 2.371026 -1.466571
H 2.271200 2.403946 -4.224898
H 3.710084 1.526752 -3.626164
H 2.223467 0.551051 1.921587
H 3.923995 3.978898 -3.122433
H 2.365272 3.944634 -2.240101
C 3.596175 -1.087717 1.565794
C 1.217022 -1.286146 2.448088
C 4.135031 -1.133502 3.011230
H 4.281231 -0.501145 0.918099
H 3.561974 -2.121449 1.162548
C 1.760384 -1.357448 3.888952
H 1.092320 -2.311174 2.039012
H 0.212138 -0.812706 2.433180
H 5.154263 -1.576389 3.022900
C 3.189290 -1.935331 3.927135
H 4.224722 -0.093544 3.397985
H 1.078996 -1.967594 4.520778
H 1.772301 -0.331348 4.320809
H 3.575715 -1.944147 4.969004
H 3.162053 -2.992772 3.579419
C 0.221381 2.436589 2.080359
C -0.299467 2.265447 0.779101
C -0.310670 3.377705 -0.090749
C 0.240131 4.610769 0.305805
C 0.794028 4.760390 1.590325
C 0.769328 3.671259 2.479888
H -0.738891 3.279010 -1.098458
H 0.235590 5.459359 -0.396139
H 1.181318 3.779568 3.495486
H 0.211812 1.597208 2.790670
C -5.474604 1.696312 0.951953
C -4.748698 0.933744 1.884706
C -3.386658 0.652292 1.659889
C -2.723710 1.105418 0.496553
C -3.457700 1.910009 -0.403076
C -4.820657 2.191871 -0.191936
H -6.538372 1.920541 1.124777
H -5.243716 0.561772 2.796183
H -2.833744 0.056528 2.403241
H -2.960577 2.321257 -1.296074
H -5.373851 2.809265 -0.917767
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87
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H -3.664365 4.540827 2.004043
P 1.101469 0.804511 -0.153396
C -0.993593 -2.878373 -1.839271
C 0.193812 -2.121765 -1.981799
C 1.246890 -2.243828 -1.034839
C 1.095671 -3.161120 0.034931
C -0.089971 -3.913133 0.180528
C -1.120189 -3.758880 -0.757825
O 0.413577 -1.246239 -3.003995
C 2.500356 -1.442380 -1.195990
O 2.152529 -3.233869 0.897433
H -0.222034 -4.599835 1.023647
H -2.058473 -4.314234 -0.628255
H -1.820940 -2.761221 -2.545370
C 3.649544 -2.097579 -1.686532
C 4.848521 -1.402058 -1.901371
C 4.912174 -0.025662 -1.626519
C 3.779891 0.634708 -1.124291
C 2.567972 -0.054418 -0.895209
H 3.587294 -3.172351 -1.906667
H 5.730470 -1.933065 -2.289105
H 5.843658 0.534526 -1.796193
H 3.848548 1.706857 -0.899461
C 1.584273 1.047510 1.643840
C -0.713923 -0.761922 -3.717823
C 1.103627 2.517646 -0.911841
H 2.141914 2.898219 -1.013530
C 2.002328 -3.961522 2.102678
H 1.854331 -5.048738 1.907344
H 1.141619 -3.580208 2.698417
H 2.941608 -3.813432 2.670517
H -1.468699 -0.353494 -3.006725
H -1.177584 -1.560399 -4.341561
H -0.339303 0.047573 -4.373195
C 0.312079 3.507709 -0.024845
C 0.481798 2.405986 -2.324148
C 0.333077 3.785819 -2.993321
H -0.520533 1.935424 -2.222485
H 1.096507 1.727164 -2.951983
C 0.158243 4.879026 -0.713140
H 0.824062 3.636926 0.950043
H -0.693650 3.094130 0.185631
H -0.452152 5.546690 -0.068338
C -0.487142 4.740718 -2.104733
H 1.160610 5.352668 -0.822673
H -0.146842 3.670771 -3.989579
H 1.342220 4.223434 -3.167652
H 0.753369 1.670242 2.039914
H -0.581300 5.736749 -2.588755
H -1.514936 4.332002 -1.983326
C 2.917942 1.768803 1.914141
C 1.537386 -0.313430 2.373221
C 3.140800 1.952038 3.431098
H 2.938232 2.754112 1.402962
H 3.748946 1.161915 1.496469
C 1.765997 -0.136657 3.886631
H 2.319960 -0.977477 1.951149
H 0.559966 -0.805223 2.177745
H 4.114027 2.456799 3.614008
C 3.090449 0.598907 4.169336
H 2.346130 2.618343 3.836025
H 1.759210 -1.128069 4.390087
H 0.922931 0.451975 4.314134
H 3.225999 0.749948 5.262023
H 3.936559 -0.034527 3.818851
C -2.235768 1.411617 2.029075
C -2.372735 1.061191 0.662462
C -3.042909 1.970209 -0.194163
C -3.495189 3.212144 0.282194
C -3.311785 3.567881 1.631592
C -2.687054 2.654817 2.502709
H -3.186268 1.712428 -1.253069
H -3.990985 3.909970 -0.410215
H -2.547366 2.913297 3.563883
H -1.749737 0.709585 2.721536
C -4.785369 -3.039374 0.513327
C -3.851630 -2.829363 1.544839
C -2.919116 -1.781546 1.450431
C -2.883129 -0.940881 0.312847
C -3.855970 -1.135386 -0.695136
C -4.788077 -2.182698 -0.605288
H -5.520985 -3.854213 0.588238
H -3.851919 -3.483804 2.430390
H -2.196862 -1.621301 2.264496
H -3.877287 -0.465887 -1.567897
H -5.525620 -2.329897 -1.409590
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InPhos

