

Supporting Information for
“Origins of the Enantioselectivity of Palladium-Catalyzed
Aziridination with BINOL-Phosphoric Acid Ligands”

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Scheme S1 The electronic structures of the C–H activation transition states.

We carried out a natural bond orbital (NBO)¹ analysis of **4HPA-SOAc-TS** and **4HPA-SPA-TS**. For other transition states, the analyses are similar.

In **4HPA-SOAc-TS**, we observed considerable electron transfers from the lone pairs of palladium (*d* electrons) and the acetate oxygen (*p* electrons) to the C–H antibonding orbital. The stabilization energies are:

$$E_2(n_{\text{O}} \rightarrow \sigma_{\text{C-H}}^*) = 70.2 \text{ kcal mol}^{-1}$$

$$E_2(n_{\text{Pd}} \rightarrow \sigma_{\text{C-H}}^*) = 6.8 \text{ kcal mol}^{-1}$$

Both weaken and activate this bond. Actually, at the transition state geometry, the acetate has a stronger effect. Thus, the old C–H has not been broken completely in the transition state.

In **4HPA-SPA-TS**, however, the old C–H has essentially been disappeared. Instead, a bond between the hydrogen and the phosphate oxygen ($\sigma_{\text{O-H}}$) with an occupancy of 1.92 has formed.

Therefore, **4HPA-SOAc-TS** and **4HPA-SPA-TS** is a reactant- and product-like transition state, respectively. This is in agreement with the discussions in the paper. In the **SOAc** scenarios, the transition state occurs earlier therefore has lower activation energy.

These NBOs are shown below, using isovalue = 0.8 au.

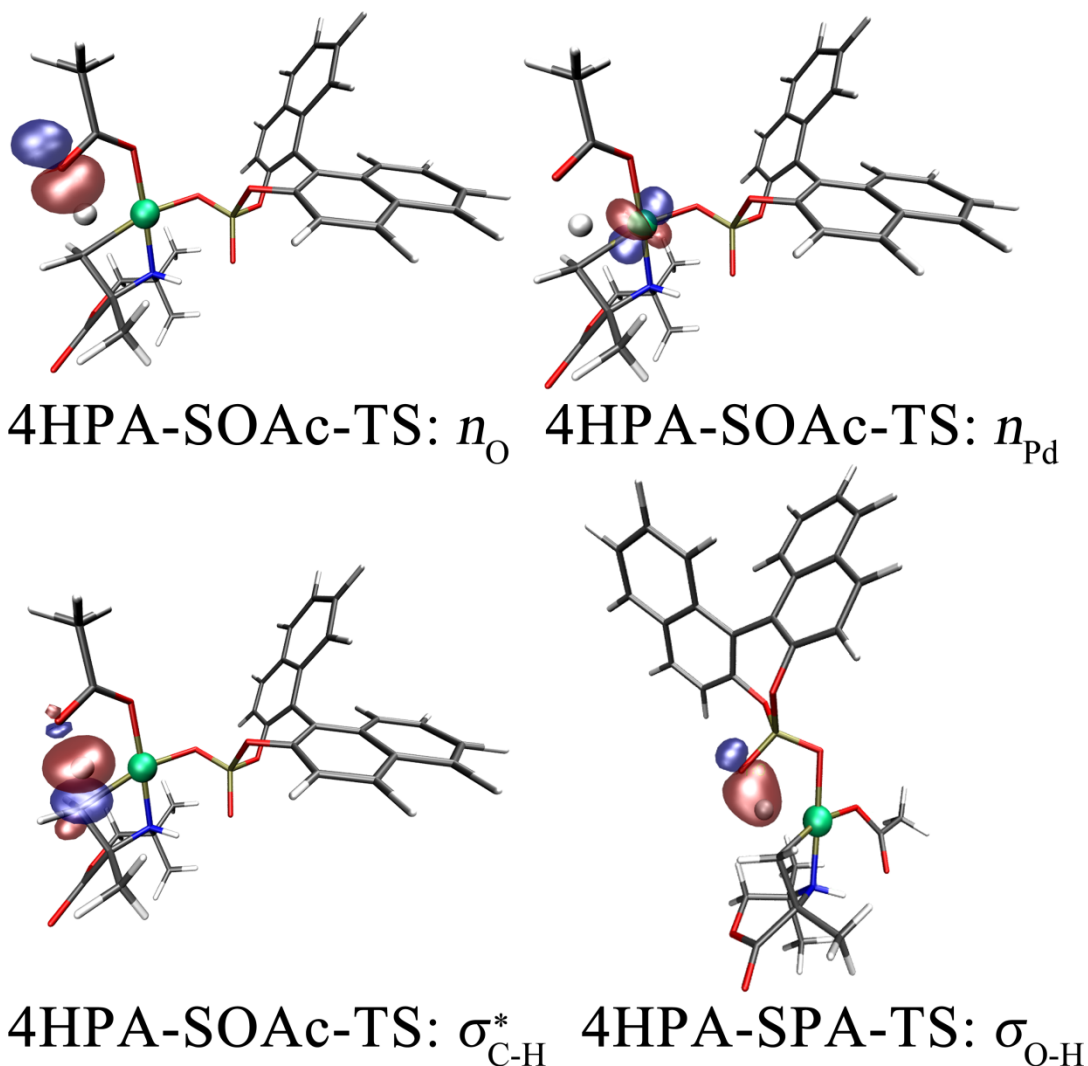


Figure S1 Scan of the potential energy surface of **1**: the activated C–H bond was stretched from 1.09 to 1.59 Å while other geometrical parameters were fixed.

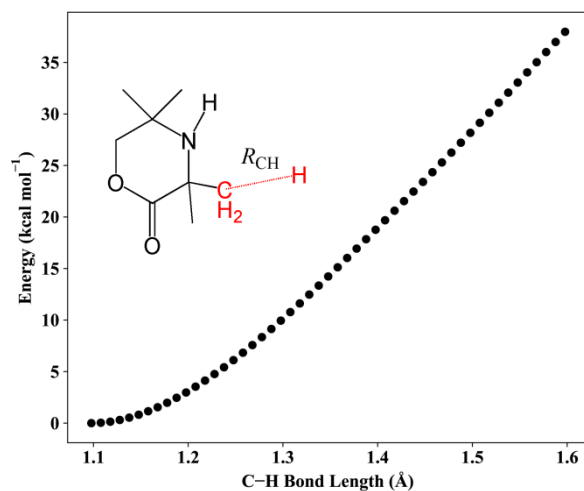


Figure S2 Scan of the potential energy surface of **3HPA**: the relative orientation of acetate and phosphate changes. The potential energy surface is very flat: energy change is less than 2.5 kcal mol⁻¹.

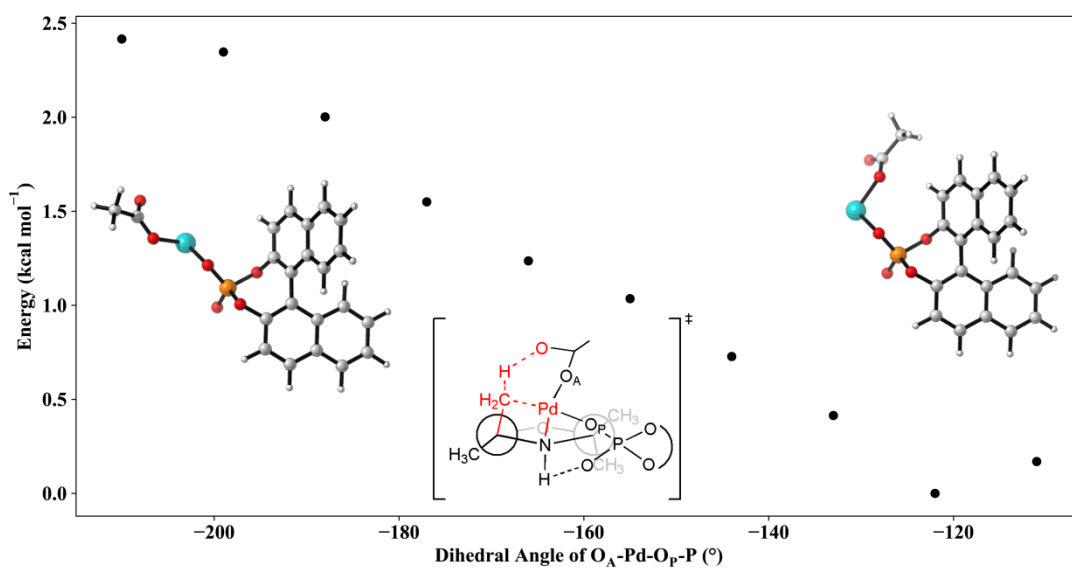


Figure S3 Superposition of **3TRIP** from **4TRIP-SOAc** (blue) and **4TRIP-ROAc** (red).

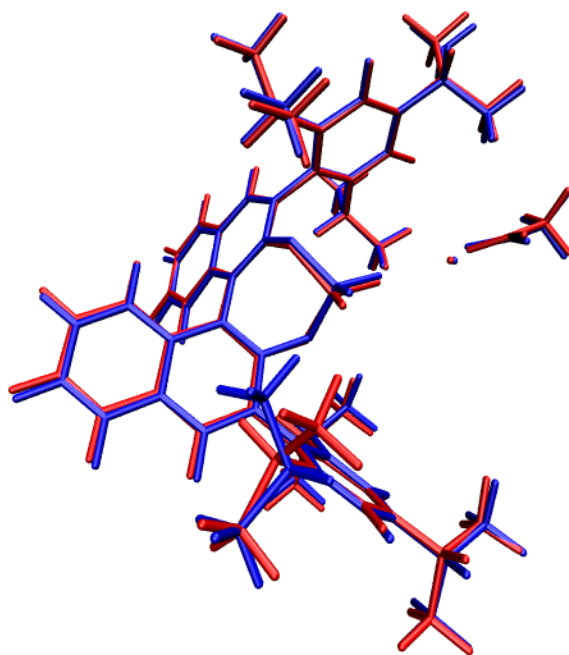


Table S1 The distortion/interaction analysis for **4X**. The energies are given in kcal mol⁻¹.

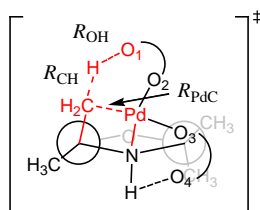
X and scenario	$\Delta E_{\text{dist}}(\mathbf{1})$	$\Delta E_{\text{dist}}(\mathbf{3X})$	$\Delta E_{\text{int}}(\mathbf{4X})$	$\Delta E(\mathbf{4X})$
4HPA-SOAc	2.6	15.5	-53.1	-35.0
4HPA-ROAc	4.1	15.5	-51.0	-31.3
4HPA-SPA	2.7	21.3	-54.2	-30.2
4HPA-RPA	3.6	20.8	-53.1	-28.7
4PhPA-SOAc	2.5	13.2	-55.6	-39.8
4PhPA-ROAc	3.9	13.4	-53.4	-36.1
4PhPA-SPA	2.7	20.6	-56.6	-33.3
4PhPA-RPA	3.7	20.4	-55.6	-31.6
4TRIP-SOAc	2.8	21.8	-59.0	-34.4
4TRIP-ROAc	4.2	17.9	-57.0	-34.8
4TRIP-SPA	2.7	21.8	-60.5	-36.0
4TRIP-RPA	3.4	20.7	-58.7	-34.7

Table S2 Key Geometrical and Electronic Parameters of Transition States **4X-TS**.

The total electrostatic potential $\varphi(\mathbf{r})$ is defined as:

$$\varphi(\mathbf{r}) = \sum_A^{\text{nuclei}} \frac{Z_A}{|\mathbf{r} - \mathbf{R}_A|} - \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$$

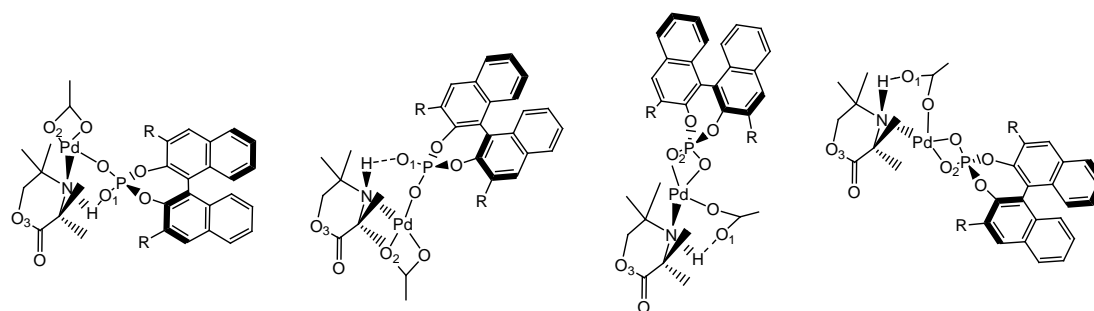
where Z_A , \mathbf{R}_A , and $\rho(\mathbf{r})$ is the nuclear charge of A , position of A , and electron density at \mathbf{r} , respectively.



X and scenario	R_{CH} (Å)	R_{OH} (Å)	R_{PdC} (Å)	$\varphi(\text{O}_1)$ (10^3 au)	$\varphi(\text{O}_2)$ (10^3 au)	$\varphi(\text{O}_3)$ (10^3 au)	$\varphi(\text{O}_4)$ (10^3 au)	$\omega_{\text{activation}}$ (cm^{-1})
4HPA-SOAc-TS	1.39	1.41	2.22	0.946	0.942	0.936	0.939	1139.53 <i>i</i>
4HPA-ROAc-TS	1.39	1.40	2.21	0.945	0.941	0.936	0.939	1148.41 <i>i</i>
4HPA-SPA-TS	1.48	1.33	2.20	0.939	0.938	0.942	0.947	1167.80 <i>i</i>
4HPA-RPA-TS	1.47	1.33	2.20	0.939	0.938	0.942	0.946	1171.12 <i>i</i>
4PhPA-SOAc-TS	1.38	1.41	2.22	0.939	0.934	0.928	0.930	1107.62 <i>i</i>
4PhPA-ROAc-TS	1.37	1.43	2.24	0.940	0.934	0.928	0.930	1077.95 <i>i</i>
4PhPA-SPA-TS	1.48	1.32	2.21	0.931	0.928	0.934	0.939	1167.00 <i>i</i>
4PhPA-RPA-TS	1.49	1.32	2.19	0.931	0.929	0.934	0.941	1134.00 <i>i</i>
4TRIP-SOAc-TS	1.39	1.40	2.21	0.929	0.923	0.914	0.917	1127.88 <i>i</i>
4TRIP-ROAc-TS	1.40	1.46	2.19	0.930	0.923	0.915	0.915	1047.12 <i>i</i>
4TRIP-SPA-TS	1.49	1.30	2.18	0.917	0.915	0.923	0.930	1134.45 <i>i</i>
4TRIP-RPA-TS	1.50	1.34	2.17	0.916	0.916	0.923	0.931	1104.20 <i>i</i>

Table S3 Key Geometrical and Electronic Parameters of **4X** and **4X-TS**.

The magnitude of ring puckering of **1** is measured with Cremer–Pople amplitude Q_2 .² For free **1**, $Q_2 = 0.508$ Å.



X and scenario	R_{PdN} (Å)	R_{O1H} (Å)	R_{O2O3} (Å)	Q_1 in 4X (Å)	Q_1 in 4X-TS (Å)	$\Delta E_{\text{int-disp}}(\mathbf{4X-TS})$ (kcal mol ⁻¹)
4HPA-SOAc	2.12	1.90	5.64	0.551	0.588	-14.7
4HPA-ROAc	2.13	1.89	3.73	0.531	0.592	-14.7
4HPA-SPA	2.10	1.75	5.53	0.543	0.603	-14.2
4HPA-RPA	2.09	1.78	4.44	0.649	0.607	-14.1
4PhPA-SOAc	2.12	1.85	5.62	0.547	0.584	-20.2
4PhPA-ROAc	2.13	1.81	3.70	0.520	0.596	-20.1
4PhPA-SPA	2.10	1.76	5.52	0.534	0.591	-21.3
4PhPA-RPA	2.09	1.78	4.46	0.653	0.603	-20.2
4TRIP-SOAc	2.12	1.75	5.51	0.548	0.590	-27.3
4TRIP-ROAc	2.15	1.78	3.56	0.521	0.625	-26.3
4TRIP-SPA	2.10	1.75	4.52	0.518	0.558	-23.9
4TRIP-RPA	2.10	1.79	4.88	0.646	0.595	-23.8

Table S4 Geometries of the Molecules Considered in This Study (Unit: Å)

All were optimized at SMD(EtOAc)/BLYP-D3/def2-TZVP level of theory.

