

Table S1

	Total electronic energy	Zero point corrected E	Gibbs Free energy
Ylide water complex	-2832.1294691	-2831.267545	-2831.376151
Trans TS1	-3177.6742178	-3176.70053	-3176.816261
Trans OP1	-3177.6926549	-3176.716344	-3176.83219
Trans OP2	-3177.692712	-3176.716881	-3176.833907
Trans PW	-3177.7770413	-3176.801006	-3176.920388
Cis TS1	-3177.6754871	-3176.700689	-3176.810672
Cis OP1	-3177.6913687	-3176.714995	-3176.830229

Table SI2. Free energies of activation for cis and trans Wittig addition at B3LYP methods with different basis sets

Level of theory	$\Delta G^\ddagger$ trans addition	$\Delta G^\ddagger$ trans addition
B3LYP/6-311G(d,p)	26.21609189	29.07126012
B3LYP/6-311+G(d)	27.79992587	32.71207024
B3LYP/6-311+G(d,p)	26.07176471	31.16023924
B3LYP/6-311++G(d,p)	26.01717138	31.12760875

Table SI 3. Comparison of free energies of activation for cis and trans Wittig on water and under neat conditions reaction at different levels of theories

	<i>Cis</i> ( $\Delta G^\ddagger$ )	<i>Trans</i> ( $\Delta G^\ddagger$ )
<b>M05-2x/6-31G(D)</b>		
On water	17.94	19.04
Neat conditions	18.95	16.82
<b>B3LYP/6-31G(D)</b>		
On water	26.24	25.12
Neat conditions	28.52	26.51
<b>B3LYP/6-311++G(D,P)</b>		
On water	26.02	31.13
Neat conditions	31.57	29.15

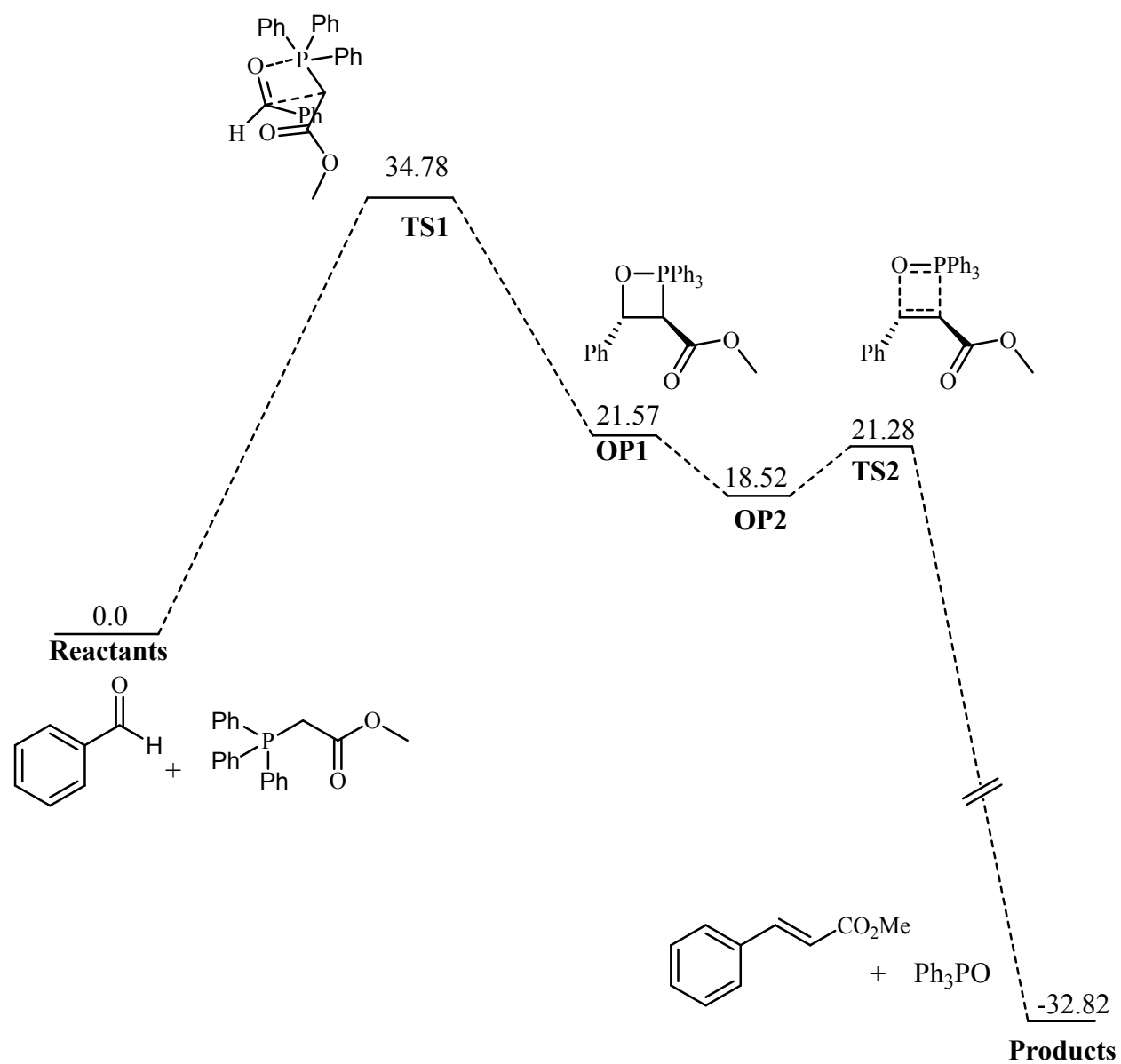


Figure S1. Gibbs free energy profile for *trans* Wittig reaction in neat conditions. All energies are relative to benzaldehyde and ylide. Unnecessary hydrogen atoms are removed for clarity