70

L(InPhos)

H 4.255067 -1.558513 -3.213396
H -3.829739 0.168648 -2.385849
H 4.598281 1.511358 0.297964
H -2.141148 -0.328836 -2.734320
H -2.516443 1.381464 -2.344715
H 4.989584 -0.273677 -1.216078
H 1.723044 4.032847 -1.927245
H -0.356541 1.923277 2.275725
H 5.608398 0.153019 0.949741
H -1.868978 2.522869 1.510751
H -0.456229 3.601499 1.671806
C 3.615409 -1.534906 -2.318798
C 4.033278 -0.808219 -1.194843
C 4.669296 0.735948 1.094836
H 1.744188 5.488982 -0.886038
H -0.560931 5.034735 -1.845801
H 4.689354 1.225751 2.088004
C 1.355510 4.450253 -0.962388
H -0.448272 2.574330 -2.026566
H 2.105551 -2.803281 -3.213850
H 1.716218 1.680853 -0.826082
H 3.003047 3.539081 0.155605
C -0.184541 4.451806 -0.977625
C 2.402225 -2.238451 -2.323147
C 3.207837 -0.781340 -0.048540
O 3.531260 -0.105036 1.094348
C -0.747796 3.015187 -1.049905
C 1.892643 3.581138 0.189863
H -1.856069 3.052675 -1.036476
C 1.329855 2.146553 0.106449
H -0.562318 4.960331 -0.064332
H -0.259699 -2.820767 -3.066346
C 1.580962 -2.203341 -1.174679
C 1.961163 -1.454665 -0.032270
H 1.622110 4.045399 1.162716
C -0.230037 2.096338 0.092859
H 1.709908 1.535142 0.947874
P -0.614671 0.264216 -0.399340
C -2.769901 0.330797 -2.100188
H 0.563322 -4.352092 -2.544154
H -2.186461 -2.102329 -0.961089
C -0.114412 -3.528856 -2.218719
O 0.391926 -2.862897 -1.077461
H -4.614519 -1.722566 -1.571385
C -0.765304 2.555342 1.462752
C -2.533911 0.030148 -0.594641
H -1.092222 -3.953303 -1.919560
C 1.073830 -1.378793 1.171831
C -2.832479 -1.473103 -0.315892
C -0.140484 -0.634261 1.172738
C -4.318367 -1.841749 -0.506952
H -4.462800 -2.914336 -0.253938
H -5.318339 0.775494 -0.932506
H 2.427719 -2.613234 2.323428
H -2.554954 -1.711062 0.729977
H -3.343937 1.977125 0.013460
C 1.481586 -2.054682 2.342384
C -3.485342 0.907338 0.264721
C -4.977334 0.534969 0.097054
C -0.904102 -0.612133 2.362932
C -5.218881 -0.960078 0.378681
H -6.289790 -1.215723 0.225752
H -1.837046 -0.039877 2.397391
H -3.236899 0.795487 1.337998
C 0.705186 -2.024257 3.509070
H -5.586226 1.159625 0.786001
H -4.984195 -1.168600 1.447394
C -0.498490 -1.299795 3.517477
H 1.038676 -2.563175 4.408423
H -1.120517 -1.261525 4.424360