1			
H	-2.88203000	-0.86056500	-1.15999000
O	-0.13793200	1.73555700	-0.32737100
C	1.49491700	-0.11396700	0.03654500
C	1.17210100	1.18502900	-0.72079400
C	-1.17077900	0.90862300	0.00662000
C	-0.99338900	-0.63456800	-0.06938600
N	0.41796700	-1.10302200	-0.24535200
H	0.53537200	-1.41371100	-1.21199600
C	1.61846900	0.14836400	1.55440500
C	2.81801000	-0.68944100	-0.50550300
H	1.15019700	1.00282000	-1.80483500
H	1.88257700	1.99269800	-0.50782500
O	-2.22560200	1.42289300	0.34674800
C	-1.58125100	-1.25777500	1.22258800
C	-1.82149600	-1.10060200	-1.29624200
H	1.78135500	-0.79807900	2.08468900
H	0.72254300	0.62295600	1.97304600
H	2.46775400	0.81556300	1.75387300
H	3.05354000	-1.63326800	0.00337700
H	3.64650500	0.01056000	-0.33529700
H	2.75601200	-0.88779400	-1.58570700
H	-2.62490600	-0.95738200	1.37007800
H	-1.00403900	-0.95512600	2.10406700
H	-1.52868400	-2.35067100	1.13906200
H	-1.72222400	-2.18926600	-1.40927700
H	-1.47096800	-0.61916400	-2.22021000

3			
Pd	0.00000000	0.00000000	0.00004400
C	0.00000000	2.47574100	-0.00003000
O	-0.00638600	1.78802800	-1.09386200
O	-0.00618200	1.78814000	1.09386500
C	0.00000000	-2.47574100	-0.00003000
O	0.00618200	-1.78814000	1.09386500
O	0.00638600	-1.78802800	-1.09386200
C	0.04644100	3.96810600	-0.00009900
H	1.09929200	4.28733500	0.00058600
H	-0.43579900	4.36515500	-0.90069000
H	-0.43694200	4.36524100	0.89984800
C	-0.04644100	-3.96810600	-0.00009900
H	-1.09929200	-4.28733500	0.00058600
H	0.43579900	-4.36515500	-0.90069000

H	0.43694200	-4.36524100	0.89984800
4			
Pd	-1.19025800	0.23027800	0.00017600
O	1.25364600	2.54317700	-0.37756600
O	-0.97802700	2.26928400	0.00111800
H	1.26160100	-2.99707100	-0.17388900
O	-2.09502700	-1.69836300	-0.02401100
O	3.55430600	-0.88830100	0.37428600
C	1.35436000	-0.53644600	1.56151500
C	2.68071300	-1.33090500	1.46339600
C	3.03428200	-0.88979700	-0.88941400
C	1.48133700	-0.95187200	-1.02153400
N	0.89228600	-0.15936300	0.14504600
H	1.21476200	0.82252500	-0.02106800
C	1.57739800	0.78172200	2.33209800
C	0.33052300	-1.42247800	2.29780700
H	2.50117500	-2.40476200	1.34178800
H	3.27016800	-1.18437200	2.37280900
O	3.78952700	-0.80968900	-1.83868200
C	1.08173400	-0.24270800	-2.33431600
C	1.01334900	-2.42472700	-1.07200800
H	0.66682300	1.39360400	2.33067200
H	2.39100400	1.37122900	1.89182000
H	1.83323900	0.55605800	3.37493400
H	-0.57007200	-0.84877100	2.54793300
H	0.77419000	-1.78265600	3.23693600
H	0.03367300	-2.29030900	1.70033500
H	1.54477600	-0.75374400	-3.18401300
H	1.40250000	0.80458300	-2.33853700
H	-0.00849500	-0.27774900	-2.45214000
H	1.49074200	-2.91623200	-1.92877600
H	-0.07245300	-2.45914900	-1.20763500
C	-3.27566600	-1.17641100	-0.13013100
O	-3.35555100	0.10756100	-0.14729100
C	-4.49149900	-2.04278200	-0.26825800
C	0.09731400	2.98870400	-0.20608600
C	-0.15447300	4.49321900	-0.20687400
H	0.29930500	4.93099400	-1.10544700
H	0.34708300	4.93182900	0.66719000
H	-1.22101900	4.73665700	-0.17247000
H	-4.67447800	-2.22345300	-1.33808600
H	-5.37041600	-1.53919200	0.15041900
H	-4.33546400	-3.00972300	0.22381000
4-TS			

Pd	0.85192700	0.01043800	-0.17674000
O	0.15197700	2.56210900	1.55246000
O	1.43237900	1.99623100	-0.25092700
H	-0.44147600	-2.15889400	-1.06349500
O	2.40929500	-2.50044200	0.25347900
O	-3.21051000	-1.35647300	-0.99336300
C	-2.18209400	0.88857500	-0.67820300
C	-2.56408600	-0.21901700	-1.66348300
C	-2.70127600	-1.78697300	0.19538900
C	-1.38050800	-1.15494200	0.69864500
N	-1.15595300	0.29685000	0.27621300
H	-1.06918200	0.92339100	1.09123700
C	-3.40010000	1.35815600	0.15299300
C	-1.58818700	2.07207100	-1.46045400
H	-1.68409800	-0.58064200	-2.21188100
H	-3.30738300	0.14103800	-2.37999500
O	-3.24440900	-2.71316800	0.77082400
C	-1.29155000	-1.24884300	2.22891600
C	-0.22363600	-1.93454500	-0.01302000
H	-3.10540000	2.18303600	0.81401700
H	-3.82379500	0.56002000	0.77375400
H	-4.19014800	1.71945800	-0.51766500
H	-1.27469400	2.86469200	-0.77386000
H	-2.35433800	2.48483400	-2.12949200
H	-0.72227300	1.76878000	-2.05932700
H	-1.36717000	-2.29276300	2.54771100
H	-2.10530300	-0.68216400	2.69835700
H	-0.33016000	-0.84652800	2.57236800
H	-0.10839100	-2.89748600	0.50614800
H	1.17432300	-1.93805200	0.19275600
C	3.22514700	-1.62851800	-0.21308900
O	2.87033100	-0.43626400	-0.52552400
C	4.66874500	-2.02696000	-0.42321100
C	0.97739400	2.83065000	0.65293100
C	1.52173200	4.25027700	0.48907300
H	1.44987400	4.79274500	1.43819000
H	0.90857500	4.77407100	-0.25935200
H	2.55787100	4.24568800	0.13159000
H	5.27995600	-1.16632100	-0.70968600
H	4.71214700	-2.78819800	-1.21464400
H	5.06208300	-2.48034500	0.49530500
3HPA			
Pd	3.76784900	-0.00624200	-0.00748400
C	6.23367700	-0.00082700	-0.00201400

O	5.54159800	0.97692900	-0.48858100
O	5.54446900	-0.98686700	0.47185400
C	7.72413600	0.02170200	0.04035900
H	8.12346100	-0.99345700	-0.07035100
H	8.11887800	0.67658200	-0.74463300
H	8.04217900	0.41354700	1.01816900
P	1.10661500	-0.00569700	-0.00474000
O	2.04012000	-1.13451700	0.54758000
O	2.03965800	1.12182800	-0.56054800
O	0.09572000	0.45387800	1.20821300
O	0.09021700	-0.46328300	-1.21372900
C	-1.03020300	-1.27926600	-0.86851000
C	-2.09949800	-0.72571000	-0.17255300
C	-0.98587900	-2.62103700	-1.30237000
C	-3.16422900	-1.61713200	0.22523600
C	-2.03926000	-3.45800100	-0.99813700
C	-4.23279600	-1.20749900	1.07700500
C	-3.13620600	-2.99259100	-0.21701200
H	-2.02779600	-4.49506300	-1.33246100
C	-5.23719400	-2.08851300	1.43714000
H	-4.25325600	-0.18913800	1.45581100
C	-4.19640700	-3.86816500	0.16172100
C	-5.22999300	-3.42718100	0.96678700
H	-6.03875700	-1.75212300	2.09429400
H	-4.16816000	-4.90101100	-0.18636300
H	-6.03155100	-4.10703200	1.25399700
C	-1.02195700	1.27518100	0.86662600
C	-2.09569300	0.72671700	0.17349900
C	-0.97012500	2.61667800	1.30048500
C	-3.15732300	1.62314200	-0.22129500
C	-2.02037800	3.45862300	0.99916900
C	-4.23010900	1.21862500	-1.07019600
C	-3.12155100	2.99846600	0.22088700
H	-2.00309200	4.49559200	1.33352900
C	-5.23123600	2.10442600	-1.42767500
H	-4.25643800	0.20038800	-1.44895100
C	-4.17857100	3.87908500	-0.15503800
C	-5.21637900	3.44305000	-0.95736400
H	-6.03613900	1.77189500	-2.08271000
H	-4.14447400	4.91180100	0.19293200
H	-6.01540700	4.12673900	-1.24249600
H	-0.11993400	-2.96636200	-1.86341700
H	-0.10103000	2.95785700	1.85920500

4HPA-SOAc

Pd	2.43409700	1.11870800	-0.14962100
H	3.73907500	-2.16598700	-2.99776200
O	3.92661300	2.45553200	0.46746900
O	4.99224100	-3.08638200	0.55200200
C	3.83979900	-1.09204400	1.52768300
C	4.03850900	-2.61565600	1.56470800
C	5.07255500	-2.48053500	-0.66142500
C	4.12269300	-1.29903900	-1.03993700
N	3.26373800	-0.81231800	0.13577300
H	2.39630900	-1.38345900	0.11160300
C	5.15876100	-0.34518700	1.79061200
C	2.78358300	-0.72401400	2.58897200
H	3.08771500	-3.14352600	1.41060700
H	4.47145800	-2.92736000	2.52063800
O	5.88807700	-2.89759900	-1.46455500
C	4.97639400	-0.15081500	-1.62420800
C	3.16045100	-1.84866800	-2.12421500
H	5.02720000	0.73361500	1.67046300
H	5.97352100	-0.67234900	1.13558800
H	5.47045200	-0.54352800	2.82396100
H	2.61805400	0.36018500	2.60844100
H	3.14211800	-1.03129100	3.57970400
H	1.82554400	-1.22037300	2.39592600
H	5.61353900	-0.54490600	-2.42246900
H	5.61189700	0.32145200	-0.86955100
H	4.31454300	0.61292700	-2.05033000
H	2.45907700	-1.06415200	-2.43007800
H	2.58493200	-2.70543500	-1.75198600
C	3.17144000	3.47092000	0.18317600
O	1.99522800	3.20681700	-0.26610800
C	3.67257600	4.87058600	0.34668400
H	4.25073000	4.96027200	1.27471500
H	2.83880500	5.58104600	0.34725700
H	4.34115900	5.10784800	-0.49396700
P	-0.10956700	-0.81189100	-0.25311100
O	0.62209600	-2.04029600	0.26233300
O	0.71705300	0.30711800	-0.97861500
O	-0.96960500	-0.15347700	1.02759800
O	-1.30848700	-1.11900300	-1.37412800
C	-2.52082500	-1.67732000	-0.91431900
C	-3.41688800	-0.89732100	-0.18505200
C	-2.78171100	-3.01921900	-1.27442700
C	-4.61053200	-1.53756000	0.31449600
C	-3.95829800	-3.61467100	-0.87075000

C	-5.52036600	-0.88656200	1.20094400
C	-4.88949300	-2.90591400	-0.05784300
H	-4.17511200	-4.64558300	-1.15051100
C	-6.65811300	-1.52817800	1.65800500
H	-5.31120500	0.12891200	1.52712500
C	-6.07894800	-3.53071800	0.42105900
C	-6.95076900	-2.85749100	1.25660800
H	-7.33321300	-1.00943800	2.33837900
H	-6.28200500	-4.56015400	0.12394400
H	-7.85345900	-3.34783500	1.62001500
C	-1.89461100	0.86511200	0.71311100
C	-3.09912000	0.53571200	0.09509400
C	-1.54613700	2.18644600	1.07241400
C	-3.97327100	1.61762800	-0.29057200
C	-2.41137400	3.21931000	0.77958300
C	-5.15546500	1.41546200	-1.06411000
C	-3.62814500	2.97156900	0.08008100
H	-2.15661000	4.24276800	1.05466100
C	-5.97009500	2.47681200	-1.41793600
H	-5.41594600	0.41047000	-1.38598100
C	-4.49817600	4.03909100	-0.29125700
C	-5.64907800	3.80034700	-1.01934600
H	-6.86427000	2.29480500	-2.01384900
H	-4.23013100	5.05492800	0.00107800
H	-6.30247700	4.62568300	-1.30106900
H	-0.58992100	2.35944900	1.56172100
H	-2.04070600	-3.55512400	-1.86444800

4HPA-SOAc-TS

Pd	-2.53359200	0.90203900	0.29357000
H	-5.15754800	1.18880900	0.56279700
O	-3.21302600	2.04723700	2.95318500
O	-6.23340300	-0.83080800	-1.23177900
C	-3.86664100	-0.86632100	-2.00546600
C	-5.22239200	-0.15948300	-2.06201500
C	-5.87192900	-1.27659500	0.00285300
C	-4.45209500	-0.93621900	0.52135500
N	-3.38343500	-0.79151500	-0.56219600
H	-2.63301900	-1.49448700	-0.44794100
C	-3.98048200	-2.36140200	-2.38765000
C	-2.89013600	-0.14883000	-2.95228500
H	-5.13724100	0.88793200	-1.74306100
H	-5.62964800	-0.18963800	-3.07613400
O	-6.69744300	-1.84701800	0.69294000
C	-3.98840800	-1.98822600	1.53986500

C	-4.53848100	0.49701500	1.14399400
H	-4.63317100	-2.92286000	-1.70840100
H	-4.38887500	-2.45428700	-3.40192700
H	-2.98633800	-2.82512300	-2.36931200
H	-1.89938000	-0.60998000	-2.90358500
H	-3.25908600	-0.23656900	-3.98252400
H	-2.78955100	0.91315400	-2.70226900
H	-4.70113200	-2.05173300	2.36736100
H	-3.91524700	-2.97496600	1.06647000
H	-3.00569300	-1.71114400	1.94185000
H	-5.00061300	0.40324800	2.13786600
H	-3.61027200	1.18644500	1.91193400
C	-2.26450300	2.75423900	2.47039900
O	-1.75850300	2.54895400	1.30564100
C	-1.69392300	3.88516300	3.29775000
H	-1.25005800	3.46684100	4.21138200
H	-0.93214700	4.43927900	2.74207600
H	-2.50475600	4.56009100	3.60071500
P	0.06804900	-0.50005100	-0.61457400
O	-0.66132100	-1.83159300	-0.68694700
O	-0.72587800	0.83876000	-0.77977200
O	1.28551100	-0.49404100	-1.76517800
O	0.94268000	-0.30211900	0.81077100
C	2.07300900	-1.12161100	0.98617300
C	3.23834700	-0.85210800	0.26899300
C	1.97685300	-2.17175800	1.92854000
C	4.34706500	-1.76401400	0.41815900
C	3.05913700	-3.00039400	2.13813000
C	5.52678900	-1.68097800	-0.38097900
C	4.25688900	-2.83580900	1.38371800
H	2.99896400	-3.80693200	2.86899600
C	6.57125500	-2.57318100	-0.21238900
H	5.60097800	-0.90773800	-1.14135700
C	5.35783500	-3.72916200	1.53892900
C	6.49549400	-3.60042100	0.76377500
H	7.45823800	-2.49027700	-0.84027100
H	5.28003400	-4.52759900	2.27774800
H	7.32747200	-4.29290700	0.88923800
C	2.31420000	0.46182000	-1.64575000
C	3.28202400	0.32403400	-0.65164300
C	2.32733400	1.51126700	-2.59312100
C	4.26787200	1.37150300	-0.52509200
C	3.31336200	2.47289200	-2.53023200
C	5.20613700	1.42120900	0.54932700