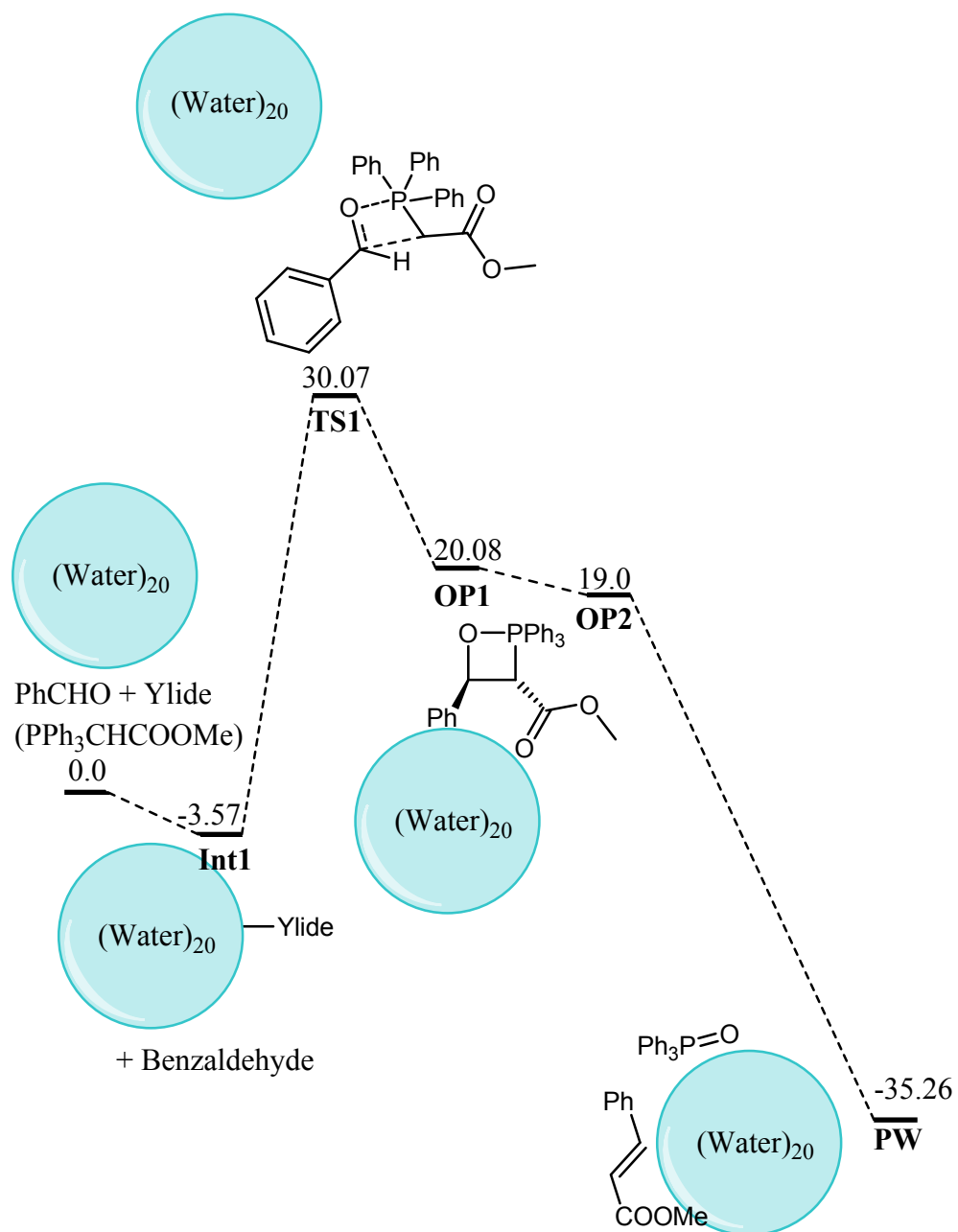


Figure S2. Gibbs free energy profile for *trans* Wittig reaction on water, all energies are Gibbs free energies relative to benzaldehyde, ylide and water 20 species

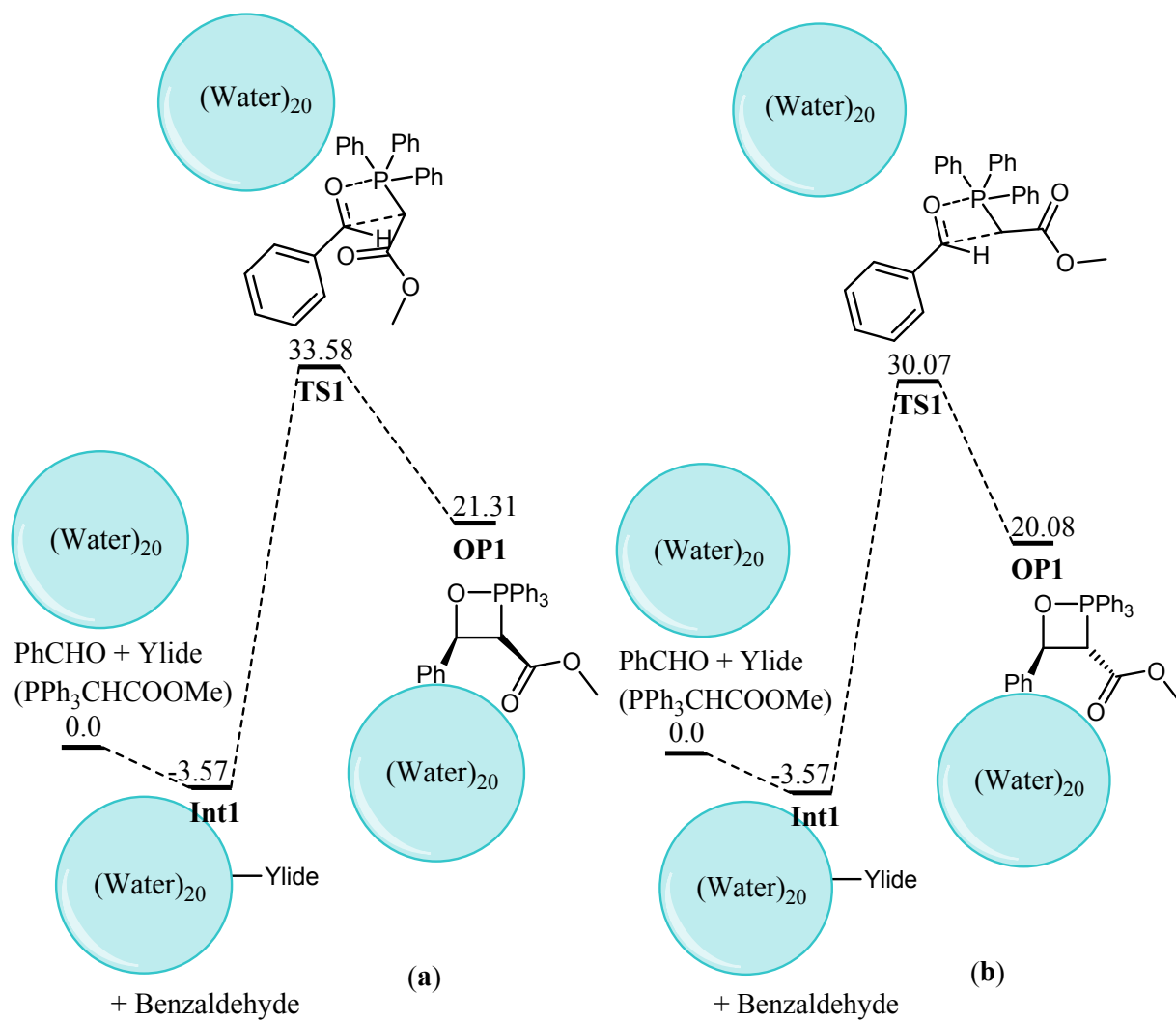


Figure S3. Comparative Gibbs free energy profile for the rate determining step cis (a) and trans (b) witting on water