71

A1(InPhos)

Pd 0.199894 -1.231534 -1.402307
H 4.053464 2.419940 0.650596
P 0.657034 0.625893 -0.181144
H 2.499743 2.682659 1.478981
C -0.936663 -3.300288 -0.983064
H 2.677734 3.104499 -0.256323
C -0.599626 -2.544551 0.196749
H -0.177680 3.308484 -2.729361
C -1.537821 -1.582182 0.722073
H 0.513658 1.651588 -2.831013
C -2.815621 -1.483510 0.143155
H 1.431704 2.974778 -2.023773
C -3.179088 -2.283119 -0.977339
C -2.238432 -3.152219 -1.535293
O 0.411101 -2.893367 1.066102
C -1.080332 -0.625259 1.772038
O -3.641903 -0.530881 0.680937
H -4.176564 -2.205556 -1.423410
H -2.514899 -3.759862 -2.409380
H -0.288968 -4.113056 -1.331082
C -1.657669 -0.723394 3.056884
C -1.290661 0.138019 4.099527
C -0.327513 1.131210 3.863382
C 0.243387 1.251349 2.587058
C -0.106666 0.392654 1.519618
H -2.409998 -1.505202 3.227620
H -1.753709 0.032848 5.091882
H -0.022641 1.819939 4.665219
H 0.976756 2.045995 2.421786
C -0.253498 2.179588 -0.844785
C 1.487802 -3.658541 0.555117
C 2.540601 0.937709 0.105312
C 2.952413 2.364655 0.521021
C -4.859265 -0.228234 0.027083
H -5.559786 -1.095391 0.041770
H -4.686427 0.077861 -1.030195
H -5.308240 0.614931 0.588381
H 1.933132 -3.154072 -0.335278
H 1.161774 -4.686895 0.273592
H 2.238239 -3.721798 1.367365
C 3.232676 0.584114 -1.250876
C 2.977113 -0.111368 1.172288
C 4.506630 -0.284693 1.273041
H 2.524068 -1.090142 0.904836
H 2.567409 0.163512 2.163438
C 4.763597 0.431764 -1.139511
H 2.978464 1.349009 -2.011843
H 2.812512 -0.378909 -1.616982
H 5.169206 0.150806 -2.135038
C 5.129229 -0.632655 -0.090204
H 5.236871 1.400437 -0.865727
H 4.729902 -1.079750 2.016732
H 4.969690 0.649399 1.660021
C 0.419721 2.549855 -2.183257
H 6.232476 -0.733995 -0.000975
H 4.734877 -1.618458 -0.426663
C -0.306210 3.392824 0.120305
C -1.710681 1.676044 -1.089280
C -1.247091 4.513080 -0.378508
H 0.708557 3.804056 0.282161
H -0.688227 3.050938 1.102932
C -2.662534 2.787347 -1.576480
H -2.113431 1.269685 -0.139040
H -1.693386 0.831739 -1.811280
H -1.256037 5.337836 0.366353
C -2.673201 3.977700 -0.600319
H -0.860519 4.943291 -1.327934
H -3.684948 2.364907 -1.682556
H -2.358423 3.139889 -2.585852
H -3.339553 4.784968 -0.974566
H -3.084577 3.637857 0.377129

141

A2(InPhos)

Pd 0.032594 -0.081268 -0.036693
H -1.531002 -3.905095 -2.819457
P -1.957203 -1.289402 -0.005883
H -1.968977 -4.225040 -1.115253
P 1.976708 1.185469 0.179678
H -0.454671 -3.338597 -1.515083
C -2.673223 2.779175 1.547035
H -2.360847 -4.513548 2.261392
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H 2.935574 3.657436 1.789135
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H 0.426534 -2.463331 0.948175
H -0.325903 -3.993213 0.443319
H -1.159700 -1.699371 4.818014
C 0.239243 -2.993144 3.737365
H -1.867573 -3.232252 4.240393
H 1.256274 -4.302614 2.313869