C	4.28941700	2.44517700	-1.49230300
H	3.33849100	3.28211300	-3.26022000
C	6.13515100	2.44276900	0.64343000
H	5.18523000	0.64639700	1.31135500
C	5.27053200	3.47345100	-1.37255000
C	6.17966400	3.47347700	-0.33081700
H	6.83639000	2.45852600	1.47765300
H	5.28165200	4.27158900	-2.11560300
H	6.92111000	4.26774600	-0.24759300
H	1.04003400	-2.30585000	2.46599900
H	1.54855700	1.53749400	-3.35292800

4HPA-SPA

Pd	-2.25768000	-0.81387700	-0.28631600
O	-5.38887400	-1.67168300	-1.17336400
O	-3.30661800	-2.49608600	-0.74648300
H	-5.25704000	-0.60918700	3.04902800
O	-5.89707100	2.41144600	0.64584200
C	-4.07559900	1.61607600	-0.87510700
C	-5.54252600	2.05299100	-0.73353000
C	-5.34938100	1.75336800	1.70140300
C	-4.32788500	0.58932800	1.48876300
N	-3.95826400	0.38248300	0.01964600
H	-4.65310400	-0.29232800	-0.37783900
C	-3.11005200	2.74754500	-0.48202200
C	-3.84344400	1.19047600	-2.33924200
H	-6.22746100	1.26084000	-1.06528900
H	-5.73620400	2.96022000	-1.31482000
O	-5.68626400	2.08088300	2.82545300
C	-3.08182700	0.87180100	2.35914200
C	-5.03064700	-0.70266500	1.98208900
H	-2.07645900	2.39019000	-0.47921000
H	-3.33289100	3.17726800	0.50084300
H	-3.19972600	3.55443800	-1.22081600
H	-2.78992000	0.92988100	-2.49911300
H	-4.09267100	2.02590100	-3.00630100
H	-4.46174600	0.32732100	-2.61312000
H	-3.40027400	1.09304000	3.38303600
H	-2.49180900	1.71073500	1.98293800
H	-2.44019100	-0.01689200	2.37535000
H	-4.36400900	-1.56204000	1.83971400
H	-5.96413400	-0.88913000	1.43743800
C	-4.56338200	-2.60911200	-1.09982400
C	-4.98545600	-4.04376600	-1.39593500
H	-4.13479000	-4.66958800	-1.68538700

H	-5.74746800	-4.04613700	-2.18386200
H	-5.43442000	-4.46507500	-0.48439900
P	0.39802400	-0.46093300	-0.15571800
O	-0.68788300	0.62034900	0.14900100
O	-0.29727100	-1.79705000	-0.54261100
O	1.38632100	-0.54051600	1.16704600
O	1.43372200	-0.05504100	-1.37901000
C	2.38218300	0.97548600	-1.13044100
C	3.47017900	0.72906400	-0.29856900
C	2.16951500	2.20238000	-1.79555300
C	4.35534400	1.83466300	-0.01557800
C	3.05902400	3.23765700	-1.59758600
C	5.40857400	1.75230600	0.94350600
C	4.15337300	3.09348900	-0.69657600
H	2.91662700	4.18788400	-2.11188400
C	6.24058200	2.83118500	1.18586500
H	5.55427200	0.82911100	1.49831200
C	5.04029500	4.17885100	-0.43275500
C	6.06714000	4.05214900	0.48405400
H	7.03341800	2.74410900	1.92841900
H	4.88386800	5.11949200	-0.96166800
H	6.73470400	4.89045300	0.68108400
C	2.63101200	-1.21616300	1.02651500
C	3.65991700	-0.62678900	0.29810900
C	2.75371700	-2.45730200	1.68760900
C	4.86965100	-1.39413700	0.11492400
C	3.93769000	-3.15776400	1.58839700
C	5.92729200	-0.97045800	-0.74394700
C	5.01025900	-2.66387100	0.79078400
H	4.05258200	-4.11302100	2.10023800
C	7.07329300	-1.73111000	-0.89553000
H	5.82639000	-0.03901700	-1.29486200
C	6.21168600	-3.41393100	0.62200500
C	7.22648800	-2.95736200	-0.19821300
H	7.86369900	-1.38797900	-1.56266500
H	6.30925000	-4.36573800	1.14496300
H	8.13743700	-3.54196300	-0.32339700
H	1.30488400	2.30371300	-2.44840500
H	1.90736800	-2.83627400	2.25690100
4HPA-SPA-TS			
Pd	2.53258500	0.58833800	-0.00270200
O	4.91854500	2.62766100	-0.70966200
O	2.77589200	2.15553700	-1.34045100
H	2.57185600	-1.93353000	1.71107700

O	5.04881900	-2.86318300	0.51828600
C	5.06340300	-0.91365400	-1.02419200
C	4.56051100	-2.33562700	-0.76426900
C	5.02687600	-2.04191000	1.60402200
C	4.35447100	-0.65439600	1.45939900
N	4.47818200	-0.03491600	0.07060100
H	4.97116300	0.87899400	0.07480000
C	6.60482900	-0.81672400	-0.93393100
C	4.58136200	-0.45721700	-2.41227200
H	3.46286400	-2.37239700	-0.77066500
H	4.94574700	-3.02882800	-1.51685800
O	5.45341400	-2.45301900	2.66751200
C	4.92593500	0.32173700	2.49625800
C	2.79749000	-0.85985600	1.62954600
H	6.92765600	0.20504500	-1.17001500
H	6.98728400	-1.07492100	0.06080300
H	7.06140200	-1.50129000	-1.65972300
H	4.86147300	0.58530000	-2.59401600
H	5.05663400	-1.07860000	-3.18211500
H	3.49292600	-0.54665100	-2.50904700
H	4.77203100	-0.07158100	3.50569300
H	6.00230200	0.46639400	2.33835600
H	4.41893200	1.29116800	2.41424400
H	2.42816200	-0.36638800	2.53382400
H	1.61101600	-0.99798000	0.75721200
C	3.88926400	2.84220300	-1.39191900
C	3.87264200	3.95907400	-2.43381600
H	4.57458100	4.75049200	-2.14803700
H	4.19898700	3.53880600	-3.39688300
H	2.86685000	4.37313500	-2.56723600
P	-0.43874300	-0.11532700	0.27344100
O	0.36450700	-1.42128700	0.56667500
O	0.43929900	1.14873800	0.11710200
O	-1.55947400	0.01598000	1.48744300
O	-1.37482700	-0.23827900	-1.08952500
C	-2.49157400	-1.11504600	-1.04635000
C	-3.61865100	-0.76466100	-0.30774300
C	-2.39852200	-2.29981900	-1.80911000
C	-4.69042800	-1.72931200	-0.22937000
C	-3.45596200	-3.18541900	-1.81171300
C	-5.81698500	-1.56013500	0.62991300
C	-4.61259600	-2.93853700	-1.01683700
H	-3.40458700	-4.09873500	-2.40413100
C	-6.82927300	-2.50251700	0.67600300

H	-5.87662800	-0.67917400	1.26386900
C	-5.68253400	-3.87973200	-0.95645800
C	-6.77274500	-3.66653400	-0.13354500
H	-7.67559200	-2.35180000	1.34574700
H	-5.61656000	-4.78321500	-1.56337000
H	-7.58070200	-4.39649800	-0.09175200
C	-2.65329100	0.89868100	1.28728900
C	-3.66870200	0.54871500	0.40161100
C	-2.66148800	2.08417400	2.05397100
C	-4.72142900	1.51271200	0.18054700
C	-3.70720300	2.97175900	1.91079800
C	-5.72960500	1.33899600	-0.81431500
C	-4.74588200	2.72527300	0.96691200
H	-3.73315100	3.88687400	2.50200800
C	-6.72550100	2.28243600	-0.99635200
H	-5.70941900	0.45432800	-1.44522000
C	-5.79582500	3.66862400	0.76147700
C	-6.77045200	3.45236900	-0.19475800
H	-7.47955900	2.12851400	-1.76785400
H	-5.80723700	4.57522400	1.36734300
H	-7.56416300	4.18346600	-0.34542000
H	-1.48992300	-2.48878000	-2.37742300
H	-1.83758900	2.27224000	2.73943300

4HPA-ROAc

Pd	2.43434900	0.91689300	-0.37063800
H	3.49503200	-0.56595900	3.36084100
O	4.04876100	2.12149100	0.19640100
O	6.00704000	-1.05495600	0.33233200
C	4.09465300	-1.49494200	-1.20491900
C	5.40342300	-0.74245200	-0.97224000
C	5.24528200	-1.34915800	1.41952000
C	3.69461700	-1.34693400	1.35123000
N	3.15638700	-1.06445400	-0.07092000
H	2.28573600	-1.62563400	-0.15367400
C	4.32109600	-3.02684500	-1.21336600
C	3.49018900	-1.07637000	-2.56061400
H	5.25980700	0.34264500	-1.02127100
H	6.15761300	-1.03983000	-1.70741300
O	5.81283900	-1.60993500	2.46668400
C	3.15173500	-2.71647700	1.84653300
C	3.20503700	-0.26396700	2.34834900
H	3.36316800	-3.55824200	-1.26385100
H	4.87673300	-3.38568200	-0.34175500
H	4.90511200	-3.28912000	-2.10435000

H	2.50097400	-1.52931100	-2.69633200
H	4.14186000	-1.42548400	-3.37140200
H	3.38475700	0.01232100	-2.64720800
H	3.52577400	-2.90187600	2.85854600
H	3.45392200	-3.55140600	1.21030900
H	2.05671500	-2.67823300	1.87208300
H	2.11148300	-0.19286100	2.31031100
H	3.64466400	0.71742500	2.14761200
C	3.37574000	3.20049200	-0.06923500
O	2.17661800	3.03963100	-0.50374700
C	3.99126900	4.55299100	0.09961300
H	4.76260400	4.52907300	0.87798700
H	3.22213500	5.29409700	0.34542500
H	4.46423100	4.84722200	-0.84928500
P	-0.20195800	-0.89661300	-0.47798100
O	0.48425100	-2.20097200	-0.10890000
O	0.64467400	0.23659100	-1.15479600
O	-0.95369200	-0.30862200	0.90269000
O	-1.47617700	-1.04200300	-1.54860100
C	-2.69318500	-1.57053100	-1.06778600
C	-3.50116200	-0.81052600	-0.22334100
C	-3.05384600	-2.85824100	-1.52642800
C	-4.70197100	-1.42696400	0.28907900
C	-4.24127300	-3.42133800	-1.10846200
C	-5.52077700	-0.80986200	1.28209700
C	-5.08331700	-2.73824000	-0.18395300
H	-4.53482800	-4.40893200	-1.46423800
C	-6.66925100	-1.42567500	1.74762500
H	-5.23161700	0.15757500	1.68440500
C	-6.28158800	-3.33625300	0.30707500
C	-7.06443100	-2.69393100	1.24841800
H	-7.27291800	-0.93444900	2.51053600
H	-6.56309500	-4.32140300	-0.06661800
H	-7.97479600	-3.16360100	1.62000200
C	-1.83378400	0.78091000	0.73367300
C	-3.08639600	0.57295000	0.15987000
C	-1.39446900	2.04307900	1.19294900
C	-3.91825100	1.72901500	-0.07395700
C	-2.21498100	3.14142300	1.04605800
C	-5.15047800	1.66069500	-0.79082900
C	-3.47886600	3.02270600	0.39807000
H	-1.89046200	4.11978000	1.40022600
C	-5.92299800	2.79029900	-0.99662700
H	-5.48285600	0.70511600	-1.18840800

C	-4.30771900	4.16275600	0.17978700
C	-5.50788700	4.05230800	-0.49781100
H	-6.85688400	2.71070600	-1.55277800
H	-3.96795600	5.13126400	0.54843100
H	-6.12870300	4.93240300	-0.66341100
H	-0.40760700	2.11954700	1.64484300
H	-2.37894200	-3.37916200	-2.20287900

4HPA-ROAc-TS

Pd	2.49574800	0.81766700	-0.25991500
H	5.09450400	1.29703900	-0.17259900
O	3.03914600	3.25478500	1.35119800
O	6.26154400	-1.32759300	-0.52963200
C	3.91629700	-1.89261600	-1.15025000
C	5.24794800	-1.28465700	-1.59474000
C	5.88329200	-1.03525200	0.74529500
C	4.44500000	-0.51061700	0.98102600
N	3.39708200	-1.03661500	-0.00146700
H	2.66085500	-1.57622500	0.48491100
C	4.08977600	-3.33620400	-0.62146600
C	2.93978800	-1.87532900	-2.33809300
H	5.11881600	-0.24573200	-1.92563600
H	5.68032900	-1.86497500	-2.41421700
O	6.70579200	-1.10739600	1.64046000
C	3.98516700	-0.82115900	2.41241200
C	4.47853600	1.02702300	0.69202600
H	3.11082000	-3.75364000	-0.35478400
H	4.73575700	-3.38705800	0.26335900
H	4.53541900	-3.96561500	-1.40210800
H	2.80163500	-0.86427600	-2.73687500
H	1.96220100	-2.26300300	-2.03669700
H	3.33415300	-2.51905600	-3.13503900
H	4.67537100	-0.37678100	3.13568400
H	3.95433500	-1.90461800	2.58089900
H	2.98363900	-0.40578000	2.58036100
H	4.91792800	1.52272300	1.57022600
H	3.50634400	1.99146400	0.95265300
C	2.09593200	3.54276000	0.53879400
O	1.66209700	2.72212000	-0.35136300
C	1.42668400	4.89601500	0.63154200
H	0.74454200	5.05829000	-0.20752600
H	2.18797600	5.68515400	0.66192200
H	0.86185600	4.94139900	1.57325500
P	-0.05939100	-0.88116800	-0.25459700
O	0.72482600	0.13177200	-1.15720400

O	0.67437200	-2.03349500	0.41093100
O	-1.29565100	-1.34789000	-1.28547600
O	-0.89882200	-0.05865500	0.95011300
C	-1.85969000	0.88513100	0.54169200
C	-3.07661400	0.45387500	0.01547100
C	-1.54289600	2.24982600	0.72888100
C	-3.99479800	1.45971000	-0.46428000
C	-2.44859300	3.21777500	0.35199100
C	-5.19322900	1.13677500	-1.16902400
C	-3.68054500	2.85694400	-0.26757300
H	-2.21650100	4.27275400	0.49809200
C	-6.05254000	2.12631300	-1.61382500
H	-5.43007100	0.09431700	-1.36610100
C	-4.59673400	3.84920100	-0.72621400
C	-5.76238800	3.49567400	-1.38063200
H	-6.95761300	1.85151300	-2.15523800
H	-4.35212700	4.89932200	-0.56221400
H	-6.45112900	4.26389200	-1.73125400
C	-2.47680500	-1.86147200	-0.71777300
C	-3.36891300	-1.00960500	-0.06678300
C	-2.71995200	-3.24404300	-0.89025900
C	-4.53278700	-1.60162500	0.55016800
C	-3.87064400	-3.80337300	-0.37619200
C	-5.42924500	-0.85907800	1.37639500
C	-4.79334600	-3.01142800	0.36668500
H	-4.07337800	-4.86553900	-0.51368000
C	-6.53970800	-1.45583500	1.94734300
H	-5.23081100	0.19264900	1.56573800
C	-5.95579800	-3.58954900	0.95737600
C	-6.81738600	-2.82985600	1.72689100
H	-7.20415500	-0.86566000	2.57826500
H	-6.14590100	-4.65188400	0.80018900
H	-7.69937200	-3.28487300	2.17696400
H	-0.57505100	2.50298000	1.15243800
H	-1.98476800	-3.83878700	-1.42919300
4HPA-RPA			
Pd	2.31014100	0.98271900	-0.14173700
O	5.43275700	2.05021700	0.26643000
O	3.46755000	2.52670400	-0.78568500
H	3.22992600	-2.36206200	-2.44732500
O	4.15403900	-3.17538000	0.77340100
C	3.95089900	-0.89209100	1.70101400
C	3.32587800	-2.28278100	1.60018800
C	4.73562500	-2.65261600	-0.34023200