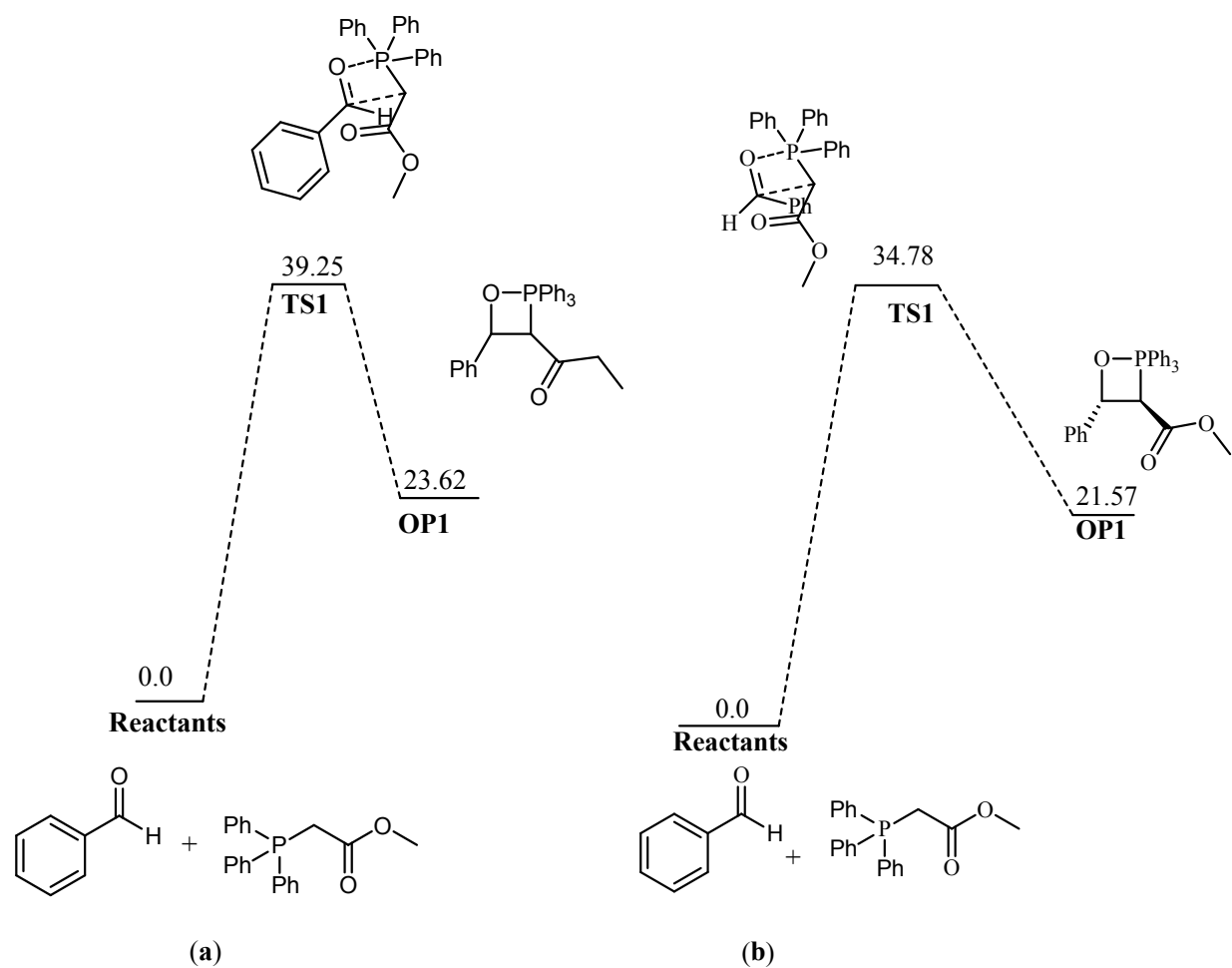


Fig S4. Comparative Gibbs free energy profile for the rate determining step *cis* (a) and *trans* (b) Wittig under neat conditions

**PPH3 Ylide water 20 complex**

O	4.55267600	2.14366600	2.99280600
O	3.48522700	3.79682900	1.24842600
O	5.10596300	3.52920500	-0.99318500
O	7.31245000	1.86107800	-0.47105200
O	6.98316500	1.07812200	2.08733200
O	6.49382900	-1.72782500	2.01147100
O	6.71743800	-2.57960100	-0.42094900
O	7.03677500	-0.26448500	-1.88039800
O	4.27798600	-3.60687500	-1.29331800
O	2.66679900	-3.58157600	0.76517500
O	4.02804300	-2.32886200	2.88563900
O	0.81331700	-1.62195800	0.28411600
O	2.18714700	-0.49251400	-1.70028900
O	3.07027500	-2.30386800	-3.46518000
O	1.29426100	1.90350900	-2.16847000
O	1.06761000	2.61048600	0.44515700
O	0.76289000	0.32135500	2.08626300
O	3.83367500	2.69994400	-3.13520600
O	4.57410400	0.05152300	-3.00256300
O	2.82861500	0.08805800	3.79389800
H	4.73875700	2.71821100	3.75096700
H	4.12626500	2.75632200	2.30771200
H	2.59993900	3.46853100	0.97677500
H	4.04222900	3.73733400	0.43605100



H	5.47528400	4.38759600	-1.25142700
H	4.60097900	3.20916100	-1.81292200
H	6.53963200	2.44527800	-0.64532600
H	7.24364800	1.61421400	0.49486900
H	6.80230600	0.11460700	2.05216800
H	6.14119100	1.47508800	2.40687400
H	7.25502700	-2.11708100	2.46850500
H	6.56722900	-2.06231100	1.04630000
H	6.89086200	-1.78003500	-0.97481400
H	5.85933500	-2.94249400	-0.74864100
H	7.77835300	-0.25345800	-2.50433100
H	7.15948700	0.57761600	-1.29713600
H	4.39866000	-4.55690000	-1.44577400
H	3.63359700	-3.55860000	-0.50609400
H	3.13687100	-3.17122800	1.52537000
H	1.89332100	-2.98521800	0.60931800
H	4.96731000	-2.13508900	2.60786400
H	4.09404600	-2.91297000	3.65603200
H	-0.11091200	-1.67558000	-0.05551000
H	1.72649500	-0.91485600	-0.91717600
H	2.30375800	-1.21118700	-2.38415800
H	1.56775000	0.93380500	-2.06173400
H	3.74295900	-1.61705700	-3.66082400
H	3.50704900	-2.85622100	-2.77496300
H	1.08678100	2.38605800	-0.52337500
H	0.50146900	1.89538100	-2.72630800

H	1.00546900	1.08830300	1.52491500
H	0.18827900	2.98437500	0.61403800
H	1.48722600	0.24459500	2.77159900
H	0.78279800	-0.94825700	1.03100300
H	4.17473600	1.78035700	-3.26763200
H	2.89058900	2.56235900	-2.89808500
H	5.49191000	-0.06728900	-2.64575200
H	3.97184300	-0.06626500	-2.23714200
H	3.44584000	0.81032200	3.53562800
H	3.25945500	-0.73569600	3.48062500
P	-4.54487700	-0.05252700	-0.30165700
C	-3.74476100	-0.60191700	-1.72144100
H	-4.27565400	-0.54300700	-2.66200600
C	-2.46850000	-1.20927700	-1.65501500
O	-2.02592700	-1.63507200	-2.87477900
O	-1.79261700	-1.37555500	-0.61957700
C	-4.85539900	-1.36261400	0.94492100
C	-0.75436600	-2.28941900	-2.89996400
H	0.04825200	-1.60621900	-2.61175100
H	-0.74137000	-3.15722700	-2.23305100
H	-0.60767100	-2.61002200	-3.93237100
C	-2.53406800	1.06764100	1.31406700
C	-3.74843400	1.30770700	0.64848700
C	-4.32605100	2.58628100	0.71169800
C	-3.70165700	3.60677400	1.43040600
C	-2.50207100	3.35886300	2.10084400

C	-1.92017400	2.08907400	2.04235300
H	-2.06192200	0.09313500	1.26011400
H	-5.26519700	2.78876300	0.20740500
H	-4.16086800	4.59076700	1.47462100
H	-2.02839400	4.14994000	2.67710400
H	-0.99309500	1.86097600	2.56022300
C	-5.36631500	-2.08880800	3.20093600
C	-5.08960800	-1.06378800	2.29573500
C	-4.89012800	-2.69587000	0.51530800
C	-5.16276100	-3.71763500	1.42425900
C	-5.40241700	-3.41534200	2.76617800
H	-5.54297600	-1.85159500	4.24639700
H	-5.04397500	-0.03632100	2.64404100
H	-4.68974000	-2.92218900	-0.52768300
H	-5.17932900	-4.74999300	1.08613400
H	-5.60972100	-4.21297500	3.47449600
C	-6.17269800	0.57035700	-0.85886300
C	-7.35033100	0.26312200	-0.16348100
C	-6.24397000	1.37719200	-2.00739100
C	-8.57898400	0.75143800	-0.61138100
H	-7.31200000	-0.36417600	0.72106000
C	-7.47373300	1.86228300	-2.45036500
H	-5.33853300	1.62106900	-2.55461900
C	-8.64314700	1.55026500	-1.75322400
H	-9.48598100	0.50217200	-0.06774900
H	-7.51777600	2.48269700	-3.34113800