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H 0.947223 -2.161190 3.535522
C 1.874419 -3.172135 -2.539385
C 2.453285 -1.946366 -2.149909
C 3.066877 -1.806074 -0.880597
C 3.056685 -2.913510 0.000331
C 2.481927 -4.144448 -0.379945
C 1.908122 -4.259700 -1.652225
O 2.528714 -0.854693 -2.961143
C 4.031280 -0.688478 -0.623413
O 3.655733 -2.706032 1.213084
H 2.477560 -4.997444 0.307399
H 1.451569 -5.213019 -1.954731
H 1.397767 -3.284626 -3.518942
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C 6.437689 -0.156411 -0.639018
C 6.144591 1.149601 -0.216627
C 4.810679 1.522274 -0.007336
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H 7.476830 -0.473933 -0.812028
H 6.948976 1.881247 -0.048885
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C 2.131660 1.619832 2.072402
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C 1.719374 2.758869 -0.930422
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H 4.741151 -3.406161 2.774151
H 4.773795 -4.473891 1.302436
H 3.308883 -4.430796 2.367144
H 2.172761 0.061197 -4.730860
H 0.923370 -1.164817 -4.268813
H 2.544020 -1.711958 -4.871897
C 1.149182 2.191121 -2.268812
C 2.947550 3.640430 -1.270009
C 2.625207 4.753343 -2.294456
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C 0.842523 3.277984 -3.319388
H 0.233273 1.600188 -2.053611
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H 0.494736 2.785237 -4.254296
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C 3.102003 2.765939 2.427571
H 1.828009 4.961889 -4.327718
H 2.866147 3.526202 -4.067375
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C 0.712669 1.932196 2.643718
C 2.583826 0.264393 4.233138
H 3.639291 0.040130 2.338994
H 1.955836 -0.539522 2.319710
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H 2.925235 -0.729853 4.594583
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H -0.399964 2.049778 4.498427
H 1.236767 2.737736 4.621035
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C -2.551545 3.875764 -1.038525
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P -1.014780 -0.801784 -0.284549
H -0.978653 -2.874005 2.040464
C 1.807916 3.167054 -1.210414
H -0.906479 -3.912810 -2.649770
C 0.776144 2.343752 -1.713201
H -1.716195 -2.367362 -3.015930
C -0.492613 2.295654 -1.074539
H -2.251828 -3.357953 -1.610713
C -0.707685 3.114356 0.066333
C 0.321227 3.939390 0.572661
C 1.562741 3.961752 -0.081093
O 0.904647 1.551166 -2.810816
C -1.643952 1.573832 -1.717578
O -1.952972 3.027458 0.614899
H 0.156382 4.563852 1.457679
H 2.363850 4.607789 0.306622
H 2.791521 3.188587 -1.691359
C -2.413800 2.350051 -2.612886
C -3.522808 1.817523 -3.283927
C -3.878784 0.477004 -3.067244
C -3.121047 -0.305966 -2.183796
C -1.999551 0.213739 -1.493607
H -2.126494 3.398397 -2.776042
H -4.104865 2.447226 -3.973026
H -4.744055 0.036652 -3.584630
H -3.410201 -1.350453 -2.038772
C -2.260148 -1.338574 1.089428
C 2.200928 1.326319 -3.341371
C -0.342570 -2.284690 -1.302566
C -1.370974 -3.016558 -2.187667
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H 1.719813 -4.913191 -0.152133
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C -1.423175 -1.888490 2.271702
H 2.956122 -4.394540 -2.308256
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83

T1OA(InPhos)

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C 2.556922 -1.002458 3.130148
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100

D1(InPhos)

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P -1.136849 -1.051171 -0.371235
H -1.605146 -3.652621 1.228437
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C 0.051016 2.824070 -1.517506
H -2.013009 -3.534856 -2.316990
C -1.170459 2.302788 -1.026678
H -1.610387 -4.229604 -0.709640
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C -2.825703 -0.808384 -2.617889
C -2.035313 -0.077984 -1.695099
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C -1.186750 -3.767449 -1.619851
C -3.596158 2.982480 1.636935
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C -4.250714 -0.786658 2.495644
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H -4.604354 -3.483192 1.674556
H -4.592063 0.156592 2.973249
H -3.905163 -1.446656 3.319493
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C -0.357357 1.214378 3.087349
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C -0.391409 1.239013 4.494749
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H -0.829988 2.106945 5.012010
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O 2.094783 0.402593 -1.233917
B 3.132843 1.148956 -0.394248
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O 3.559480 2.368193 -1.060817
H 4.462858 2.242576 -1.397136
O 2.260439 1.520672 0.845570
H 2.719873 1.348196 1.687968
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C 6.645624 -0.010988 1.011770
C 5.586466 0.770442 0.512846
C 4.360597 0.195079 0.097192
C 4.245145 -1.208681 0.215861
C 5.292433 -2.004767 0.711554
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H 7.585311 0.469391 1.326369
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H 3.309717 -1.686710 -0.092059
H 5.166833 -3.096612 0.784446
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100
T1TM(InPhos)