C	4.22967500	-1.27270000	-0.85443800
N	3.92164500	-0.28352500	0.29186500
H	4.66859700	0.44546500	0.29282800
C	5.43048100	-0.95248800	2.15946200
C	3.14493500	-0.04117200	2.70140700
H	2.31206000	-2.23332300	1.18523600
H	3.28886000	-2.76567100	2.58089000
O	5.54425900	-3.32168100	-0.95728900
C	5.28715200	-0.61927800	-1.76030300
C	2.96088000	-1.62166500	-1.68340800
H	5.81450400	0.06382100	2.30863500
H	6.08458100	-1.45603000	1.43823600
H	5.49991300	-1.49662200	3.10994400
H	3.48485500	1.00117000	2.68091700
H	3.31246500	-0.43071100	3.71445300
H	2.06983400	-0.07057400	2.49541500
H	5.49768500	-1.26362700	-2.61907600
H	6.22408500	-0.44548300	-1.21836100
H	4.90970400	0.34155700	-2.13125700
H	2.59157400	-0.72111800	-2.18987400
H	2.15228800	-2.02870700	-1.06877800
C	4.71219100	2.77510500	-0.45365600
C	5.26388500	4.05805700	-1.06524900
H	5.85986600	4.59019700	-0.31383800
H	4.47116800	4.70858500	-1.44826900
H	5.93265200	3.78491800	-1.89428500
P	-0.35122700	0.66479800	-0.07080500
O	0.72112200	-0.37794100	0.38774500
O	0.35016700	1.97852100	-0.51224200
O	-1.42370800	0.81934200	1.17611800
O	-1.29567700	0.13742100	-1.32272500
C	-2.18248500	-0.94112200	-1.04620600
C	-3.32605800	-0.71551100	-0.28624600
C	-1.84673600	-2.19592900	-1.59918600
C	-4.13684600	-1.86182500	0.05168000
C	-2.66437200	-3.27925500	-1.35325200
C	-5.23392800	-1.78738100	0.96074700
C	-3.80705700	-3.15130800	-0.51130900
H	-2.42580900	-4.25348700	-1.77948700
C	-5.98647000	-2.90788700	1.26607900
H	-5.47603900	-0.83659500	1.42854500
C	-4.61432000	-4.28123000	-0.18577500
C	-5.68586100	-4.16461800	0.67982300
H	-6.81455000	-2.82552600	1.96968200

H	-4.36015000	-5.24644800	-0.62479700
H	-6.29148900	-5.03651100	0.92530400
C	-2.70084800	1.38667100	0.91206100
C	-3.64475500	0.66399200	0.18835300
C	-2.94719000	2.66393700	1.46016500
C	-4.89893400	1.31647100	-0.10706500
C	-4.17380000	3.25948700	1.25296300
C	-5.87998500	0.74479100	-0.97117200
C	-5.16821900	2.61904500	0.45846900
H	-4.38355200	4.24075900	1.67799400
C	-7.07384800	1.39610500	-1.22725300
H	-5.68275000	-0.21455600	-1.44252700
C	-6.41606600	3.25340200	0.18485000
C	-7.35425700	2.65467300	-0.63508100
H	-7.80358500	0.94055300	-1.89615900
H	-6.61094400	4.23108500	0.62650300
H	-8.30137200	3.15253700	-0.84086800
H	-2.16003500	3.15184200	2.03161000
H	-0.94540700	-2.28069100	-2.20297900

4HPA-RPA -TS

Pd	2.50939100	0.41011300	-0.41580400
O	4.85278900	2.57773200	-0.81002000
O	2.65636700	2.46747000	-0.19619900
H	2.66353400	-2.62993500	-0.33535600
O	5.01209300	-2.63382600	1.33048700
C	4.90883500	-0.15591100	1.49423800
C	4.41117000	-1.49573200	2.04211600
C	5.10218400	-2.57004700	-0.02677000
C	4.43078800	-1.37445200	-0.74666500
N	4.44136900	-0.07241000	0.05002600
H	4.95230600	0.69260100	-0.43087900
C	6.45335200	-0.06869400	1.49334700
C	4.31026700	0.98681400	2.33319500
H	3.31747500	-1.56955000	1.97421600
H	4.71430500	-1.62551300	3.08444400
O	5.62274100	-3.49011000	-0.63060300
C	5.09530100	-1.13286700	-2.10829200
C	2.89190800	-1.70428800	-0.88422700
H	6.77063100	0.92199800	1.14439300
H	6.91794900	-0.82258800	0.84688800
H	6.83326300	-0.21568900	2.51227000
H	4.58552200	1.95834000	1.91000600
H	4.70823600	0.93273400	3.35462900
H	3.21657200	0.92364000	2.37685700

H	5.02461400	-2.03462400	-2.72386000
H	6.15528800	-0.87882200	-1.98115000
H	4.58996400	-0.31048000	-2.62974000
H	2.60898900	-1.85041800	-1.93137300
H	1.63234800	-1.35878000	-0.19960000
C	3.77111500	3.10292100	-0.45740000
C	3.67797500	4.61334200	-0.24767800
H	4.38864500	5.12799300	-0.90417100
H	3.95023900	4.83505300	0.79516000
H	2.66204000	4.98511100	-0.42149900
P	-0.42390700	-0.37819100	-0.36026100
O	0.37005300	-1.63085500	0.12717900
O	0.45060200	0.71471700	-1.02035300
O	-1.27741800	0.14265100	0.96379500
O	-1.61022000	-0.73995100	-1.45667500
C	-2.74645700	-1.45584700	-0.99486300
C	-3.68783300	-0.82068700	-0.18924200
C	-2.87021500	-2.79251800	-1.43275700
C	-4.78088400	-1.62042400	0.31327000
C	-3.95698800	-3.53777500	-1.02619900
C	-5.71521600	-1.13035000	1.27409500
C	-4.92344600	-2.98671000	-0.13587400
H	-4.07191100	-4.56745700	-1.36410600
C	-6.75435700	-1.92225500	1.73031600
H	-5.60399400	-0.11996600	1.65887300
C	-6.01520700	-3.76874300	0.34476100
C	-6.91769100	-3.24875500	1.25369700
H	-7.45103000	-1.52494900	2.46813300
H	-6.11698000	-4.79451900	-0.01084700
H	-7.74493700	-3.85799900	1.61671900
C	-2.33452900	1.06322100	0.73998700
C	-3.52153500	0.62215100	0.16116300
C	-2.12245700	2.39132900	1.16949700
C	-4.53780000	1.61172300	-0.11120000
C	-3.12218600	3.32435000	0.99075000
C	-5.72558300	1.31597800	-0.84459700
C	-4.33780800	2.97125700	0.33649100
H	-2.97880600	4.35158900	1.32519400
C	-6.68115200	2.28851800	-1.08145600
H	-5.87841300	0.31115100	-1.22947800
C	-5.35153200	3.94353500	0.08836400
C	-6.50315600	3.61156900	-0.60054600
H	-7.57649300	2.03733900	-1.64963500
H	-5.19243500	4.96298400	0.44133200

H	-7.26775700	4.36475400	-0.78850200
H	-1.16943900	2.64966800	1.62683100
H	-2.09989100	-3.20566300	-2.08103300
3PhPA			
Pd	-3.51587400	0.04250400	-0.00792300
C	-5.98063600	0.04076600	-0.00791100
O	-5.28825200	-0.48691200	-0.96384400
O	-5.29070300	0.57735200	0.94523100
C	-7.47153400	0.01252500	0.01009100
H	-7.86181100	0.99312600	0.31046500
H	-7.86218600	-0.26619000	-0.97462500
H	-7.80440800	-0.72721100	0.75282800
P	-0.85483900	0.02468800	-0.00422000
O	-1.78731300	0.63562800	1.09523800
O	-1.79326600	-0.56188000	-1.11185100
O	0.12942500	-1.04493600	0.75836900
O	0.16467600	1.06626300	-0.75835100
C	1.30190500	1.55822700	-0.05489800
C	2.33704700	0.67859000	0.24239300
C	1.34214000	2.95876500	0.21073900
C	3.43629100	1.17428400	1.03567700
C	2.45937300	3.44194600	0.87775100
C	4.45650300	0.32891600	1.56300600
C	3.49574400	2.58378200	1.33468400
H	2.52846200	4.50835500	1.09088500
C	5.49549200	0.84996500	2.31420900
H	4.41228600	-0.74146500	1.37967200
C	4.58922500	3.08894400	2.09970800
C	5.57281600	2.24270700	2.57597400
H	6.25877700	0.18297200	2.71407400
H	4.62610600	4.15761900	2.31276400
H	6.40030500	2.63857700	3.16397400
C	1.24836200	-1.57800900	0.05550100
C	2.31171500	-0.73475300	-0.24749100
C	1.24136800	-2.98020000	-0.20386200
C	3.39118700	-1.27020700	-1.04181800
C	2.34115300	-3.50397800	-0.86903800
C	4.43638700	-0.46098700	-1.57680300
C	3.40395600	-2.68251700	-1.33313800
H	2.37489500	-4.57331100	-1.07601100
C	5.45551600	-1.01936000	-2.32841300
H	4.42703200	0.61124600	-1.39897600
C	4.47832100	-3.22691700	-2.09828300
C	5.48702500	-2.41533600	-2.58239700

H	6.23864400	-0.37965200	-2.73448200
H	4.48047500	-4.29735500	-2.30540800
H	6.29945300	-2.84103600	-3.17056100
C	0.14371800	-3.87665800	0.27272600
C	0.45570200	-4.94810800	1.13452400
C	-1.19413500	-3.70085700	-0.13208200
C	-0.54617000	-5.81647300	1.58706800
H	1.48572700	-5.08938900	1.46105600
C	-2.19392500	-4.56971100	0.32137400
H	-1.45391500	-2.89360200	-0.81184300
C	-1.87549800	-5.62834300	1.18419300
H	-0.28786600	-6.63522000	2.25861500
H	-3.22323200	-4.41850000	-0.00381600
H	-2.65626200	-6.30072700	1.53920200
C	0.27597700	3.89490800	-0.26030200
C	0.62753400	4.96772300	-1.10529300
C	-1.06950600	3.75676200	0.13397400
C	-0.34288800	5.87426700	-1.55117800
H	1.66337700	5.07986100	-1.42457900
C	-2.03777200	4.66402500	-0.31262100
H	-1.35990700	2.94922800	0.80092900
C	-1.67998900	5.72392800	-1.15826300
H	-0.05428600	6.69325700	-2.20999300
H	-3.07341000	4.54195800	0.00464900
H	-2.43640000	6.42612000	-1.50821900
4PhPA-SOAc			
Pd	-2.67515900	-0.66919500	-0.78616000
H	-2.90659400	3.76298200	-1.68168900
O	-4.49939800	-1.65847000	-1.06282300
O	-4.45008600	3.16453600	1.83010400
C	-3.85625100	0.73708800	1.72564900
C	-3.76298400	2.05614400	2.50663900
C	-4.46770500	3.25006800	0.47409500
C	-3.72927000	2.19690300	-0.41342600
N	-3.15613700	1.02520100	0.39584500
H	-2.20279900	1.32465000	0.68214600
C	-5.31558800	0.28353200	1.54918800
C	-3.04552300	-0.33211900	2.48179200
H	-2.71633900	2.34895900	2.66497200
H	-4.26283600	1.97051800	3.47688600
O	-5.05459500	4.18636400	-0.03938100
C	-4.70475100	1.70823800	-1.50726500
C	-2.53359200	2.93997100	-1.06391500
H	-5.37176200	-0.60094500	0.90829600

H	-5.96000200	1.06273900	1.12735400
H	-5.72064400	0.02325200	2.53533900
H	-3.09778200	-1.29122200	1.95630800
H	-3.46442100	-0.47175400	3.48643600
H	-1.99149300	-0.04953900	2.58168500
H	-5.12688500	2.57507400	-2.02580900
H	-5.52372000	1.10954200	-1.09849600
H	-4.15797300	1.09662200	-2.23462500
H	-1.96843500	2.25020300	-1.70166600
H	-1.85375300	3.34533500	-0.30636000
C	-3.93331900	-2.55681200	-1.80874800
O	-2.67447100	-2.41870600	-2.02354400
C	-4.72810200	-3.67923500	-2.39770300
H	-5.46645900	-4.04243400	-1.67247900
H	-4.06603600	-4.49487400	-2.70789700
H	-5.27040700	-3.30794100	-3.27973700
P	0.20561900	0.52607500	0.20697100
O	-0.42469300	1.54032300	1.14952500
O	-0.67883700	-0.12858800	-0.90424700
O	0.93506400	-0.63494800	1.16715100
O	1.48205800	1.09769400	-0.70752300
C	2.74973700	1.27089700	-0.12347000
C	3.48146700	0.14905400	0.26469600
C	3.27167500	2.60113400	-0.06831800
C	4.74753000	0.35075800	0.92317500
C	4.53790400	2.77185400	0.47424400
C	5.48798700	-0.71194600	1.52129800
C	5.28325100	1.68677900	1.00893500
H	4.96201900	3.77452900	0.52550400
C	6.70302700	-0.47517900	2.14039900
H	5.08557600	-1.72162300	1.49676900
C	6.54540900	1.89322900	1.64218500
C	7.24522700	0.83575900	2.19317200
H	7.24601900	-1.30215500	2.59750000
H	6.94320800	2.90726400	1.69367000
H	8.20532100	1.00605600	2.67972800
C	1.71347800	-1.60456900	0.50437100
C	2.95508400	-1.22808900	0.00206900
C	1.17274500	-2.91984400	0.38085100
C	3.68373400	-2.17954200	-0.80002200
C	1.91159500	-3.84766500	-0.33897900
C	4.89282700	-1.85682200	-1.48489600
C	3.14635200	-3.50993400	-0.95780200
H	1.53546200	-4.86569400	-0.43990000

C	5.55372200	-2.80098200	-2.25158100
H	5.29663100	-0.85055500	-1.41034500
C	3.86265400	-4.46234400	-1.74283000
C	5.04370100	-4.11966200	-2.37445200
H	6.47172400	-2.52748000	-2.77128300
H	3.45185400	-5.46721500	-1.84547700
H	5.57795100	-4.85420400	-2.97651400
C	-0.12924800	-3.29327200	1.00569200
C	-0.37800300	-3.05331800	2.37351200
C	-1.12513300	-3.93036700	0.24088100
C	-1.57986100	-3.46144700	2.96085300
H	0.37709600	-2.55280300	2.97689300
C	-2.33568600	-4.32229800	0.82621400
H	-0.96631300	-4.08248100	-0.82405800
C	-2.56512500	-4.09675000	2.18941000
H	-1.75445500	-3.27078700	4.01951600
H	-3.10328000	-4.79156700	0.21076900
H	-3.50721100	-4.39996400	2.64573200
C	2.53121100	3.77205200	-0.62929300
C	3.15272400	4.57600700	-1.60761700
C	1.23783400	4.12006000	-0.19096300
C	2.49886600	5.69675400	-2.13568700
H	4.14686900	4.30945000	-1.96562000
C	0.58754000	5.24241700	-0.71820600
H	0.74323100	3.51651100	0.56602600
C	1.21266100	6.03422900	-1.69251800
H	2.99253400	6.30114700	-2.89679000
H	-0.41060700	5.50107400	-0.36524100
H	0.70153600	6.90470900	-2.10352000

4PhPA-SOAc-TS

Pd	-2.53089800	-0.18279700	0.93608800
H	-5.13698000	-0.42912400	1.32742000
O	-3.14707300	-2.74050000	2.33305500
O	-6.27477900	1.16143900	-0.84778100
C	-3.90674300	1.90718600	-1.06078300
C	-5.23672200	2.06060100	-0.32018000
C	-5.93414200	-0.12193900	-1.14776400
C	-4.50195100	-0.60522700	-0.81000900
N	-3.42899600	0.48496600	-0.81516900
H	-2.69438200	0.25817400	-1.50666600
C	-4.07226400	2.09361900	-2.58801800
C	-2.90202800	2.92979900	-0.50510200
H	-5.11407500	1.86951100	0.75449400
H	-5.64295900	3.06617800	-0.45857200