H -9.60089500 1.92777900 -2.10081900

**Trans TS1 (on water)**

O 4.89304200 -3.62182200 0.43803800  
O 4.89658900 -2.54176900 2.83162900  
O 6.91442300 -0.65359400 2.84034000  
O 8.22626300 -0.64910100 0.35388100  
O 7.01238200 -2.58283400 -1.08833400  
O 5.68272000 -1.26910700 -3.23308700  
O 6.23747900 1.25270000 -3.16353700  
O 7.58562300 1.55774600 -0.78929300  
O 3.92364600 2.74478500 -2.75436000  
O 1.96656400 0.99162900 -2.86938700  
O 3.02651700 -1.60840800 -3.09109400  
O 1.16271300 0.79983300 -0.29285200  
O 3.04621400 2.18253200 1.01178400  
O 3.80382500 4.32805500 -0.39543700  
O 3.19273600 1.52452700 3.51399300  
O 2.51591200 -1.08640900 3.30018700  
O 1.09621600 -1.56040700 0.87798900  
O 6.02938700 1.74334000 3.42718500  
O 5.76019100 2.72305000 0.87765600  
O 2.43611300 -3.20844700 -0.79542200  
H 5.07189100 -4.55777200 0.61622500  
H 4.88239500 -3.18439600 1.35200500  
H 4.07579000 -2.02512400 2.98527300

H	5.62908800	-1.88033300	2.87009900
H	7.58645600	-0.83644900	3.51474700
H	6.56275700	0.27152700	3.06785900
H	7.77184000	-0.66785200	1.22646100
H	7.83461900	-1.40600700	-0.16648800
H	6.55189200	-2.11763600	-1.81902000
H	6.28708700	-2.96339900	-0.54416300
H	6.14397200	-1.58229100	-4.02627900
H	5.88267800	-0.26400400	-3.19398200
H	6.78417300	1.39051300	-2.35149000
H	5.42991000	1.80360200	-3.02378400
H	8.41080800	2.06395200	-0.83939800
H	7.84479200	0.66129100	-0.35124800
H	3.78220700	3.30617000	-3.53228900
H	3.16944800	2.06648100	-2.78741400
H	2.30914200	0.09458600	-3.08057800
H	1.64955600	0.89566700	-1.93295700
H	4.01750400	-1.51669900	-3.18314300
H	2.73955900	-2.12920100	-3.85612800
H	0.22422900	1.08524700	-0.30184400
H	2.32428400	1.69202300	0.53028800
H	3.10712100	3.08492500	0.58902900
H	3.07237800	1.87458700	2.56843500
H	4.68545700	4.13003700	-0.01489000
H	3.81928300	3.84713300	-1.25456400
H	2.71585200	-0.11881000	3.43284600

H	2.68354700	2.12062600	4.08415600
H	1.59664100	-1.48082100	1.71589800
H	2.17532800	-1.41005700	4.14735100
H	1.58861200	-2.21127200	0.30524700
H	1.14739000	-0.12525300	0.10980400
H	6.06120600	2.23311200	2.56665100
H	5.06913600	1.68814000	3.62290600
H	6.42787700	2.31606100	0.26806200
H	4.93272000	2.20505800	0.77156200
H	3.30768500	-3.41416500	-0.38231700
H	2.64619700	-2.63489800	-1.56418700
P	-3.86086200	-0.95989700	-0.00988300
C	-2.61761600	1.30061500	-0.99083300
O	-2.70606100	2.01819400	-2.12268900
O	-1.56507000	1.15727600	-0.36706400
C	-1.49885100	2.67052500	-2.56018800
H	-1.16274600	3.38912600	-1.80791500
H	-0.70594300	1.94255900	-2.75397200
H	-1.77230800	3.18962500	-3.47898500
C	-4.47188600	1.62996900	0.98064900
O	-5.49009700	0.96255100	1.42049500
C	-3.91310000	0.79845700	-0.50369200
C	-4.69349700	3.08808800	0.57766900
C	-3.63408000	4.00170900	0.51255200
C	-3.86093400	5.33227200	0.15641200
C	-5.15660000	5.76624200	-0.13369500

C	-6.22082300	4.86417500	-0.05443400
C	-5.98926800	3.53601300	0.30363000
H	-3.52476000	1.56255200	1.56583400
H	-4.72490500	0.94766500	-1.21550000
H	-2.62629200	3.66927600	0.75671500
H	-3.02987100	6.03282800	0.11566900
H	-5.33699300	6.80313000	-0.40672100
H	-7.23383800	5.20134500	-0.26273400
H	-6.80399500	2.82531000	0.40489700
C	-1.03348300	-3.04410000	-3.03422500
C	-2.09846800	-2.24809500	-3.46539500
C	-2.92224600	-1.62427300	-2.53295100
C	-1.63215400	-2.60515900	-0.73194600
C	-0.79662200	-3.21734100	-1.67177300
H	-0.38678500	-3.52573100	-3.76339400
H	-2.28441900	-2.10674800	-4.52652200
H	-3.74092300	-0.99970300	-2.87923200
H	-1.42121200	-2.73907400	0.32165900
H	0.05646900	-3.79634200	-1.33128300
C	-2.69715800	-1.80014500	-1.15435600
C	-3.31052300	-1.23223700	1.70457500
C	-4.22269800	-1.69884400	2.66236200
C	-1.98146500	-0.97136500	2.07157100
C	-3.79961300	-1.92493200	3.97005900
H	-5.25838300	-1.86525900	2.39169100
C	-1.56738800	-1.20651000	3.38335800

H	-1.26889400	-0.59764800	1.34799200
C	-2.47197200	-1.68278100	4.33166800
H	-4.51072800	-2.28321900	4.70881700
H	-0.53005100	-1.01875200	3.64697000
H	-2.14761900	-1.86378700	5.35330100
C	-6.68177300	-1.14126200	-0.10007000
C	-7.87685300	-1.82052900	-0.34384300
C	-7.86529800	-3.14613600	-0.77906600
C	-6.64948700	-3.80559700	-0.97214100
C	-5.44807800	-3.13730500	-0.74309700
H	-6.66141700	-0.12384600	0.28899100
H	-8.82142400	-1.30738100	-0.18515700
H	-8.80067800	-3.66741600	-0.96580000
H	-6.63339900	-4.83925400	-1.30636500
H	-4.50987500	-3.65639600	-0.90861800
C	-5.45926700	-1.80033000	-0.30709800

### **Trans OPI**

O	4.75727100	-3.45696000	-1.03534300
O	4.44918600	-3.57440000	1.57199000
O	6.43924900	-1.96003600	2.63316600
O	8.13770500	-1.04210100	0.59250100
O	7.13166500	-2.09721900	-1.67872100
O	6.25403300	0.11222700	-3.24842700
O	6.83640000	2.32531500	-2.05045700
O	7.74598700	1.48520800	0.39975200