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H 3.026971 -2.874167 -3.180332
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H 3.882905 -2.171613 -1.795353
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H 3.304698 -1.119059 -3.128144
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C -1.096108 1.773321 3.466844
C -2.159694 0.915971 3.775544
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C 1.541613 -0.761652 2.313663
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H -3.084798 1.333061 4.198315
H -2.916852 -1.118770 3.757375
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C 3.454241 -1.867333 3.416672
C 4.085076 -2.021148 2.172947
C 3.449127 -1.545305 1.020229
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H 1.698324 -1.125731 4.439704
H 3.930956 -2.229931 4.339180
H 5.067235 -2.509436 2.093929
H 3.957916 -1.676551 0.063089
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C 1.680010 -1.867512 -1.803577
C 3.052777 -1.995679 -2.504754
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H 0.374833 3.831873 2.169287
H 2.145927 3.765173 2.534772
H -2.609087 -3.201809 2.880154
H -1.655978 -3.084475 4.437259
H -1.158616 -4.260395 3.142473
C 0.582110 -1.693591 -2.905177
C 1.415368 -3.171380 -0.988243
C 1.170010 -4.412509 -1.875181
H 0.521062 -3.029722 -0.359811
H 2.273108 -3.365982 -0.315794
C 0.363530 -2.951524 -3.772053
H 0.831523 -0.823302 -3.545009
H -0.386262 -1.456152 -2.419300
H -0.469857 -2.749261 -4.479519
C 0.041216 -4.171842 -2.891665
H 1.259810 -3.163547 -4.395047
H 0.913162 -5.266594 -1.213009
H 2.099464 -4.699626 -2.414658
C 2.231852 1.449034 -2.599640
H -0.111344 -5.074236 -3.521841
H -0.906987 -3.987111 -2.342677
C 4.139613 0.814988 -1.014075
C 2.296894 2.287321 -0.194868
C 5.005238 2.055517 -1.337698
H 4.450648 -0.027327 -1.656318
H 4.356980 0.535064 0.035113
C 3.135974 3.546456 -0.493466
H 2.519205 1.958403 0.836834
H 1.223538 2.536358 -0.236571
H 6.075046 1.784251 -1.208529
C 4.642512 3.240345 -0.424409
H 4.878727 2.347678 -2.401939
H 2.868187 4.335699 0.241219
H 2.876139 3.952696 -1.493741
H 5.241897 4.137389 -0.692188
H 4.904209 2.972349 0.624412
C -1.240136 2.852360 -0.050067
C -1.036698 1.848249 -1.020507
C -1.107908 2.214986 -2.381367
C -1.305760 3.556730 -2.761160
C -1.460498 4.555906 -1.784353
C -1.440411 4.193981 -0.425356
H -1.015034 1.445567 -3.161571
H -1.347959 3.817787 -3.830200
H -1.591737 4.959537 0.352518
H -1.251029 2.579244 1.012506
O -3.578716 -2.433754 0.824010
B -2.764430 -2.076638 -0.286741
H -4.502590 -2.494359 0.523784
O -3.097949 -2.697737 -1.524029
H -2.464724 -2.420446 -2.207840
O -1.332027 -2.151486 0.051810
H -1.159079 -2.336353 1.002996
C -5.138737 1.859004 -0.959298
C -4.604978 1.180436 -2.071732
C -3.612117 0.210271 -1.881779
C -3.119701 -0.134482 -0.592205
C -3.691508 0.567579 0.504072
C -4.682356 1.546262 0.334293
H -5.908859 2.632351 -1.103232
H -4.957777 1.422220 -3.085881
H -3.201671 -0.300852 -2.766638
H -3.340904 0.330341 1.515078
H -5.093138 2.076393 1.207698
```

93

G1(InPhos)