O	-6.78364600	-0.87551400	-1.58823700
C	-4.07422000	-1.72248400	-1.77296600
C	-4.53994500	-1.08074400	0.67997900
H	-4.74250300	1.34953700	-3.03491900
H	-4.48513500	3.08854700	-2.79744000
H	-3.09461100	2.01290400	-3.07988800
H	-1.91749600	2.80021000	-0.96269800
H	-3.25317500	3.94242200	-0.73774000
H	-2.78269300	2.83875400	0.57976200
H	-4.76889000	-2.56483400	-1.70739000
H	-4.06891500	-1.35552900	-2.80665600
H	-3.06727700	-2.07006500	-1.51716400
H	-5.00589300	-2.07686200	0.70090800
H	-3.59352400	-1.76539600	1.41349000
C	-2.09539400	-2.25505000	2.86764700
O	-1.62197400	-1.09560000	2.56756800
C	-1.32175700	-3.08311600	3.86762300
H	-0.67179400	-3.76269900	3.29661000
H	-0.69460300	-2.45126800	4.50397700
H	-2.00308400	-3.68971500	4.47407100
P	0.04935200	0.30163300	-0.52402300
O	-0.68434000	-0.20092500	-1.75862700
O	-0.76081000	0.93833300	0.65316200
O	1.20296700	1.38894700	-1.05039300
O	0.99384700	-0.85631300	0.24850400
C	2.09368500	-1.37971800	-0.44242100
C	3.20831300	-0.56715200	-0.64885800
C	2.05535300	-2.76276000	-0.80487200
C	4.28076200	-1.07459400	-1.46492700
C	3.13899600	-3.26973200	-1.50859000
C	5.37701800	-0.26833900	-1.89162600
C	4.23579100	-2.45112700	-1.89497200
H	3.14189800	-4.32019000	-1.79932500
C	6.38502100	-0.79466800	-2.68098000
H	5.41339700	0.77786600	-1.59682500
C	5.29786500	-2.96344800	-2.69831600
C	6.35286500	-2.15600300	-3.08234300
H	7.20845900	-0.15709000	-3.00228300
H	5.25624800	-4.00668700	-3.01343800
H	7.15502700	-2.55792600	-3.70080000
C	2.27350700	1.71998500	-0.20351800
C	3.27613100	0.77748600	0.01022800
C	2.27206800	3.02341600	0.38118300
C	4.32430400	1.09754400	0.94917600

C	3.32081600	3.34421300	1.23063700
C	5.32111700	0.16097100	1.35617400
C	4.34640900	2.41189200	1.54571200
H	3.36074300	4.33718200	1.67810700
C	6.30813500	0.51317200	2.26062500
H	5.30089100	-0.84904200	0.95602700
C	5.38788600	2.74618600	2.46239600
C	6.35389300	1.82059600	2.81051300
H	7.05411000	-0.22346000	2.55830200
H	5.39952400	3.74706500	2.89529200
H	7.14128900	2.08598800	3.51554000
C	1.18406700	4.00509900	0.09996200
C	0.80985700	4.32746600	-1.22115700
C	0.52428700	4.65258600	1.16400400
C	-0.18277400	5.28203300	-1.46836200
H	1.30492500	3.83338900	-2.05476100
C	-0.47585400	5.60130400	0.91532700
H	0.78393600	4.39411600	2.19004800
C	-0.83023100	5.92267900	-0.40173000
H	-0.45381600	5.52354600	-2.49613800
H	-0.98107500	6.08434900	1.75174400
H	-1.60945000	6.65948800	-0.59604600
C	0.94786100	-3.65614600	-0.34542300
C	1.26787100	-4.81463500	0.39349100
C	-0.41036500	-3.37608500	-0.60315300
C	0.26036400	-5.66376300	0.87046600
H	2.31152200	-5.03589900	0.61560700
C	-1.41399700	-4.22501200	-0.12419900
H	-0.67679400	-2.49701100	-1.18430800
C	-1.08581900	-5.36807900	0.61842700
H	0.52842300	-6.54762000	1.44947800
H	-2.45840000	-3.98938400	-0.32119700
H	-1.87263900	-6.01702500	1.00203400

4PhPA-SPA

Pd	-2.24866200	-0.17562200	-0.67826300
O	-5.40879000	-0.80584000	-1.67276100
O	-3.24467700	-1.50088100	-1.85525700
H	-4.85859900	-1.95608400	2.47086400
O	-5.92620000	1.79621700	1.97545500
C	-4.24311600	2.04319600	0.13686900
C	-5.70440300	2.21042500	0.58320900
C	-5.25358500	0.74163400	2.50782200
C	-4.18899600	-0.04344000	1.67662200
N	-3.96937400	0.54651700	0.28259400

H	-4.66669800	0.09175400	-0.35205900
C	-3.29479700	2.92268700	0.97054200
C	-4.15104200	2.41785600	-1.35673600
H	-6.38386100	1.62929200	-0.05503400
H	-6.00152600	3.26372200	0.55760300
O	-5.50336100	0.41609900	3.65509700
C	-2.87740300	-0.08983700	2.49593900
C	-4.73773900	-1.48222400	1.49165400
H	-2.25161900	2.70865300	0.72346900
H	-3.43180800	2.79230900	2.04946800
H	-3.50144100	3.97542000	0.73921200
H	-3.11153700	2.35576100	-1.70181000
H	-4.49692500	3.44994800	-1.49775900
H	-4.76413300	1.75483100	-1.97889700
H	-3.09615000	-0.46884400	3.49953700
H	-2.40494500	0.89135300	2.58409600
H	-2.16819700	-0.76912800	2.01232600
H	-4.02595800	-2.07345700	0.90413000
H	-5.70542000	-1.48227700	0.97594400
C	-4.52353000	-1.56345400	-2.12922600
C	-4.88177900	-2.71392100	-3.06371200
H	-4.05017000	-2.97109300	-3.72842400
H	-5.77129000	-2.45326000	-3.64823100
H	-5.11737100	-3.59529500	-2.44915900
P	0.37688600	0.11765500	-0.35851200
O	-0.71534000	0.98806600	0.33887100
O	-0.27886500	-0.73841900	-1.47822000
O	1.11367800	-0.74579500	0.84231500
O	1.63430300	0.94682000	-1.02943800
C	2.74020200	1.37318200	-0.24869900
C	3.59669600	0.42779000	0.31561900
C	2.96135400	2.78191000	-0.18102000
C	4.68156800	0.90540300	1.13838300
C	4.07463100	3.22146200	0.52030000
C	5.50690100	0.03594800	1.91182200
C	4.93273600	2.32351000	1.21026200
H	4.27568700	4.29082000	0.58054300
C	6.54628000	0.53308900	2.67829100
H	5.31067700	-1.03305700	1.90381000
C	6.02251300	2.80084000	1.99836300
C	6.81835100	1.92570200	2.71348100
H	7.15832700	-0.15103500	3.26551500
H	6.20780700	3.87475600	2.03536000
H	7.64465000	2.30149200	3.31622700

C	2.14927500	-1.60537700	0.38961900
C	3.38045700	-1.03651800	0.08670000
C	1.83229600	-2.98699400	0.23104900
C	4.39107800	-1.88709000	-0.49331100
C	2.84236300	-3.80955000	-0.24771400
C	5.63637000	-1.39584000	-0.98444800
C	4.11417500	-3.29805800	-0.62642000
H	2.65163800	-4.87621800	-0.36433600
C	6.57665600	-2.25256600	-1.53003900
H	5.84711200	-0.33085000	-0.93546100
C	5.11482700	-4.15447200	-1.17635600
C	6.32343600	-3.64635800	-1.61422600
H	7.51864900	-1.85209900	-1.90383100
H	4.89986900	-5.22016600	-1.25964300
H	7.07648700	-4.30977200	-2.03856800
C	0.45581000	-3.49987800	0.49298600
C	-0.23776600	-3.19944600	1.68398500
C	-0.19402100	-4.27674900	-0.48732300
C	-1.54306800	-3.66164200	1.88443300
H	0.24451700	-2.59833800	2.45176700
C	-1.50030300	-4.73732100	-0.28577100
H	0.31542000	-4.48835500	-1.42638800
C	-2.18143700	-4.42861400	0.89922900
H	-2.06642700	-3.41347900	2.80718300
H	-1.99221400	-5.32036000	-1.06402100
H	-3.20363700	-4.77421400	1.05095400
C	2.06092100	3.76108800	-0.86355000
C	2.59195400	4.65091900	-1.81872600
C	0.68938900	3.84304000	-0.55096700
C	1.77041500	5.59340100	-2.45150500
H	3.64952300	4.59223100	-2.07500800
C	-0.13032000	4.78390600	-1.18468600
H	0.26211800	3.17435900	0.19157200
C	0.40580900	5.66161300	-2.13838600
H	2.19626800	6.26946100	-3.19287000
H	-1.18885700	4.83188600	-0.92977600
H	-0.23413400	6.39187100	-2.63335800

4PhPA-SPA-TS

Pd	-2.50633900	-0.19141700	-0.34891400
O	-4.79021600	-2.31656700	-1.11955200
O	-2.89184200	-1.39733400	-1.99581500
H	-2.37249000	1.68297200	2.07684400
O	-5.04004800	2.79351800	1.30874800
C	-5.26772400	1.20013800	-0.58449100

C	-4.77901600	2.57399400	-0.12169900
C	-4.81023400	1.76993100	2.17438700
C	-4.15765400	0.47005200	1.63998200
N	-4.44747300	0.16939600	0.17490400
H	-4.86312200	-0.77141700	0.02936000
C	-6.76003800	0.96773200	-0.24403400
C	-5.04656700	1.07059600	-2.10178400
H	-3.70280800	2.69192600	-0.30683900
H	-5.32243400	3.37411600	-0.63143600
O	-5.04618400	1.93177900	3.35832700
C	-4.60045300	-0.72576100	2.49284700
C	-2.59275400	0.68082500	1.68024600
H	-7.08496900	-0.00429400	-0.63575400
H	-6.95784000	0.98308300	0.83436600
H	-7.37035900	1.75124700	-0.71052800
H	-5.30128400	0.06124400	-2.44072500
H	-5.69914600	1.78347900	-2.62208200
H	-4.00642500	1.27673300	-2.37844900
H	-4.30835300	-0.57261000	3.53612700
H	-5.69009500	-0.84999000	2.44784000
H	-4.11950000	-1.63715000	2.12288700
H	-2.11966900	-0.05635500	2.33664500
H	-1.46173000	1.10794000	0.83280000
C	-3.87054200	-2.26480600	-1.96924900
C	-3.81639500	-3.26260000	-3.12587600
H	-4.62519500	-3.99547500	-3.03826900
H	-3.90890200	-2.72838100	-4.08155700
H	-2.84671900	-3.77736600	-3.13111400
P	0.50122400	0.40256300	-0.01869500
O	-0.21929900	1.54570300	0.75972900
O	-0.43230400	-0.45595300	-0.89910500
O	1.30932700	-0.49575100	1.12109500
O	1.73458700	0.92961300	-0.98310400
C	2.95542900	1.32639800	-0.37583500
C	3.78651500	0.35143300	0.17364800
C	3.25500800	2.72179700	-0.37401500
C	4.97529400	0.78196000	0.86465100
C	4.44123300	3.11426800	0.23215000
C	5.82245100	-0.11315600	1.58339900
C	5.30819500	2.18581600	0.86781100
H	4.71474300	4.16900100	0.23294800
C	6.95753100	0.34331500	2.23013900
H	5.56894400	-1.16917800	1.62738400
C	6.49498500	2.61928600	1.53196200

C	7.30707600	1.71870300	2.19524400
H	7.58678100	-0.35933100	2.77588100
H	6.74259800	3.68112700	1.51677400
H	8.20774200	2.06212600	2.70336400
C	2.16041600	-1.49311400	0.57696000
C	3.39873500	-1.09312000	0.08580700
C	1.66452000	-2.82909000	0.51117500
C	4.22665600	-2.07979800	-0.55931600
C	2.50018500	-3.78421100	-0.05090600
C	5.45607200	-1.76164300	-1.20902800
C	3.77168400	-3.44979900	-0.59205800
H	2.16364300	-4.81935200	-0.10490700
C	6.21895500	-2.74550600	-1.81355100
H	5.79528000	-0.72931500	-1.23429100
C	4.59262500	-4.44047600	-1.20993900
C	5.79379700	-4.09968800	-1.80313600
H	7.15263600	-2.47745700	-2.30741600
H	4.24568900	-5.47418800	-1.21746300
H	6.40872000	-4.86448200	-2.27677500
C	0.27558100	-3.16250400	0.94031300
C	-0.22635600	-2.78406200	2.20203200
C	-0.57942600	-3.84050400	0.04819400
C	-1.54490200	-3.08480100	2.56168500
H	0.41715000	-2.25234800	2.90017300
C	-1.90072700	-4.13101200	0.40492700
H	-0.21758300	-4.10064100	-0.94554000
C	-2.38691300	-3.75760900	1.66447000
H	-1.91833900	-2.78429700	3.54040800
H	-2.55720900	-4.62852100	-0.30784900
H	-3.41768700	-3.97879700	1.93864600
C	2.32874000	3.72813200	-0.97017000
C	1.81478400	3.57774100	-2.27508300
C	1.96631300	4.87255600	-0.23022800
C	0.96824400	4.54762400	-2.82352200
H	2.08552500	2.70335400	-2.86329100
C	1.11570900	5.84030800	-0.77902200
H	2.33647700	4.99193200	0.78744800
C	0.61347300	5.68171600	-2.07788800
H	0.58626000	4.41814500	-3.83616900
H	0.84020000	6.71374700	-0.18799400
H	-0.05018400	6.43330000	-2.50509500
4PhPA-ROAc			
Pd	-2.65245400	-0.44563200	-0.84532200
H	-4.26060700	-0.78212200	2.95836800

O	-4.56738000	-1.18494700	-1.22608100
O	-5.81683800	1.88904900	0.41456000
C	-3.52129600	2.43585900	-0.39432100
C	-4.96834600	2.11893700	-0.76609000
C	-5.32779300	1.32997100	1.55464200
C	-3.83876200	0.92221600	1.68419600
N	-3.02173500	1.23449400	0.41498600
H	-2.06254200	1.46650200	0.74661900
C	-3.42655000	3.75712700	0.40855500
C	-2.67140100	2.58008800	-1.67283600
H	-5.03657600	1.22854800	-1.40076300
H	-5.43127100	2.96626700	-1.28167700
O	-6.09610000	1.16010200	2.48647400
C	-3.20975900	1.65407800	2.90428200
C	-3.79346500	-0.59702500	1.98502600
H	-2.41285300	3.90006900	0.80087400
H	-4.13738400	3.80892500	1.23890200
H	-3.65131600	4.59122200	-0.26776000
H	-1.62026100	2.76036800	-1.41793800
H	-3.03137700	3.43858900	-2.25368300
H	-2.72487500	1.68578300	-2.30624500
H	-3.77733900	1.39725200	3.80450300
H	-3.20706600	2.74104700	2.79833700
H	-2.17482300	1.31463800	3.02909500
H	-2.75139600	-0.92926300	2.03628200
H	-4.32392700	-1.18905500	1.23416000
C	-4.09293800	-2.11796100	-1.99672800
O	-2.82071700	-2.13438900	-2.16591900
C	-4.99860900	-3.10732100	-2.65924400
H	-5.99709000	-3.08082700	-2.20987400
H	-4.57354000	-4.11567800	-2.57991400
H	-5.07886700	-2.85906400	-3.72761400
P	0.29277100	0.52875400	0.22140800
O	-0.30252800	1.57719900	1.14941000
O	-0.60868800	-0.11955600	-0.87717200
O	0.98846100	-0.64287400	1.19197300
O	1.59043900	1.05180800	-0.69541800
C	2.85476500	1.20485100	-0.09848100
C	3.55802700	0.07168100	0.31039800
C	3.40269200	2.52463800	-0.04835700
C	4.81934100	0.25391000	0.98231100
C	4.66584400	2.67484700	0.50719400
C	5.52982100	-0.81832600	1.59942700
C	5.38137700	1.57960900	1.06201400