O	4.52390700	3.74233200	-1.40807200
O	2.55789300	2.38911600	-2.53102500
O	3.60801700	0.01692600	-3.63271400
O	1.30501700	1.35651400	-0.34842900
O	2.98321900	1.86727900	1.68952600
O	4.10707400	4.27509900	1.36386900
O	2.69934400	0.19412200	3.65953500
O	2.14526100	-2.09920000	2.25626200
O	1.22973000	-1.24188600	-0.25367300
O	5.53000800	0.08202000	4.01158100
O	5.71533200	2.07116300	2.12730700
O	2.58266000	-2.29083100	-2.32428600
H	4.87629700	-4.38903800	-1.27383500
H	4.61607600	-3.46882000	-0.03176200
H	3.61151300	-3.15457600	1.86260900
H	5.16144700	-3.02592000	1.97935800
H	6.98985600	-2.44596600	3.26609100
H	6.07240800	-1.17447700	3.15959600
H	7.54816000	-1.38197300	1.30363700
H	7.82077500	-1.48125400	-0.24664200
H	6.82045800	-1.33187600	-2.20728400
H	6.31157200	-2.58833400	-1.44650100
H	6.83830600	0.10422900	-4.02204600
H	6.46734500	0.99170500	-2.76626200
H	7.23039600	2.06173900	-1.18282200
H	6.02844900	2.84319000	-1.81797900

H	8.57838400	1.88777700	0.69098900
H	7.90507200	0.46733900	0.45514800
H	4.54404600	4.58322900	-1.89069100
H	3.76288700	3.22319800	-1.83194100
H	2.93071600	1.59386200	-2.97393800
H	2.06560500	2.01889900	-1.75419900
H	4.60378100	0.03942300	-3.54531500
H	3.42897200	-0.08018300	-4.58018100
H	0.37857500	1.66501800	-0.27567700
H	2.34664000	1.70219500	0.94241700
H	3.17555200	2.84667800	1.68074500
H	2.73770700	0.92752000	2.96233000
H	4.89897500	3.83591100	1.73971700
H	4.22955800	4.16575500	0.39320600
H	2.31176100	-1.30654200	2.82643700
H	2.20879800	0.55523700	4.41291900
H	1.65435200	-1.54697000	0.57679600
H	1.27765200	-2.43965000	2.52871000
H	1.73195200	-1.65915600	-1.00891500
H	1.26134300	0.34219100	-0.34738900
H	5.72478600	0.87856900	3.45599700
H	4.54935900	0.05306300	4.02896800
H	6.44940500	1.86553800	1.49300200
H	4.88578800	1.74573200	1.71468100
H	3.35339300	-2.75252300	-1.91825000
H	2.96002200	-1.50598700	-2.77737100

P	-3.95397900	-0.67874000	0.09586700
C	-2.38218900	1.64822000	-0.99975800
O	-2.30785900	1.68882700	-2.33222600
O	-1.45674300	1.96779600	-0.26008200
C	-1.03298700	2.05408800	-2.90177100
H	-0.72406400	3.04121900	-2.55087500
H	-0.27307300	1.31873400	-2.63359000
H	-1.19423500	2.06092500	-3.97900500
C	-4.24891600	1.64416500	0.83905300
O	-4.85045000	0.41698300	1.23605200
C	-3.71374800	1.16742000	-0.51447200
C	-5.21942700	2.80669000	0.79496200
C	-4.79534400	4.08283300	1.18196000
C	-5.66001500	5.17628300	1.10576100
C	-6.96593200	5.00348000	0.64593600
C	-7.39972600	3.73182000	0.26284700
C	-6.53279500	2.64228300	0.33633600
H	-3.41181600	1.90944400	1.50000600
H	-4.45813200	1.29612800	-1.30680300
H	-3.77987700	4.21995400	1.54735500
H	-5.31451100	6.16026400	1.41212700
H	-7.64322400	5.85165500	0.59077600
H	-8.41775200	3.58822100	-0.09052700
H	-6.87596700	1.65386600	0.04576500
C	-1.79431600	-2.09875100	-3.85741500
C	-3.12877200	-1.68202000	-3.87199700

C	-3.75819700	-1.31924600	-2.68315300
C	-1.74099500	-1.79190600	-1.45498500
C	-1.10063900	-2.14813500	-2.64957700
H	-1.30061500	-2.38133200	-4.78403400
H	-3.67818000	-1.63771000	-4.80942800
H	-4.79890000	-1.00146700	-2.71675200
H	-1.16174800	-1.83137300	-0.53931200
H	-0.05875200	-2.45738200	-2.62356500
C	-3.07915000	-1.37629700	-1.45192200
C	-2.80497900	-1.26614900	1.42327900
C	-3.06236400	-2.47985700	2.07952800
C	-1.71430000	-0.48999100	1.84285800
C	-2.25492600	-2.90292100	3.13548100
H	-3.90170600	-3.09644500	1.77711800
C	-0.91106600	-0.91445700	2.90371600
H	-1.47990800	0.44530300	1.34819900
C	-1.17911400	-2.11905800	3.55747300
H	-2.47653300	-3.84196000	3.63547000
H	-0.07202200	-0.29612200	3.21264800
H	-0.56884700	-2.43852500	4.39967200
C	-6.67842900	-1.45440500	0.55938100
C	-7.75731200	-2.33994700	0.52744700
C	-7.61246700	-3.60935400	-0.03092800
C	-6.37842500	-3.99102100	-0.55984200
C	-5.30472000	-3.10098800	-0.54900300
H	-6.78269700	-0.48484200	1.02602400

H	-8.71137000	-2.03447700	0.94890800
H	-8.45269900	-4.29860100	-0.05145700
H	-6.24930500	-4.98061000	-0.98998400
H	-4.36008600	-3.41304900	-0.97890600
C	-5.43602800	-1.81641500	0.01099100

### Trans OP2

O	-5.16059200	3.18192900	1.72310100
O	-5.20236600	1.42520100	3.67289900
O	-7.18366700	-0.40323800	3.02836000
O	-8.49706600	0.40002600	0.67911400
O	-7.29662300	2.70899800	-0.03958200
O	-6.01026200	2.16701500	-2.51955000
O	-6.51103200	-0.25014200	-3.27764600
O	-7.85299800	-1.30494100	-1.12698000
O	-4.14960400	-1.72200800	-3.35348200
O	-2.20299300	-0.01845800	-2.87854100
O	-3.35868200	2.48193500	-2.30337000
O	-1.34724300	-0.72118000	-0.40705400
O	-3.29086600	-2.38854300	0.34451500
O	-4.01580200	-4.00573700	-1.66670600
O	-3.44370300	-2.62913200	2.91714400
O	-2.82394000	-0.07351500	3.57447400
O	-1.25328500	1.09679900	1.50000400
O	-6.26825600	-2.84901000	2.78038300

O	-5.98777500	-2.91669200	0.05023000
O	-2.70683600	3.11794500	0.39860000
H	-5.32422300	4.02173900	2.17877500
H	-5.16584600	2.48639800	2.46085400
H	-4.37060100	0.90157600	3.66227500
H	-5.91803200	0.77356800	3.47940500
H	-7.85533300	-0.46663900	3.72450800
H	-6.81765700	-1.34560000	2.93444300
H	-8.04235300	0.13218800	1.51000300
H	-8.10975000	1.28900600	0.43985800
H	-6.84930200	2.51078100	-0.88969300
H	-6.56169600	2.88365100	0.59081200
H	-6.47786100	2.71540000	-3.16802500
H	-6.19459900	1.20116000	-2.81125800
H	-7.05411100	-0.65000200	-2.55477000
H	-5.68504200	-0.79081800	-3.30792600
H	-8.67457700	-1.77818300	-1.32842000
H	-8.11239200	-0.60181800	-0.41841000
H	-3.99679400	-1.98187500	-4.27507500
H	-3.40150600	-1.06774000	-3.14632700
H	-2.55596400	0.89442300	-2.79287800
H	-1.85597800	-0.22666400	-1.97043000
H	-4.34923900	2.39826300	-2.40904400
H	-3.11498000	3.29471800	-2.77071000
H	-0.45435200	-1.12002300	-0.50238700
H	-2.55948600	-1.76869300	0.06087200