```
Pd 0.913615 0.139445 -0.221750
H -1.878591 0.352885 -3.746456
H 2.022066 5.831076 -1.650375
H -0.407294 0.287322 -2.717708
P -1.458697 0.183118 0.032248
H -1.554607 1.649337 -2.555039
H -4.048900 2.658048 1.568636
C 2.674341 -1.368762 2.425939
C 1.279059 -1.208499 2.334916
H -3.763354 0.990395 2.125985
C 0.513027 -1.941230 1.371674
H -4.348027 1.299228 0.449823
C 1.212133 -2.844382 0.512458
C 2.611159 -2.994984 0.600095
C 3.318380 -2.264782 1.561687
O 0.554473 -0.404597 3.157059
C -0.967628 -2.107879 1.586811
O 0.428943 -3.541414 -0.354639
H 3.151994 -3.655824 -0.083803
H 4.409603 -2.371993 1.615093
H 3.259213 -0.793479 3.151053
C -1.338573 -3.251730 2.330032
C -2.679059 -3.532217 2.623349
C -3.680170 -2.658341 2.168674
C -3.324967 -1.521582 1.428403
C -1.974257 -1.220261 1.129685
H -0.547125 -3.930476 2.677773
H -2.940802 -4.429997 3.202478
H -4.739779 -2.861700 2.382625
H -4.123423 -0.866430 1.071851
C -2.238104 -0.266233 -1.670904
C 1.232501 0.603827 3.887148
C -2.211927 1.774907 0.781418
C -3.677577 1.663069 1.250545
C 1.050282 -4.332372 -1.356316
H 1.608649 -5.186132 -0.908423
H 1.749128 -3.720593 -1.968700
H 0.229318 -4.717920 -1.991734
H 1.852078 1.229190 3.205995
H 1.881179 0.168057 4.681126
H 0.446054 1.228183 4.352352
C -2.057045 2.921302 -0.261175
C -1.301534 2.072964 2.011464
C -1.561306 3.464108 2.624351
H -0.243322 2.025769 1.688184
H -1.445016 1.275727 2.768594
C -2.285383 4.324070 0.345098
H -2.769077 2.762386 -1.096407
H -1.034617 2.894761 -0.684640
H -2.077872 5.082738 -0.438888
C -1.381849 4.570094 1.567772
H -3.350713 4.450560 0.637215
H -0.856583 3.622076 3.469809
H -2.586479 3.511983 3.052056
C -1.479784 0.561263 -2.733044
H -1.596069 5.567589 2.009065
H -0.324711 4.574804 1.228900
C -3.768415 -0.035832 -1.782405
C -1.923486 -1.774843 -1.895819
C -4.368355 -0.598077 -3.092549
H -3.996949 1.046526 -1.708665
H -4.278650 -0.541717 -0.939667
C -2.501085 -2.314451 -3.219689
H -2.360744 -2.374486 -1.073232
H -0.825506 -1.926569 -1.848691
H -5.470404 -0.456909 -3.073226
C -4.024159 -2.087522 -3.278151
H -3.990159 -0.020051 -3.962254
H -2.270516 -3.398966 -3.297473
H -2.016065 -1.821450 -4.089113
H -4.440965 -2.464289 -4.237000
H -4.503474 -2.672149 -2.460395
C 1.259403 2.509587 -2.140656
C 1.356066 2.027120 -0.818032
C 1.766837 2.934279 0.185686
C 1.997774 4.291685 -0.105713
C 1.843964 4.770427 -1.418616
C 1.485949 3.867729 -2.435677
H 1.905872 2.581258 1.218197
H 2.301378 4.976672 0.701202
H 1.391361 4.218139 -3.475450
H 1.008774 1.826297 -2.961068
C 5.511392 -0.858889 -1.510860
C 4.413861 -1.263528 -2.293077
C 3.109442 -0.868794 -1.936918
C 2.868297 -0.094476 -0.778511
C 3.983822 0.338888 -0.032023
C 5.291844 -0.044396 -0.385019
H 6.533088 -1.158257 -1.790217
H 4.574337 -1.882554 -3.190378
H 2.263332 -1.185903 -2.568139
H 3.833827 0.984439 0.845723
H 6.146134 0.301735 0.218502
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93