H	5.10996100	3.66908000	0.55431500
C	6.74165100	-0.60080500	2.23162900
H	5.10647700	-1.81955400	1.57846100
C	6.63951100	1.76573500	1.70933300
C	7.30999900	0.69926000	2.27917100
H	7.26183900	-1.43430200	2.70316900
H	7.05791400	2.77163400	1.75680400
H	8.26717200	0.85445300	2.77640200
C	1.74052600	-1.63215500	0.52639200
C	3.00225800	-1.29394400	0.04780000
C	1.14652400	-2.91883200	0.36204400
C	3.71316600	-2.26492000	-0.74678800
C	1.86372300	-3.86614700	-0.35328000
C	4.94794500	-1.98136200	-1.40288700
C	3.12983900	-3.57262500	-0.93070100
H	1.44381300	-4.86306200	-0.48670000
C	5.59191600	-2.94364600	-2.16138600
H	5.38622300	-0.99103200	-1.31168600
C	3.82938000	-4.54508500	-1.70619700
C	5.03752000	-4.24203000	-2.30607900
H	6.53109600	-2.70005900	-2.65767700
H	3.38386500	-5.53286100	-1.82780200
H	5.55899100	-4.99169400	-2.90064800
C	-0.19721000	-3.23520100	0.92859000
C	-0.47135700	-3.05452900	2.30038000
C	-1.21175900	-3.74939500	0.09881200
C	-1.71804200	-3.40593900	2.82919900
H	0.29876300	-2.64609000	2.95256500
C	-2.46451700	-4.08619600	0.62749000
H	-1.03070300	-3.84905100	-0.96923200
C	-2.71994200	-3.92426900	1.99464600
H	-1.91270000	-3.26440500	3.89210900
H	-3.24427200	-4.46132300	-0.03473100
H	-3.69622700	-4.18026200	2.40539100
C	2.68913600	3.70414400	-0.62679100
C	3.32950500	4.48364400	-1.61240200
C	1.40025500	4.08181600	-0.19928400
C	2.69751500	5.60777100	-2.16005500
H	4.32092000	4.19546300	-1.96113500
C	0.77114800	5.20640700	-0.74717200
H	0.89171500	3.49883500	0.56449100
C	1.41441900	5.97296000	-1.73005700
H	3.20589800	6.19288200	-2.92651500
H	-0.22441700	5.48651100	-0.40230500

H	0.92069900	6.84581000	-2.15714900
4PhPA-ROAc-TS			
Pd	-2.67489000	-0.32617200	-0.69925500
H	-5.47399700	0.00039200	-0.69781600
O	-4.42809000	-2.66250200	-1.36374500
O	-5.75469000	2.61573900	0.31901600
C	-3.31990100	2.72877600	-0.19394300
C	-4.74832200	2.77767300	-0.74033800
C	-5.55319000	1.65453600	1.26272100
C	-4.33764400	0.70977500	1.08691100
N	-3.11911300	1.34984900	0.43807100
H	-2.32964300	1.43534800	1.09947100
C	-3.09909500	3.78241700	0.91692300
C	-2.33902300	2.95820300	-1.35649600
H	-4.90869300	2.01038200	-1.50884700
H	-4.95667100	3.75953800	-1.17389200
O	-6.37328100	1.51210600	2.15125100
C	-3.92102400	0.11351000	2.43848800
C	-4.78326000	-0.39275900	0.05528100
H	-2.06043000	3.74015000	1.26476000
H	-3.76020300	3.62389100	1.77825600
H	-3.29551100	4.78595800	0.51854200
H	-2.48440900	2.22479500	-2.15865000
H	-1.30554800	2.89547300	-1.00764900
H	-2.49816600	3.96301600	-1.76878700
H	-4.75817500	-0.43033200	2.88586300
H	-3.61320800	0.90831100	3.12930200
H	-3.08750300	-0.58467300	2.29919500
H	-5.29879700	-1.18005100	0.62151700
H	-4.25748600	-1.43941700	-0.64835200
C	-3.32335200	-2.82592800	-1.97820300
O	-2.34265300	-1.99831200	-1.89212000
C	-3.13414100	-4.04977200	-2.84763500
H	-2.15620300	-4.04293400	-3.33671300
H	-3.92907200	-4.08387500	-3.60400700
H	-3.23119000	-4.94875700	-2.22479800
P	0.23625700	0.66343300	0.15271200
O	-0.63963500	0.08053900	-1.00177100
O	-0.34166000	1.70054800	1.10280100
O	1.57934200	1.15775800	-0.71668200
O	0.87028300	-0.53980800	1.13311500
C	1.62085800	-1.56054600	0.53095800
C	2.89319000	-1.25606600	0.05423900
C	1.03822500	-2.86531100	0.46557900

C	3.60214400	-2.26739600	-0.68961100
C	1.76995300	-3.85349200	-0.17950300
C	4.83341300	-2.01764700	-1.36495500
C	3.02593900	-3.58683800	-0.78929100
H	1.37415700	-4.86775100	-0.22627000
C	5.47998700	-3.02066500	-2.06654500
H	5.26521000	-1.02048700	-1.33492900
C	3.72929700	-4.60178700	-1.50496200
C	4.93290600	-4.32889800	-2.12820000
H	6.41531000	-2.80252800	-2.58168100
H	3.29073100	-5.59851700	-1.56252400
H	5.45674500	-5.11085000	-2.67742100
C	2.83278700	1.25600800	-0.09524500
C	3.48887200	0.09463800	0.31306200
C	3.42576500	2.55610300	-0.02215200
C	4.74810700	0.22857900	1.00442300
C	4.68681700	2.65777800	0.54721100
C	5.41249700	-0.86961800	1.62805100
C	5.35659700	1.53275100	1.09953400
H	5.16463000	3.63537900	0.61029900
C	6.62372600	-0.69832300	2.27575800
H	4.95510300	-1.85526000	1.60078500
C	6.61290000	1.67102700	1.76196700
C	7.23890800	0.57941100	2.33461600
H	7.10688400	-1.55201500	2.75063800
H	7.06593300	2.66132900	1.81907300
H	8.19547100	0.69842900	2.84286100
C	2.75355600	3.76518300	-0.58838600
C	1.46931800	4.16785600	-0.16956400
C	3.42547900	4.54591100	-1.55160600
C	0.87429000	5.31635400	-0.70513100
H	0.93799200	3.58431500	0.57793000
C	2.82821400	5.69512400	-2.08624000
H	4.41355200	4.23925500	-1.89411200
C	1.54874100	6.08404400	-1.66602300
H	-0.11964600	5.61218300	-0.36895400
H	3.36031500	6.28092400	-2.83592800
H	1.08177100	6.97571600	-2.08432500
C	-0.29087700	-3.16362900	1.07358100
C	-0.63397300	-2.70104300	2.36281300
C	-1.23183500	-3.94626700	0.37331600
C	-1.87751100	-3.00756700	2.92595000
H	0.07712200	-2.10364000	2.92810300
C	-2.47692600	-4.24869000	0.93644100

H	-0.99893300	-4.28639000	-0.63347000
C	-2.80859800	-3.77609900	2.21265800
H	-2.12156800	-2.64056700	3.92264200
H	-3.19847500	-4.83372900	0.36824900
H	-3.78237100	-4.00202400	2.64656100
4PhPA-RPA			
Pd	-2.34910100	-0.28551200	-0.73923200
O	-5.18124500	-2.02353800	-0.64801000
O	-3.41331800	-1.48789900	-1.98383100
H	-4.00065600	3.54444500	-0.47320200
O	-4.36361900	2.15666300	2.65587200
C	-3.75555000	-0.15063600	2.00586300
C	-3.30339300	1.13602900	2.69465100
C	-5.10263200	2.26270700	1.51759400
C	-4.56672000	1.56914800	0.23166700
N	-3.95383300	0.18209100	0.51830600
H	-4.61824800	-0.54182200	0.16766700
C	-5.11225000	-0.65713300	2.55877200
C	-2.68772100	-1.24348200	2.20716700
H	-2.39229700	1.53482000	2.23297500
H	-3.11949600	0.96384800	3.75907800
O	-6.08525800	2.98117800	1.51194400
C	-5.70074100	1.37062700	-0.78781400
C	-3.51573200	2.57137600	-0.32618800
H	-5.35395900	-1.62884200	2.11225900
H	-5.94430400	0.02546200	2.34875400
H	-5.04471300	-0.77794200	3.64727700
H	-2.91297600	-2.12417800	1.59528200
H	-2.69558000	-1.55543200	3.26005600
H	-1.68057100	-0.89125500	1.96266800
H	-6.12473200	2.33725000	-1.07608500
H	-6.50391800	0.74912000	-0.37447800
H	-5.30253100	0.88402700	-1.68693000
H	-3.14276200	2.21889100	-1.29545200
H	-2.66182300	2.70263200	0.34404800
C	-4.51361300	-2.14228600	-1.69819000
C	-4.95869200	-3.10256800	-2.79561100
H	-5.10675700	-4.09743600	-2.35528100
H	-4.23409600	-3.16361500	-3.61335400
H	-5.92755700	-2.76407300	-3.18779700
P	0.26758900	0.11188900	-0.55660600
O	-0.81893000	0.86020100	0.28316700
O	-0.40371100	-0.60344500	-1.76216000
O	1.02950500	-0.87686200	0.52908000

O	1.47942100	1.04288500	-1.16232200
C	2.51589900	1.51673800	-0.31570900
C	3.42159300	0.60797800	0.22620300
C	2.61891200	2.93231100	-0.16402500
C	4.41988200	1.11618300	1.13800600
C	3.65576600	3.41204200	0.62338600
C	5.27398600	0.26937000	1.90486500
C	4.54530800	2.54248100	1.30972400
H	3.76992900	4.48801600	0.75274900
C	6.22582900	0.79953900	2.75833700
H	5.16930400	-0.80926500	1.82420100
C	5.54886000	3.05559300	2.18502500
C	6.37781500	2.20428800	2.89107600
H	6.86111300	0.13115500	3.33896500
H	5.64008200	4.13639300	2.29642100
H	7.13714200	2.60689800	3.56083100
C	2.18584700	-1.57124600	0.09717500
C	3.35698100	-0.84976400	-0.11177000
C	2.09053200	-2.99024300	-0.00806900
C	4.49758900	-1.55917900	-0.63951700
C	3.23018100	-3.67500400	-0.40116900
C	5.68658500	-0.90267800	-1.07414200
C	4.42830900	-2.99579900	-0.75806700
H	3.19729100	-4.76172300	-0.47724000
C	6.76141400	-1.62437400	-1.56328000
H	5.74511600	0.18177000	-1.02777900
C	5.56126900	-3.70873800	-1.25227300
C	6.70693700	-3.04029400	-1.64189900
H	7.65618800	-1.09978000	-1.89737800
H	5.50091400	-4.79465800	-1.32997900
H	7.56362200	-3.59529900	-2.02316100
C	0.83069200	-3.71704700	0.34753100
C	0.81944900	-4.60327400	1.44261100
C	-0.35345900	-3.54005200	-0.39401400
C	-0.35381600	-5.28445000	1.79603900
H	1.72922900	-4.74723800	2.02517400
C	-1.52517600	-4.21756300	-0.03758300
H	-0.35724900	-2.87124000	-1.24985300
C	-1.53157300	-5.08883400	1.06102000
H	-0.34770300	-5.96231000	2.64969900
H	-2.43292800	-4.05863900	-0.61905000
H	-2.44569200	-5.61212400	1.34101400
C	1.69752300	3.88106300	-0.86192800
C	2.23661500	4.86815100	-1.71233600

C	0.30147600	3.84086100	-0.67323100
C	1.40154900	5.78675100	-2.36165200
H	3.31335600	4.90336700	-1.87645100
C	-0.53125200	4.75985100	-1.32236900
H	-0.13561000	3.09712900	-0.01238900
C	0.01402000	5.73482000	-2.17027300
H	1.83554300	6.53769700	-3.02177700
H	-1.60803000	4.71466500	-1.16180600
H	-0.63671100	6.44682100	-2.67758100

4PhPA-RPA-TS

Pd	-2.62652900	-0.13550800	-0.55787300
O	-5.07613900	-1.58042700	-2.08411900
O	-2.93158700	-1.99484200	-1.42273500
H	-2.53398600	2.50339000	0.97013700
O	-5.01493400	1.87907500	2.38482400
C	-5.13666500	-0.33443100	1.26134600
C	-4.57918200	0.47529300	2.43439800
C	-4.99015300	2.52093500	1.18485300
C	-4.36897100	1.78559000	-0.02879000
N	-4.55099000	0.26902400	-0.00648900
H	-5.07571500	-0.08827800	-0.82654700
C	-6.67692000	-0.22726900	1.16539800
C	-4.70928200	-1.80449400	1.41718300
H	-3.48174100	0.44366100	2.45287900
H	-4.96351400	0.09617100	3.38491900
O	-5.37210400	3.67546900	1.12134700
C	-4.94757700	2.33850000	-1.33713900
C	-2.80251000	1.96567200	0.04884600
H	-7.04483200	-0.85252600	0.34229900
H	-7.01668600	0.80070600	0.99214000
H	-7.13097400	-0.58127400	2.09952500
H	-5.01781200	-2.38788000	0.54394700
H	-5.19607300	-2.23009800	2.30416300
H	-3.62367800	-1.89830700	1.53319600
H	-4.74730100	3.41164200	-1.41088200
H	-6.03295200	2.18155200	-1.37706300
H	-4.48085600	1.83398100	-2.19241000
H	-2.42141300	2.53804900	-0.80223600
H	-1.64858500	1.17851000	0.56469800
C	-4.05565700	-2.30316400	-2.02028700
C	-4.03505200	-3.67461200	-2.69301600
H	-3.84590600	-3.53014700	-3.76678600
H	-5.01372700	-4.15766100	-2.58515500
H	-3.24670400	-4.31697400	-2.28624900

P	0.35344900	0.25441000	-0.01371900
O	-0.41993800	1.09926600	1.04856600
O	-0.54728000	-0.34671100	-1.11869800
O	1.20517400	-0.84234800	0.88358500
O	1.51783600	1.09839100	-0.82876500
C	2.68705700	1.50931100	-0.14444800
C	3.60666600	0.54379000	0.25567300
C	2.89818600	2.91388300	-0.00260000
C	4.75056300	0.97658400	1.02226000
C	4.06074000	3.32113100	0.63569200
C	5.65404500	0.06797200	1.64867900
C	4.98133200	2.39043200	1.18957200
H	4.25732700	4.38692100	0.75041300
C	6.74266200	0.52704400	2.36942100
H	5.47892900	-1.00145800	1.56555300
C	6.12231300	2.82881900	1.92590900
C	6.98956000	1.91848700	2.50042600
H	7.41380700	-0.18701700	2.84605000
H	6.29016100	3.90041900	2.03813100
H	7.85448000	2.26475700	3.06552300
C	2.24825400	-1.57031800	0.25897700
C	3.41276300	-0.89766300	-0.10070800
C	2.07424300	-2.98085800	0.13373200
C	4.42705600	-1.63741000	-0.81280700
C	3.10735900	-3.69901600	-0.45033500
C	5.57061200	-1.01912700	-1.39951200
C	4.26907500	-3.06284700	-0.96632000
H	3.01004200	-4.77962200	-0.55220500
C	6.52245400	-1.76868100	-2.06856200
H	5.68971700	0.05896400	-1.32829700
C	5.27805100	-3.80702400	-1.64778400
C	6.38508100	-3.17655000	-2.18437300
H	7.38272800	-1.27228300	-2.51688000
H	5.15125000	-4.88522400	-1.74962200
H	7.14607800	-3.75420200	-2.70834800
C	0.86645200	-3.68203900	0.66916000
C	1.02519800	-4.66279800	1.66973200
C	-0.42767200	-3.40892100	0.18541200
C	-0.08564100	-5.34683100	2.18148300
H	2.02161500	-4.87794000	2.05531700
C	-1.53596800	-4.09449700	0.69696800
H	-0.57651100	-2.67389400	-0.59997500
C	-1.37089200	-5.06230800	1.69837000
H	0.05369300	-6.09744500	2.95960100

H	-2.52257100	-3.86222000	0.30051500
H	-2.23553100	-5.59245100	2.09806000
C	1.95054200	3.92323300	-0.56923900
C	2.41350200	4.84465600	-1.53036100
C	0.60779100	4.00131100	-0.14964500
C	1.55400900	5.81464600	-2.06334600
H	3.44778200	4.79030800	-1.86931900
C	-0.24935500	4.97176400	-0.68225600
H	0.23804100	3.30941400	0.60189600
C	0.21856800	5.88028000	-1.64282500
H	1.92773300	6.51477200	-2.81046200
H	-1.28360800	5.02093200	-0.34175300
H	-0.45123500	6.63297000	-2.05826800