H	-3.32944100	-3.11433800	-0.33849800
H	-3.32095300	-2.63019700	1.90818400
H	-4.89593600	-3.94700500	-1.23835400
H	-4.03768500	-3.26759200	-2.31778100
H	-3.00959900	-1.03232600	3.37970400
H	-2.90858000	-3.36522300	3.25053000
H	-1.77856300	0.72383500	2.23878000
H	-2.36282000	-0.06092800	4.42652100
H	-1.79084300	1.85470100	1.14546000
H	-1.26382400	-0.00441500	0.30096300
H	-6.29436600	-3.01997800	1.80499800
H	-5.30753200	-2.84816500	2.98325100
H	-6.66963600	-2.34604100	-0.38804500
H	-5.17132700	-2.37450700	0.11773500
H	-3.55898100	3.20512400	0.88573300
H	-2.96000600	2.82624200	-0.50291900
C	2.54995100	1.43706600	-0.85110000
O	3.98224400	-0.47874200	1.28116400
C	3.72939400	-1.76666200	0.62425800
C	3.56767400	-1.36272000	-0.81523900
P	3.94949600	0.66874100	0.07846100
C	4.81746500	-2.76509400	0.97180000
C	5.00771100	-3.89889400	0.17066900
C	5.95902800	-4.86065100	0.51193700
C	6.73825000	-4.70175000	1.65944300
C	6.55325700	-3.57747400	2.46527000

C	5.59558500	-2.61885600	2.12804600
H	2.77196400	-2.11898600	1.02228800
H	4.40763400	-4.02751200	-0.72626400
H	6.09449000	-5.73236000	-0.12308200
H	7.48270200	-5.44832700	1.92307100
H	7.15335200	-3.44499200	3.36200000
H	5.45103900	-1.74656000	2.75737900
H	4.37624900	-1.62845400	-1.49366900
C	2.23988900	-1.61721300	-1.37037500
O	1.21255600	-1.75006600	-0.70376300
O	2.22886800	-1.66716100	-2.72392100
C	0.94251700	-1.84761600	-3.34091900
H	1.14880000	-1.95905600	-4.40655400
H	0.45447600	-2.74611000	-2.95393800
H	0.29542500	-0.98280300	-3.17112800
C	5.54649000	0.85091700	-0.81808100
C	6.64279300	0.11064400	-0.35022900
C	5.72602500	1.71734000	-1.90675500
C	7.88785800	0.22629200	-0.96757500
H	6.52545800	-0.55948100	0.49479700
C	6.97527400	1.82939500	-2.52034100
H	4.89878600	2.31137600	-2.27964000
C	8.05831500	1.08323400	-2.05595800
H	8.72515400	-0.35700800	-0.59430000
H	7.09757500	2.50462000	-3.36307100
H	9.02868700	1.17050900	-2.53700100



C	4.15382100	2.03281800	1.36966100
C	4.63881500	3.29096500	0.97817700
C	3.78207500	1.85979300	2.71285000
C	4.75947500	4.33628600	1.89331100
H	4.93827900	3.46413100	-0.05098000
C	3.89737600	2.90726300	3.63011200
H	3.40313900	0.90030200	3.04278300
C	4.38815300	4.14793200	3.22547100
H	5.14442500	5.29802500	1.56397600
H	3.60248500	2.74820200	4.66432800
H	4.48051000	4.96146800	3.94032100
C	0.46236300	2.67834500	-0.87914100
C	1.52462300	2.10939900	-0.17141300
C	2.48912500	1.33227900	-2.25199600
C	1.44929000	1.93372700	-2.95694500
C	0.43244300	2.60249500	-2.27052400
H	-0.33939400	3.17061900	-0.33712400
H	1.53197000	2.18119800	0.91014700
H	3.24167700	0.76932800	-2.79172900
H	1.42366000	1.86234000	-4.04101900
H	-0.39004400	3.04859500	-2.82284100

### **Trans PW complex**

O	-2.56987300	-3.56389900	-2.03920000
O	-1.31028700	-1.67529000	-3.31941600

O	-3.34760100	0.05518600	-4.13134700
O	-5.87423300	-0.97189700	-3.48973200
O	-5.34926200	-3.30969100	-2.24603600
O	-6.16584100	-2.97828200	0.46659600
O	-7.31474300	-0.67332200	0.71000200
O	-6.89604100	0.56284600	-1.70893700
O	-5.87552100	0.87569700	2.52757000
O	-4.03037800	-0.68795000	3.53159100
O	-4.08611600	-3.15470600	2.15468000
O	-1.71434900	0.32479200	2.47868700
O	-2.78355200	1.76796000	0.49340400
O	-4.75459800	3.26363700	1.56115100
O	-1.03698200	2.27786100	-1.40756500
O	0.06111500	-0.26669600	-1.37498600
O	-0.43780800	-1.44839500	1.06426300
O	-3.14374100	2.52241500	-3.25465700
O	-4.92178800	2.36346100	-1.12902500
O	-1.76477500	-3.76405400	0.61066600
H	-2.29812300	-4.36032800	-2.52028100
H	-2.08119600	-2.80465800	-2.51257600
H	-0.73152400	-1.18442300	-2.68762300
H	-1.99258600	-1.02569900	-3.60891100
H	-3.30999400	0.14239200	-5.09613100
H	-3.26284000	1.00492900	-3.78476600
H	-4.98406700	-0.62058000	-3.72398800
H	-5.70417300	-1.86940600	-3.08552300

H	-5.61746300	-3.17981100	-1.31181900
H	-4.36961100	-3.40238500	-2.20787900
H	-6.89267000	-3.61239100	0.56336000
H	-6.60453300	-2.05820200	0.56669200
H	-7.23411300	-0.22346900	-0.16703900
H	-6.81508200	-0.10141100	1.34038000
H	-7.68392200	0.93887400	-2.12994600
H	-6.48882800	-0.07040500	-2.41584900
H	-6.45681700	1.02974900	3.28826400
H	-5.13864300	0.27543800	2.88990200
H	-4.03816500	-1.55405500	3.06456000
H	-3.14650300	-0.30392700	3.31730600
H	-4.87696800	-3.13139600	1.54458500
H	-4.27158000	-3.85659900	2.79678500
H	-1.05100700	1.00287600	2.71165700
H	-2.44318100	1.13556300	1.18510600
H	-3.33168900	2.43267700	0.98921300
H	-1.65903500	2.16366700	-0.62674000
H	-5.07350100	3.26076700	0.63235100
H	-5.19891600	2.47617200	1.95524800
H	-0.23569200	0.67454600	-1.41346700
H	-0.45606300	3.01860100	-1.17149100
H	-0.34022600	-1.02389300	0.17643400
H	1.03925100	-0.25180100	-1.24197000
H	-0.94375700	-2.29314700	0.90557200
H	-1.19889700	-0.40620500	2.00051300