T1RE(InPhos)

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Pd 0.902433 0.077827 -0.303632
H -3.312385 2.498802 2.667483
H 2.168639 5.796448 -1.153979
H -3.399541 0.719952 2.571734
P -1.411058 0.244488 0.108778
H -3.964500 1.733557 1.195048
H -2.004317 1.680918 -3.349784
C 2.519743 -2.421067 1.803833
C 1.145296 -2.145928 1.939407
H -0.553125 0.928455 -2.599038
C 0.240102 -2.396446 0.868950
H -1.266286 2.395376 -1.880427
C 0.758418 -2.941107 -0.339701
C 2.138032 -3.208783 -0.479165
C 2.995182 -2.953634 0.596455
O 0.576923 -1.647270 3.073342
C -1.240027 -2.388016 1.125305
O -0.165969 -3.190061 -1.309765
H 2.546043 -3.594778 -1.418145
H 4.069497 -3.144816 0.479215
H 3.219972 -2.209621 2.618955
C -1.767096 -3.578414 1.675846
C -3.133768 -3.716062 1.951357
C -4.003518 -2.647779 1.675559
C -3.491171 -1.459497 1.135859
C -2.112524 -1.301881 0.855834
H -1.077927 -4.408870 1.884540
H -3.518755 -4.654366 2.377333
H -5.080647 -2.736240 1.880627
H -4.185104 -0.638762 0.931823
C -2.409722 0.532567 -1.516311
C 1.418434 -1.113682 4.079080
C -1.763724 1.612693 1.408520
C -3.194791 1.634729 1.981886
C 0.285942 -3.560234 -2.601208
H 0.797839 -4.549954 -2.584013
H 0.983034 -2.796206 -3.012973
H -0.619442 -3.623158 -3.235760
H 2.093612 -0.332735 3.660910
H 2.034264 -1.907648 4.561315
H 0.746905 -0.657292 4.831909
C -1.394011 2.978862 0.763900
C -0.758662 1.308032 2.561407
C -0.687383 2.438321 3.608085
H 0.254547 1.177741 2.124959
H -1.027327 0.344426 3.037627
C -1.278589 4.123670 1.795496
H -2.148893 3.253148 -0.000330
H -0.420315 2.874050 0.247545
H -0.928404 5.036847 1.269485
C -0.309127 3.773448 2.940228
H -2.279331 4.360471 2.218405
H 0.065060 2.168049 4.380776
H -1.660426 2.542137 4.135534
C -1.510385 1.442506 -2.385748
H -0.289220 4.593615 3.690362
H 0.714039 3.684472 2.519667
C -3.818172 1.162362 -1.350203
C -2.547651 -0.857755 -2.202768
C -4.614225 1.218944 -2.675033
H -3.732634 2.182963 -0.928031
H -4.412845 0.559916 -0.636666
C -3.316026 -0.787063 -3.538392
H -3.094607 -1.549873 -1.531040
H -1.538570 -1.292306 -2.348759
H -5.629753 1.619595 -2.467491
C -4.713097 -0.170520 -3.331973
H -4.132297 1.928659 -3.380311
H -3.406372 -1.811623 -3.959568
H -2.748496 -0.184574 -4.279676
H -5.259328 -0.104590 -4.297621
H -5.304171 -0.841221 -2.667745
C 1.675260 2.500308 -2.006108
```

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C 1.827232 1.879118 -0.742377
C 2.175087 2.707254 0.355455
C 2.287047 4.099703 0.212523
C 2.081010 4.705958 -1.040090
C 1.784626 3.892795 -2.150529
H 2.339851 2.254438 1.342989
H 2.534352 4.715883 1.090573
H 1.640417 4.346206 -3.143492
H 1.461070 1.885287 -2.890030
C 5.450098 -1.010393 -1.450480
C 4.446571 -0.939602 -2.435808
C 3.201091 -0.363051 -2.134177
C 2.911999 0.115621 -0.832290
C 3.939142 0.056897 0.138078
C 5.192186 -0.500991 -0.164025
H 6.433273 -1.442629 -1.689811
H 4.641399 -1.322822 -3.449666
H 2.435100 -0.282463 -2.920117
H 3.754449 0.462104 1.142739
H 5.974982 -0.536965 0.609670
```