3TRIP

Pd	-1.23641000	-2.76834500	0.03321300
C	-2.49688600	-4.88829300	-0.04136600
O	-2.53569400	-4.09998600	0.98231700
O	-1.73290800	-4.50537200	-1.01115700
C	-3.30866000	-6.13692800	-0.12034400
H	-2.71985100	-6.94320600	-0.57477100
H	-3.65692100	-6.43339900	0.87503300
H	-4.18090500	-5.94578500	-0.76265100
P	-0.05122600	-0.40108300	0.01287000
O	0.11583300	-1.52540500	-1.06159000
O	-0.83405000	-1.03702300	1.20813600
O	-0.78544200	0.85798900	-0.74074800
O	1.30344200	0.27970800	0.63239900
C	2.02565200	1.25233700	-0.11659700
C	1.46816400	2.50775900	-0.34458900
C	3.33212700	0.86454000	-0.52509800
C	2.21320000	3.42233400	-1.17807100
C	4.08209900	1.79739300	-1.22028900
C	1.67371600	4.65571800	-1.64990400
C	3.54854500	3.06266400	-1.58974400
H	5.09612900	1.54378600	-1.52537900
C	2.42471300	5.50792900	-2.44060000
H	0.65329000	4.92601600	-1.39132100
C	4.30183500	3.97447700	-2.38781400
C	3.75634700	5.17542900	-2.80132400
H	1.98689300	6.44069200	-2.79522200
H	5.31472200	3.69604500	-2.68011300
H	4.33871800	5.86030400	-3.41705000
C	-0.96357000	2.05139300	0.01189400
C	0.13621600	2.87164900	0.22999200

C	-2.29036400	2.33198500	0.44558400
C	-0.06455000	4.04989800	1.03981600
C	-2.48939100	3.52852100	1.11252000
C	1.00556700	4.88108800	1.48447100
C	-1.40723500	4.39075400	1.44624300
H	-3.49395400	3.80047400	1.43136600
C	0.76244700	6.01280500	2.24340700
H	2.02828400	4.61835300	1.22680100
C	-1.62249000	5.57521900	2.21202200
C	-0.56285900	6.37484400	2.59847800
H	1.59748500	6.62911000	2.57568600
H	-2.64241200	5.82972500	2.50166300
H	-0.73999700	7.27377600	3.18830300
C	-3.38296200	1.33067700	0.19880300
C	-3.85292300	1.10792800	-1.12193900
C	-3.89074600	0.55549300	1.27618200
C	-4.81642800	0.11239600	-1.34337800
C	-4.85850700	-0.42445500	0.99840100
C	-5.32733500	-0.67139500	-0.29865700
H	-5.16936100	-0.06068000	-2.35885600
H	-5.25000800	-1.03029400	1.81490300
C	3.86400200	-0.50120200	-0.19655300
C	4.27390500	-0.79671200	1.12963200
C	3.95206100	-1.49002000	-1.20917400
C	4.77800000	-2.07430500	1.41389700
C	4.47293700	-2.75212500	-0.87246200
C	4.88889500	-3.06718700	0.42799000
H	5.09224100	-2.30002600	2.43231800
H	4.54933500	-3.51790800	-1.64432700
C	5.43104000	-4.45776200	0.76246400
C	4.53181300	-5.18818000	1.79004200
C	6.89815800	-4.40083800	1.25323700
H	5.41479800	-5.04532300	-0.16841600
H	3.49355500	-5.24848000	1.43524800
H	4.89453000	-6.21170700	1.96458300
H	4.52702300	-4.66454700	2.75664900
H	7.54470800	-3.90547100	0.51540700
H	6.97967200	-3.84628300	2.19907900
H	7.28958000	-5.41434400	1.42411600
C	4.19484700	0.24257500	2.25484600
C	5.60491800	0.62991800	2.76422200
C	3.28806900	-0.23164500	3.41568900
H	3.74384900	1.15522000	1.84696400
H	6.23366900	1.00173100	1.94279100

H	5.53640100	1.41990000	3.52650400
H	6.11778100	-0.23027700	3.21745300
H	2.28915800	-0.49898300	3.04799900
H	3.71082600	-1.10902800	3.92533500
H	3.17555200	0.56629400	4.16415500
C	3.50470100	-1.21894900	-2.65142700
C	2.61257400	-2.34439000	-3.22677700
C	4.72705800	-0.96481800	-3.56897200
H	2.90016100	-0.30292600	-2.64755500
H	1.76376500	-2.54841600	-2.56380300
H	2.21599500	-2.04258900	-4.20712400
H	3.17304200	-3.27830700	-3.37340700
H	5.33966400	-0.13178400	-3.19945100
H	5.36822600	-1.85701300	-3.62025300
H	4.40213100	-0.72172800	-4.59130000
C	-6.31805900	-1.80689800	-0.55855700
C	-5.58692700	-3.02576800	-1.17663800
C	-7.52089100	-1.37936700	-1.43062400
H	-6.71211100	-2.12126300	0.42046200
H	-4.75870400	-3.34433000	-0.53199400
H	-6.27589700	-3.87359900	-1.30385900
H	-5.16827300	-2.77431400	-2.16164000
H	-8.03248900	-0.50548600	-1.00346300
H	-7.20892300	-1.12185100	-2.45276100
H	-8.25063400	-2.19873600	-1.50463600
C	-3.35803400	1.94149300	-2.31057000
C	-4.46683000	2.89937900	-2.81328800
C	-2.81225300	1.06252100	-3.46059100
H	-2.52903700	2.57080100	-1.96635800
H	-4.80903900	3.56479100	-2.00805200
H	-4.09358400	3.52502800	-3.63741000
H	-5.33876500	2.33986900	-3.18137400
H	-2.05006900	0.36487400	-3.09185100
H	-3.61053400	0.47695300	-3.93779000
H	-2.35484000	1.69244400	-4.23724300
C	-3.43665800	0.76926400	2.72657800
C	-3.17806600	-0.54811700	3.49545400
C	-4.46408400	1.64099600	3.49483700
H	-2.48607400	1.31631200	2.70246100
H	-2.49847900	-1.20138000	2.93885000
H	-2.71920200	-0.32577400	4.46991100
H	-4.10804400	-1.09957400	3.69235400
H	-4.64518600	2.59847600	2.98989200
H	-5.42851700	1.11837100	3.57610300

H	-4.10694900	1.85415200	4.51318700
4TRIP-SOAc			
Pd	2.54459400	-1.44846800	-0.67079800
H	-0.49810600	-4.77073500	0.11614700
O	4.29693600	-2.48935600	-1.15567400
O	1.61688100	-4.26246800	3.32186500
C	2.82386900	-2.33646900	2.27644200
C	1.99066800	-2.84933800	3.46151000
C	1.33754500	-4.78913900	2.10130600
C	1.37078300	-3.90763100	0.81010300
N	1.90226800	-2.49051700	1.06547600
H	1.06294800	-1.92161800	1.31358800
C	4.14463100	-3.11042700	2.12746300
C	3.09475900	-0.83667700	2.50225000
H	1.07040500	-2.26171900	3.57843000
H	2.56692500	-2.80477300	4.39123300
O	1.03138000	-5.96696600	2.03610800
C	2.19282800	-4.65275400	-0.26442600
C	-0.10212600	-3.77838300	0.34507300
H	4.68083400	-2.79188200	1.22863500
H	4.00327800	-4.19571000	2.08022900
H	4.77411500	-2.89833100	3.00107400
H	3.67958000	-0.42118300	1.67472800
H	3.66707500	-0.70053600	3.42835800
H	2.16437000	-0.26722300	2.58349600
H	1.81652300	-5.67668500	-0.35426700
H	3.25908900	-4.68656900	-0.02679400
H	2.07028500	-4.15045400	-1.23028700
H	-0.15771700	-3.16384800	-0.56121600
H	-0.73287000	-3.31674900	1.11074900
C	4.51995900	-1.76050800	-2.20874600
O	3.66769300	-0.84111500	-2.46901500
C	5.71933400	-2.01987900	-3.06617700
H	6.60917300	-2.14761800	-2.43696400
H	5.87166100	-1.19578500	-3.77096300
H	5.56499700	-2.95214000	-3.62848700
P	-0.18496500	0.14688100	0.42885000
O	-0.25209800	-0.80248100	1.61691900
O	0.93911100	-0.07852300	-0.63026200
O	-0.13541100	1.68275300	1.07011700
O	-1.56178900	0.23513000	-0.50960300
C	-2.76286700	0.70004500	0.05998700

C	-2.89448400	2.04859300	0.39404600
C	-3.83531600	-0.24119100	0.14580600
C	-4.11118100	2.45883400	1.05600200
C	-5.05581600	0.21992900	0.60604500
C	-4.26819900	3.73905600	1.66440000
C	-5.21621900	1.53589100	1.11912100
H	-5.90650800	-0.45821900	0.62226900
C	-5.46167100	4.10408900	2.26343500
H	-3.43255300	4.43492000	1.66229900
C	-6.44054500	1.95275900	1.72090300
C	-6.56539800	3.21194700	2.27901800
H	-5.55327400	5.08382000	2.73184000
H	-7.27259400	1.24847800	1.75087200
H	-7.50211000	3.51592200	2.74556100
C	-0.49860400	2.81680900	0.32923700
C	-1.83814000	3.03703200	0.01685600
C	0.55351000	3.72363000	0.00206600
C	-2.16259000	4.22422300	-0.74554300
C	0.20472500	4.93043300	-0.57687200
C	-3.44915000	4.46253400	-1.31496200
C	-1.13228700	5.20846900	-0.97515700
H	0.98476500	5.65355400	-0.81221100
C	-3.72184200	5.62739200	-2.01196800
H	-4.22853100	3.71319600	-1.20884200
C	-1.45306800	6.40774800	-1.67821200
C	-2.72383600	6.62160100	-2.17928000
H	-4.71177700	5.77800800	-2.44220100
H	-0.66618300	7.14700500	-1.83128600
H	-2.95464000	7.53811600	-2.72177600
C	1.97951200	3.28773300	0.16498700
C	2.56177900	3.15392800	1.44860500
C	2.71569600	2.92839900	-0.99803500
C	3.86462700	2.63905400	1.55013700
C	4.01447700	2.42004200	-0.84040800
C	4.60432100	2.25626400	0.42203300
H	4.31886000	2.53022200	2.53574500
H	4.57567000	2.13538700	-1.72896800
C	-3.65115000	-1.66320800	-0.29864800
C	-3.45688700	-1.92821800	-1.68507700
C	-3.67902500	-2.74075500	0.62854100
C	-3.28256500	-3.25090300	-2.11636000
C	-3.49521800	-4.04702200	0.13179500
C	-3.28878200	-4.33004300	-1.22213400
H	-3.13874900	-3.44183200	-3.17894600

H	-3.49091700	-4.87430600	0.84401600
C	1.82723000	3.61267900	2.71378000
C	2.50761000	4.86884700	3.31421400
C	1.68978200	2.49359600	3.77040200
H	0.81093000	3.90742200	2.42400800
H	2.57088400	5.67636600	2.57122200
H	1.93729900	5.24215600	4.17752900
H	3.52841000	4.64397600	3.65536100
H	1.15690900	1.63124300	3.35438900
H	2.66977800	2.15504700	4.13487400
H	1.12118900	2.85870600	4.63827100
C	2.15109600	3.11326400	-2.41484500
C	2.21341500	1.83216200	-3.27351200
C	2.85664000	4.29587700	-3.12578400
H	1.09198700	3.37571400	-2.32719200
H	1.69753000	1.00559700	-2.77409200
H	1.72805200	2.01233300	-4.24459200
H	3.24348700	1.50977500	-3.46625200
H	2.77615200	5.22231200	-2.54017800
H	3.92602100	4.08606200	-3.27463200
H	2.40745800	4.47672800	-4.11351700
C	6.02823900	1.71593200	0.57188600
C	7.07114800	2.73913900	0.05607800
C	6.21892800	0.34517900	-0.11836200
H	6.20735700	1.57393700	1.64914900
H	6.97222500	3.70305600	0.57437400
H	8.09442800	2.36786100	0.21517300
H	6.94185600	2.92149300	-1.02060400
H	5.49061300	-0.38998400	0.24446800
H	6.09734600	0.42804400	-1.20649300
H	7.22700000	-0.04860600	0.07604000
C	-3.47166800	-0.81653800	-2.74407400
C	-4.71627300	-0.93762900	-3.65878500
C	-2.16568900	-0.78288400	-3.57300200
H	-3.55143500	0.14932500	-2.23439900
H	-5.64351500	-0.91440800	-3.06864400
H	-4.74791500	-0.10555600	-4.37750300
H	-4.70489300	-1.87634400	-4.23091100
H	-1.29059200	-0.69883900	-2.91754100
H	-2.05258900	-1.68637200	-4.18881800
H	-2.16650500	0.08238600	-4.25191900
C	-3.09211700	-5.77015800	-1.69742500
C	-1.83548400	-5.94105900	-2.58415500
C	-4.35610600	-6.28881800	-2.42793300

H	-2.94962800	-6.38895200	-0.79788100
H	-0.93673100	-5.55745300	-2.08330000
H	-1.67032400	-7.00355600	-2.81412100
H	-1.94113600	-5.40866800	-3.53994100
H	-5.24508500	-6.20826900	-1.78688100
H	-4.54613600	-5.70622200	-3.34105400
H	-4.23656000	-7.34323100	-2.71739500
C	-3.90343200	-2.65459300	2.15564300
C	-5.40748500	-2.77627300	2.51769600
C	-3.24478000	-1.48295300	2.91872600
H	-3.42653900	-3.56680900	2.54592500
H	-5.87163700	-3.63789500	2.01790200
H	-5.52641600	-2.90786400	3.60354800
H	-5.96351900	-1.87540900	2.22970600
H	-2.21084300	-1.32135900	2.59733800
H	-3.78808700	-0.54016000	2.79639500
H	-3.23785300	-1.71810800	3.99388600
4TRIP-SOAc-TS			
Pd	1.35354100	-2.08265100	1.13949600
H	2.75491900	-4.32600400	1.42325400
O	3.56141600	-1.77254400	3.10913600
O	2.25430200	-5.70662400	-1.08213000
C	0.52235600	-3.93147600	-1.31506400
C	0.90388100	-5.27551300	-0.69077900
C	3.25128700	-4.77916200	-1.10420800
C	2.94193500	-3.35294700	-0.58557400
N	1.49465800	-2.89796900	-0.76412800
H	1.43323400	-2.05262700	-1.35946700
C	0.67562800	-3.94626600	-2.85471600
C	-0.92827400	-3.59848800	-0.92862700
H	0.84915600	-5.23056000	0.40519900
H	0.24290000	-6.06917100	-1.04940200
O	4.37055900	-5.11934300	-1.44386600
C	3.86754000	-2.32518600	-1.24967500
C	3.12476500	-3.40002800	0.96914800
H	1.70705500	-4.13442200	-3.17641400
H	0.03948900	-4.73175200	-3.28193100
H	0.35857100	-2.98075200	-3.26761200
H	-1.22788300	-2.62730800	-1.33122200
H	-1.59479500	-4.35893700	-1.35199900
H	-1.06961200	-3.57609400	0.15570700
H	4.91387600	-2.58120800	-1.06261200
H	3.70277100	-2.30198100	-2.33321600
H	3.67295600	-1.32855400	-0.84192200

H	4.20270600	-3.33973500	1.17856200
H	3.12979000	-2.38136200	1.91714400
C	2.50889300	-1.28424800	3.64278700
O	1.36267600	-1.28087500	3.05996600
C	2.58004400	-0.71794800	5.04382600
H	3.56422400	-0.27515800	5.22705100
H	1.79051400	0.02147800	5.20644500
H	2.43812900	-1.54514000	5.75493700
P	-0.23950200	0.04787800	-0.40162000
O	0.48400200	-0.35627900	-1.67430700
O	-0.39615500	-0.97244800	0.77167400
O	-1.75817600	0.58063900	-0.84301700
O	0.38490100	1.41303000	0.34659400
C	0.27207900	2.63673300	-0.33015800
C	-0.96996500	3.26694800	-0.38030700
C	1.46858200	3.19495500	-0.86951100
C	-1.07747000	4.48714600	-1.14211100
C	1.37310200	4.41922200	-1.50735900
C	-2.32230200	5.13139500	-1.40897100
C	0.12253300	5.07341800	-1.69090400
H	2.27373000	4.88577800	-1.90345200
C	-2.37882700	6.30643000	-2.13847000
H	-3.24199200	4.68721600	-1.03678400
C	0.02882100	6.29361000	-2.42430400
C	-1.19345100	6.90277800	-2.64180900
H	-3.34319200	6.77546900	-2.33295100
H	0.94348700	6.73212700	-2.82496000
H	-1.25155300	7.83161500	-3.20876700
C	-2.51368100	1.34131300	0.06228100
C	-2.14415600	2.65990100	0.32250800
C	-3.67933900	0.72107300	0.60089100
C	-2.90981800	3.39244600	1.30113800
C	-4.47274500	1.47619600	1.44680500
C	-2.52371600	4.67727500	1.78682600
C	-4.10579300	2.79275000	1.84241000
H	-5.39033500	1.04520900	1.84398500
C	-3.29483500	5.35235500	2.71720700
H	-1.60386100	5.12868500	1.42378000
C	-4.88677700	3.52472800	2.78580900
C	-4.49568300	4.78065100	3.21264800
H	-2.97362000	6.32979400	3.07682600
H	-5.79490700	3.06528800	3.17794400
H	-5.09709100	5.32634400	3.93938900
C	-4.03315100	-0.69060700	0.22287100