H	-3.86467000	2.61730200	-2.58524300
H	-2.32056600	2.54786200	-2.71677800
H	-5.67314500	1.75737700	-1.35384100
H	-4.25655800	1.80225700	-0.67370000
H	-2.05762700	-3.70794300	-0.33021600
H	-2.58052300	-3.63148200	1.13976400
O	2.71274000	-0.18624300	-0.63435800
C	1.71237300	3.52167100	0.14318900
C	0.86033900	4.25853900	0.88790000
P	3.55611700	-1.21608200	0.10526200
C	2.58475900	3.98902300	-0.93398000
C	2.71492000	5.34773000	-1.28520800
C	3.55964900	5.73246600	-2.31960400
C	4.29291300	4.77053800	-3.02384600
C	4.17538000	3.42246900	-2.68446100
C	3.32959500	3.03075500	-1.64793700
H	1.75760300	2.45308700	0.34741800
H	2.15794600	6.10593900	-0.74240500
H	3.65074600	6.78361000	-2.57914100
H	4.95271100	5.07537800	-3.83175500
H	4.74478600	2.67196400	-3.22568500
H	3.23513700	1.97947400	-1.38404400
H	0.72369200	5.32515100	0.74160300
C	0.04533000	3.64820300	1.95308100
O	0.12941700	2.48612100	2.33623600
O	-0.81011500	4.55193100	2.46152900

C	-1.73697900	4.11660000	3.47453900
H	-1.97334600	5.00651600	4.05927200
H	-2.64436100	3.73873900	2.99542800
H	-1.28501700	3.34928400	4.10573100
C	5.32455300	-0.94112400	-0.28112600
C	6.35899500	-1.09548600	0.65165600
C	5.63701400	-0.54348200	-1.59182000
C	7.68399100	-0.86510700	0.27762600
H	6.13400500	-1.38092100	1.67423800
C	6.96224300	-0.31976200	-1.96366300
H	4.83668500	-0.40153900	-2.31220400
C	7.98767400	-0.48089200	-1.02915600
H	8.47792700	-0.98122200	1.01035600
H	7.19427900	-0.01557100	-2.98082100
H	9.01998800	-0.30186000	-1.31765300
C	3.34353700	-1.11140000	1.91286300
C	2.64653400	-0.01735000	2.43969100
C	3.83041000	-2.10267200	2.78042200
C	2.45908400	0.09910400	3.81723000
H	2.22685000	0.72808800	1.77486000
C	3.65019100	-1.97834400	4.15748300
H	4.33107000	-2.98131300	2.38198200
C	2.96700200	-0.87539500	4.67679000
H	1.90456700	0.94767700	4.20706100
H	4.02922500	-2.74891800	4.82330900
H	2.81977900	-0.78559100	5.74987200

C	3.17200800	-2.94484500	-0.33043700
C	1.91935400	-3.45028300	0.05939400
C	4.04596900	-3.75451200	-1.07086400
C	1.54592600	-4.74577200	-0.29527900
H	1.22888500	-2.83207900	0.62800500
C	3.66954700	-5.05380400	-1.41594500
H	5.01683700	-3.37725300	-1.37718600
C	2.42195200	-5.54841100	-1.03063300
H	0.56728200	-5.10944900	0.00611700
H	4.35182100	-5.67778500	-1.98716800
H	2.13342900	-6.56021400	-1.30440200

#### **Cis TS1**

O	4.98583300	-2.05897800	3.19823500
O	3.77882000	0.12585500	4.00787800
O	5.19907500	2.15944500	2.74788400
O	7.44368800	1.17396200	1.37743900
O	7.32456100	-1.49438200	1.75931900
O	6.83077300	-2.63275400	-0.80421600
O	6.87450500	-0.76162900	-2.59082300
O	7.11233600	1.56349100	-1.13687200
O	4.37369000	-0.62089500	-3.82599300
O	2.92632600	-2.59171500	-2.87197700
O	4.44693900	-3.86199600	-0.88707400
O	1.10093800	-1.49686400	-1.12188500
O	2.44417000	0.81208400	-1.02237900

O	2.95056400	1.76934900	-3.48063000
O	1.38507600	2.12780500	0.98409700
O	1.27083800	0.09884600	2.74651000
O	1.08586000	-2.34303800	1.36993500
O	3.74803700	3.64548700	1.14623300
O	4.56237500	2.53420900	-1.26021400
O	3.33027200	-3.77646400	1.74235100
H	5.24680900	-2.48368500	4.02958500
H	4.50305400	-1.21402500	3.48493000
H	2.86164700	0.15042900	3.65485600
H	4.24795400	0.87826600	3.57473500
H	5.53622500	2.77756500	3.41439800
H	4.63231800	2.73147000	2.12911900
H	6.65614000	1.51736800	1.85871600
H	7.45451200	0.19204400	1.56071600
H	7.13730000	-1.87924000	0.87693100
H	6.51278500	-1.67815800	2.28485800
H	7.62757100	-3.15311500	-0.98883600
H	6.83356600	-1.88803300	-1.50692300
H	7.00896700	0.09088100	-2.10835400
H	5.99386100	-0.68052000	-3.02847600
H	7.83670700	2.15292300	-1.39592200
H	7.25271500	1.38795100	-0.12992100
H	4.49801600	-0.88845500	-4.74965300
H	3.79831100	-1.35609400	-3.42561800
H	3.46464400	-3.07823600	-2.20675600

H	2.15559200	-2.26135600	-2.35322400
H	5.35825300	-3.45377000	-0.86091700
H	4.58518200	-4.80518200	-1.06162600
H	0.23725000	-1.04194300	-1.19285500
H	2.06433800	-0.10969700	-1.02961600
H	2.41370500	1.13393300	-1.96441600
H	1.69188000	1.65869300	0.14833600
H	3.60265500	2.31057900	-2.98460400
H	3.46643700	0.96845100	-3.73375600
H	1.24752300	0.86655400	2.10843200
H	0.54358900	2.56438600	0.75909300
H	1.25618800	-1.50181500	1.84944300
H	0.41601800	0.11351600	3.20511300
H	1.87646800	-2.92732600	1.55579900
H	1.10432900	-1.90097300	-0.19496000
H	4.08797700	3.43783800	0.24149800
H	2.84796100	3.24771800	1.15515800
H	5.51713300	2.26982200	-1.25499500
H	4.07211900	1.72648800	-0.99300000
H	3.92071500	-3.19139100	2.27119800
H	3.72310500	-3.78174200	0.84384800
O	-3.87735500	1.96696100	1.28165500
C	-3.70827800	2.38679500	0.07287300
P	-4.17030900	-0.42981200	0.00327000
C	-3.46648000	0.90873300	-1.01912200
C	-2.56312100	3.36052400	-0.17786100



C	-1.68626600	3.64340700	0.87638800
C	-0.67383000	4.59540700	0.72104000
C	-0.52114300	5.26522900	-0.49746800
C	-1.39736800	4.99159600	-1.54989200
C	-2.41655100	4.05133800	-1.38601200
H	-4.61082300	2.75031500	-0.47220900
H	-4.14014500	1.07298900	-1.86167400
H	-1.85492700	3.12878100	1.81788200
H	-0.01251000	4.82897500	1.55241200
H	0.26694700	6.00340600	-0.61900300
H	-1.29275400	5.51829100	-2.49515000
H	-3.10526500	3.85387000	-2.20463200
C	-2.09014000	0.68408200	-1.48034500
O	-1.87878300	1.22980800	-2.69653000
O	-1.20345500	0.11820500	-0.84095300
C	-3.95876700	-1.99542700	-0.93866300
C	-0.51926100	1.22829800	-3.17547600
H	0.15495900	1.65337600	-2.43203800
H	-0.20010200	0.20993300	-3.41539100
H	-0.52502300	1.84172300	-4.07548600
C	-2.19444100	-1.39421100	1.73934800
C	-3.45920900	-0.79417100	1.64704200
C	-4.21667200	-0.59224000	2.81048200
C	-3.71071600	-0.98209400	4.04834100
C	-2.44960800	-1.57635600	4.13941500
C	-1.69279200	-1.78077600	2.98457200

H	-1.58939400	-1.56168000	0.85760300
H	-5.18983600	-0.12094100	2.75507100
H	-4.30503900	-0.81792700	4.94285100
H	-2.06353700	-1.88736100	5.10680300
H	-0.71854700	-2.25948000	3.01599100
C	-3.92540000	-4.42421500	-0.98998200
C	-4.03299800	-3.23165100	-0.27541000
C	-3.78000900	-1.98140100	-2.33133200
C	-3.66973500	-3.17701100	-3.04188800
C	-3.74169300	-4.39955200	-2.37351600
H	-3.97677900	-5.37208700	-0.46198800
H	-4.16391800	-3.26500700	0.80102900
H	-3.71274900	-1.04038000	-2.86733900
H	-3.52116600	-3.14960300	-4.11758500
H	-3.65018600	-5.32960700	-2.92753100
C	-5.98769900	-0.16812600	0.09815100
C	-6.85176300	-1.09806800	-0.50487400
C	-6.52790800	0.95929000	0.74450900
C	-8.23270800	-0.90404700	-0.46166000
H	-6.45862400	-1.97317200	-1.00866900
C	-7.91046600	1.13870300	0.78307400
H	-5.83792300	1.66215800	1.21155400
C	-8.76511300	0.21295300	0.18200700
H	-8.88939300	-1.63035500	-0.93238400
H	-8.31869400	2.01129500	1.28570700
H	-9.84128700	0.36116900	0.21442600

**Cis OP1**

O	4.50567700	-3.79884200	-0.44987800
O	4.14576900	-3.47276200	2.13275200
O	6.13624900	-1.71334100	2.93326900
O	7.85692500	-1.13960600	0.79015000
O	6.87721200	-2.55040800	-1.29116200
O	6.01293000	-0.62739600	-3.20815200
O	6.59123000	1.75270500	-2.38553100
O	7.46677300	1.32099900	0.18000700
O	4.27139600	3.25006700	-1.99748100
O	2.30942600	1.72739200	-2.88956600
O	3.36988800	-0.78604000	-3.59834300
O	1.04715100	1.04341800	-0.58818000
O	2.69810900	1.89454700	1.35187400
O	3.82453300	4.22303100	0.64824600
O	2.41066700	0.57733000	3.57734800
O	1.84718000	-1.89888700	2.54298100
O	1.00599500	-1.50974000	-0.09046000
O	5.22727200	0.52234000	3.96420300
O	5.42280200	2.17497700	1.77892100
O	2.35479300	-2.88735900	-1.96471400
H	4.63509100	-4.75695700	-0.52063200
H	4.34123400	-3.63856100	0.53749600
H	3.30591600	-3.01080100	2.34278800
H	4.85524400	-2.86551900	2.45204000

H	6.67965800	-2.09428600	3.63999500
H	5.76810200	-0.85310900	3.32621100
H	7.25757600	-1.35909900	1.53963200
H	7.55000200	-1.70955700	0.02968900
H	6.56754700	-1.88077300	-1.93741800
H	6.05685200	-2.99994900	-0.98659200
H	6.60564400	-0.76528100	-3.96283800
H	6.22462300	0.31936500	-2.87636200
H	6.97422700	1.63329900	-1.48178100
H	5.78155600	2.30094000	-2.24867900
H	8.29483000	1.76704400	0.41481100
H	7.62487900	0.32624900	0.40313600
H	4.28864200	4.00328300	-2.60796400
H	3.51322000	2.66679800	-2.33290000
H	2.68314500	0.87281600	-3.20266900
H	1.81705700	1.48130600	-2.06353800
H	4.36463700	-0.74726100	-3.50749300
H	3.19874500	-1.03286000	-4.51973700
H	0.11253300	1.33515100	-0.56405400
H	2.06725100	1.60233200	0.63859300
H	2.88292500	2.86020100	1.18335200
H	2.44544200	1.18033300	2.76527000
H	4.60955100	3.84842700	1.10067200
H	3.95831900	3.95562400	-0.28950400
H	2.00322600	-1.02310200	2.97931100
H	1.90332300	1.05371600	4.25111900

H	1.43331600	-1.65851600	0.78052800
H	0.94986600	-2.16569000	2.80309600
H	1.50778400	-2.04804300	-0.76415400
H	1.02009000	0.04039700	-0.43739800
H	5.42645300	1.21721600	3.28724100
H	4.24581300	0.49735600	3.97829600
H	6.15884800	1.86960200	1.18907000
H	4.59451300	1.78574000	1.42195100
H	3.12260400	-3.26716200	-1.47690600
H	2.73025000	-2.17586000	-2.52706200
O	-4.46093800	0.91163100	1.10879300
C	-4.67430300	1.85068900	0.06579700
P	-4.04926000	-0.51963400	0.06831300
C	-4.04026700	1.04914200	-1.08738200
C	-4.13763700	3.23555400	0.37486700
C	-3.59106900	3.53407300	1.62563500
C	-3.13480300	4.82364500	1.90693100
C	-3.21950600	5.82776700	0.94190600
C	-3.77076500	5.53714300	-0.30836800
C	-4.23144600	4.25070300	-0.58668900
H	-5.75235600	1.94889500	-0.15243800
H	-4.65072300	0.93031500	-1.98411800
H	-3.53401100	2.74727400	2.36997400
H	-2.71150400	5.04356700	2.88384700
H	-2.86124100	6.83007400	1.16113200
H	-3.84462100	6.31320400	-1.06598500

H	-4.66652600	4.03423100	-1.56091000
C	-2.63412900	1.42314500	-1.46731200
O	-2.48579900	1.57590200	-2.78749800
O	-1.72389200	1.55646200	-0.66162100
C	-1.15086800	1.87148200	-3.25299000
H	-0.79162000	2.80482300	-2.81407400
H	-0.46740700	1.06239600	-2.99265100
H	-1.23878000	1.96525500	-4.33478600
C	-1.34727200	-2.71234700	-2.32282600
C	-1.95541300	-2.08226800	-1.22933300
C	-3.95010100	-1.75276100	-2.53262100
C	-3.35764300	-2.39766200	-3.61654600
C	-2.05009700	-2.88132900	-3.51368300
H	-0.31985500	-3.05599500	-2.23361200
H	-1.36143200	-1.95394000	-0.33189400
H	-4.96612600	-1.37921900	-2.64206400
H	-3.91461800	-2.51648800	-4.54295300
H	-1.58295700	-3.37713700	-4.36103800
C	-3.27027900	-1.60138400	-1.30714000
C	-2.96898100	-1.12817700	1.46474100
C	-3.07536200	-2.45894300	1.89302200
C	-2.06958900	-0.27346200	2.11402900
C	-2.32522600	-2.91855700	2.97582000
H	-3.75945800	-3.13940600	1.39540100
C	-1.30162100	-0.74074500	3.18285500
H	-1.97429600	0.75303800	1.78292300

C	-1.43749600	-2.05876300	3.62797900
H	-2.43968800	-3.94503100	3.31353300
H	-0.60073600	-0.06774700	3.67086500
H	-0.87156700	-2.41072900	4.48826700
C	-5.71344300	-1.32709000	0.22812100
C	-6.73376600	-0.67656500	0.94322000
C	-5.96962900	-2.61408400	-0.27572000
C	-7.97852400	-1.28119000	1.11989700
H	-6.52940500	0.29201200	1.38200600
C	-7.21113000	-3.22203500	-0.08510600
H	-5.20196600	-3.14930700	-0.82120200
C	-8.22308500	-2.55430600	0.60489600
H	-8.75447000	-0.75642900	1.67085200
H	-7.38431200	-4.21946400	-0.48024800
H	-9.19206600	-3.02590500	0.74620400