C	-4.55416100	-0.96136500	-1.06900000
C	-3.84376800	-1.74969500	1.14913400
C	-4.89258800	-2.28179600	-1.40522000
C	-4.20554800	-3.05244800	0.76401800
C	-4.73130700	-3.34309200	-0.50272200
H	-5.29998800	-2.48187900	-2.39550800
H	-4.07082400	-3.87144500	1.47060000
C	2.77547300	2.47100900	-0.70928800
C	3.40013500	2.42944800	0.56408200
C	3.37153600	1.81045900	-1.81562400
C	4.60157700	1.71847000	0.71156500
C	4.58425100	1.12916600	-1.61689400
C	5.20766400	1.05385600	-0.36334900
H	5.06932400	1.67905300	1.69410900
H	5.04647400	0.61106500	-2.45690200
C	2.73340600	1.82298600	-3.21108100
C	2.74749700	0.43802300	-3.89970700
C	3.41020000	2.88256300	-4.11741600
H	1.68057500	2.10584200	-3.09076700
H	2.29057100	-0.31710600	-3.25286300
H	2.16875400	0.48068300	-4.83390400
H	3.76583400	0.11785200	-4.16155500
H	3.36810900	3.88426900	-3.67063700
H	4.46867900	2.63320800	-4.28374000
H	2.91344500	2.92777600	-5.09793100
C	2.80817200	3.14247000	1.78593500
C	3.75287200	4.25476000	2.30364900
C	2.44554200	2.14388900	2.91030000
H	1.87848900	3.63522700	1.47780000
H	3.99259600	4.97363800	1.50748700
H	3.28002000	4.80565700	3.12996800
H	4.69926700	3.83788800	2.67665000
H	1.75912600	1.37448700	2.54033600
H	3.34170800	1.64614900	3.30577000
H	1.95747400	2.66629900	3.74622100
C	6.50892400	0.26752100	-0.19335300
C	6.49299800	-0.65626100	1.04705600
C	7.73307200	1.21656400	-0.15707700
H	6.61269300	-0.37429400	-1.08231600
H	5.59298100	-1.28267900	1.07180900
H	7.37226400	-1.31649100	1.04460600
H	6.51711500	-0.07952600	1.98210800
H	7.78497400	1.83260500	-1.06572000
H	7.67423400	1.89447300	0.70698000

H	8.66968700	0.64494600	-0.07749800
C	-3.27576400	-1.50655200	2.55410000
C	-2.24053400	-2.56924300	2.98991800
C	-4.41476800	-1.41518800	3.60221800
H	-2.75311400	-0.54236700	2.53683300
H	-1.45508600	-2.68131100	2.23668000
H	-1.76256600	-2.25961300	3.92954200
H	-2.70542400	-3.55004200	3.16434100
H	-5.13683800	-0.62857300	3.35044300
H	-4.96302600	-2.36709300	3.66289600
H	-4.00629200	-1.19449100	4.59948000
C	-5.15395800	-4.77002000	-0.86044600
C	-4.58659200	-5.24947700	-2.21714000
C	-6.69750800	-4.90856400	-0.83474300
H	-4.74991900	-5.43192200	-0.07843700
H	-3.49346400	-5.14990000	-2.25197100
H	-4.83812500	-6.30640300	-2.38645600
H	-5.00243500	-4.67301800	-3.05531100
H	-7.10543900	-4.61562600	0.14265300
H	-7.15934400	-4.26603400	-1.59841300
H	-7.00065700	-5.94666200	-1.03591400
C	-4.77458800	0.14774400	-2.10571500
C	-6.27252100	0.29433100	-2.47037500
C	-3.90558900	-0.06740300	-3.36823600
H	-4.46386300	1.09905400	-1.65836400
H	-6.88272400	0.46635200	-1.57248700
H	-6.42147800	1.14472300	-3.15181200
H	-6.65573700	-0.60639300	-2.97060700
H	-2.84522700	-0.14870900	-3.09916800
H	-4.19742100	-0.98110200	-3.90587400
H	-4.01877300	0.77863600	-4.06188700

4TRIP-SPA

Pd	-2.04876900	0.69915600	-0.67217300
O	-5.34635300	1.11031400	-1.40027400
O	-3.41698400	0.07645700	-2.03776600
H	-4.91376800	-0.16364300	2.70456300
O	-4.68427600	3.74169000	2.21046700
C	-3.17976800	3.40299300	0.23543000
C	-4.45573400	4.05121900	0.79382600
C	-4.39675400	2.51001000	2.70890600
C	-3.70513800	1.41928900	1.83159400
N	-3.39460000	1.90033700	0.41017300
H	-4.24589700	1.68496000	-0.16040600
C	-1.91803900	3.91513700	0.95013300

C	-3.11367600	3.72027200	-1.27336200
H	-5.34221700	3.72982700	0.23018500
H	-4.38575100	5.14297700	0.75611200
O	-4.68281900	2.27669700	3.87041000
C	-2.44011000	0.94566000	2.58231200
C	-4.69457800	0.23277100	1.70836800
H	-1.03125300	3.37500400	0.60805500
H	-1.98344500	3.82255300	2.03908400
H	-1.78520700	4.97891400	0.71703800
H	-2.19359200	3.31397800	-1.71014200
H	-3.11087800	4.80771400	-1.41843300
H	-3.97049900	3.29978400	-1.81324700
H	-2.71414700	0.66691900	3.60450200
H	-1.66454100	1.71210300	2.62040700
H	-2.02954600	0.06640200	2.07993700
H	-4.22991500	-0.55964500	1.11198700
H	-5.63369000	0.53126500	1.22878100
C	-4.69215100	0.34618500	-2.14519700
C	-5.35755900	-0.35152500	-3.32649900
H	-4.80976100	-1.25101400	-3.62433700
H	-5.37327500	0.34644900	-4.17623900
H	-6.39263900	-0.60207200	-3.06848500
P	0.47820900	-0.07635000	-0.39161700
O	-0.20437200	1.06467200	0.42430600
O	-0.41727000	-0.44771000	-1.60674800
O	0.76101900	-1.31508500	0.66520100
O	1.98870800	0.24091800	-0.95526100
C	3.11801900	0.13557300	-0.10297900
C	3.55354000	-1.11929600	0.31658900
C	3.76267700	1.36147000	0.22763500
C	4.69476600	-1.16713800	1.20223800
C	4.93075200	1.28681700	0.96656800
C	5.12745200	-2.36181600	1.85153100
C	5.41418100	0.05259900	1.48107300
H	5.45908600	2.20526300	1.21884300
C	6.23470900	-2.36497400	2.68208800
H	4.57467100	-3.28458700	1.69846200
C	6.56212200	0.00987200	2.32754500
C	6.97170500	-1.17429400	2.91125500
H	6.53920500	-3.29043700	3.17029900
H	7.10144100	0.93784600	2.51992600
H	7.84573700	-1.19335900	3.56174500
C	1.44004400	-2.44181700	0.13536700
C	2.81297400	-2.35715900	-0.07992000

C	0.65301500	-3.60518000	-0.10420500
C	3.46329600	-3.49027300	-0.69262000
C	1.32010300	-4.72876800	-0.56226000
C	4.81796300	-3.46384200	-1.13770500
C	2.70315000	-4.70006400	-0.89441200
H	0.76451300	-5.65114400	-0.71896000
C	5.40479700	-4.58104900	-1.70626000
H	5.39589000	-2.54930700	-1.03261700
C	3.34541700	-5.83890200	-1.46580400
C	4.66981400	-5.78547200	-1.85926200
H	6.43958800	-4.53390000	-2.04468800
H	2.76371600	-6.75086300	-1.60357000
H	5.14695800	-6.65936300	-2.30205200
C	-0.83520100	-3.57213900	0.10624200
C	-1.36726400	-3.47296500	1.41850200
C	-1.70938700	-3.59538600	-1.01551500
C	-2.75917000	-3.38897700	1.58124700
C	-3.09497100	-3.53203000	-0.79227600
C	-3.64312400	-3.41835800	0.49232000
H	-3.17190900	-3.30697600	2.58758900
H	-3.76057200	-3.55505200	-1.65178500
C	3.12678600	2.67322100	-0.13067200
C	3.11065600	3.13027200	-1.47352800
C	2.49802900	3.43375800	0.89046100
C	2.47236800	4.34381000	-1.76957900
C	1.86901100	4.64056700	0.53825900
C	1.84092800	5.11330600	-0.77973300
H	2.46617600	4.69724500	-2.80006200
H	1.37960600	5.22912400	1.31448800
C	-1.19631100	-3.70337900	-2.45857900
C	-1.92671000	-2.75752600	-3.44212900
C	-1.28934400	-5.16502100	-2.96960100
H	-0.13922000	-3.41169600	-2.45922000
H	-1.97826900	-1.73692900	-3.05360900
H	-1.39135400	-2.73990600	-4.40286400
H	-2.95104300	-3.09974900	-3.64847900
H	-0.74051000	-5.86359100	-2.32574600
H	-2.33821900	-5.49503700	-3.00182100
H	-0.87797100	-5.24514900	-3.98683700
C	-0.47300000	-3.50624000	2.66528400
C	-0.72767600	-4.79267400	3.49065000
C	-0.62499700	-2.24188000	3.54306500
H	0.57207700	-3.54533200	2.33528600
H	-0.59102500	-5.69221600	2.87406500

H	-0.03005000	-4.85109100	4.33892900
H	-1.75006100	-4.81287600	3.89405700
H	-0.39292800	-1.33841500	2.96867500
H	-1.64397500	-2.14508400	3.94295300
H	0.06561700	-2.28868700	4.39793100
C	-5.15465400	-3.39023400	0.73422400
C	-5.70047900	-4.83392100	0.88695800
C	-5.94727600	-2.62099800	-0.34561200
H	-5.31487400	-2.87398500	1.69385800
H	-5.18635100	-5.37023200	1.69657100
H	-6.77729800	-4.82342100	1.11211200
H	-5.55185400	-5.40310100	-0.04253000
H	-5.54226600	-1.61548600	-0.50176900
H	-5.93462300	-3.14573300	-1.31083000
H	-6.99871900	-2.51741600	-0.04251800
C	3.79225500	2.34809700	-2.60247300
C	5.01232500	3.12100500	-3.16164500
C	2.80379600	1.97401400	-3.73247300
H	4.17498300	1.40966100	-2.18306200
H	5.73213800	3.35574300	-2.36492300
H	5.53080400	2.52279200	-3.92519200
H	4.70457700	4.06798200	-3.62751000
H	1.94052400	1.42756100	-3.33335800
H	2.43314100	2.86645900	-4.25653400
H	3.29954300	1.33369900	-4.47661800
C	1.14148600	6.42904700	-1.12309000
C	-0.02486600	6.21487800	-2.11788800
C	2.13784700	7.48611300	-1.65834900
H	0.71359300	6.82119000	-0.18741000
H	-0.73310900	5.46659500	-1.74066500
H	-0.57241300	7.15442500	-2.28302800
H	0.34306600	5.86606000	-3.09333400
H	2.95750200	7.65645400	-0.94643800
H	2.58073300	7.16564900	-2.61218900
H	1.62969000	8.44628200	-1.83017600
C	2.49297100	2.99686800	2.36248500
C	1.07332500	2.97689400	2.97483900
C	3.45125100	3.88037300	3.19933400
H	2.86895300	1.96873200	2.41416300
H	0.41397600	2.33936300	2.37782800
H	1.10905300	2.57705400	3.99872400
H	0.63133100	3.98136800	3.02762100
H	4.47098400	3.86264600	2.79061900
H	3.11271300	4.92658200	3.21040000

H	3.49476500	3.52718100	4.23999600
4TRIP-SPA-TS			
Pd	2.39425200	-0.93525000	0.34397700
O	4.30738000	-2.73520100	2.08188500
O	2.63190100	-1.21715500	2.38335000
H	2.29760600	-0.57103700	-2.72131600
O	4.96484800	1.16490100	-2.13782300
C	5.27871500	0.25698500	0.15642700
C	4.81605300	1.43504200	-0.70068600
C	4.70227400	-0.07715800	-2.61833500
C	4.13648900	-1.17287000	-1.67865100
N	4.37304400	-0.91319200	-0.18902500
H	4.71446100	-1.75889300	0.29806200
C	6.73957200	-0.14992300	-0.15526300
C	5.14526300	0.63004600	1.64281800
H	3.76730800	1.68713600	-0.49768100
H	5.43825100	2.31415200	-0.51890100
O	4.85448200	-0.29255400	-3.80805900
C	4.72360400	-2.54002300	-2.05633800
C	2.57351500	-1.13710600	-1.81991300
H	7.03231500	-1.00200200	0.47107400
H	6.89187900	-0.42810600	-1.20428100
H	7.40826100	0.69038500	0.07014100
H	5.40953900	-0.22445500	2.27493300
H	5.83721500	1.45041200	1.86941000
H	4.12691300	0.94317300	1.89328000
H	4.45368600	-2.79301200	-3.08638700
H	5.81765400	-2.53344800	-1.96855400
H	4.31633800	-3.30777700	-1.38814900
H	2.15417900	-2.14371700	-1.92872600
H	1.52576600	-0.18820600	-1.33764100
C	3.47957700	-2.12594300	2.79666700
C	3.36844800	-2.43242700	4.28949100
H	4.36423400	-2.62135100	4.70842800
H	2.87195700	-1.62406000	4.83690600
H	2.76971000	-3.34724400	4.40640800
P	-0.47986000	-0.07181900	-0.27103500
O	0.38823100	0.43650800	-1.46270700
O	0.27399600	-0.96263900	0.73784600
O	-1.78204700	-0.80002400	-0.97331900
O	-1.18121000	1.15247600	0.59358500
C	-2.12098200	1.96443300	-0.09051700

C	-3.38039800	1.44673600	-0.38744200
C	-1.71412600	3.29882000	-0.37472400
C	-4.26928000	2.26637900	-1.17450500
C	-2.61807600	4.10935900	-1.03954800
C	-5.50686000	1.78713900	-1.69745600
C	-3.87820800	3.62075200	-1.48396200
H	-2.35549900	5.14644200	-1.24257400
C	-6.33178500	2.60781100	-2.44675800
H	-5.80168600	0.75799900	-1.50956700
C	-4.76148800	4.44437300	-2.24361700
C	-5.96548100	3.95282200	-2.71301000
H	-7.26891500	2.21563200	-2.84119700
H	-4.46003100	5.46959400	-2.46081600
H	-6.62797300	4.58964700	-3.29865900
C	-2.94600700	-1.00972300	-0.19896800
C	-3.76182200	0.07927000	0.08857800
C	-3.22076900	-2.35311900	0.18665200
C	-4.93615000	-0.16140000	0.89222900
C	-4.41054500	-2.58622900	0.85348800
C	-5.76683100	0.88516900	1.39175000
C	-5.27626100	-1.52250100	1.23481200
H	-4.67512700	-3.60426200	1.13384400
C	-6.89695400	0.60564500	2.14049100
H	-5.50493000	1.91933800	1.18423900
C	-6.45827000	-1.77440100	1.99326000
C	-7.25803500	-0.73533700	2.43201100
H	-7.51267900	1.42364200	2.51386300
H	-6.71133800	-2.80715900	2.23499900
H	-8.15514400	-0.94116400	3.01535900
C	-2.20716300	-3.42492200	-0.10164500
C	-2.02850300	-3.89434300	-1.42673100
C	-1.36736800	-3.89857900	0.94420500
C	-1.00933600	-4.82588700	-1.68514100
C	-0.36229600	-4.82661100	0.62986100
C	-0.15647300	-5.29432600	-0.67642600
H	-0.86384800	-5.18721300	-2.70402700
H	0.29330600	-5.17626900	1.42402900
C	-0.38625200	3.81942600	0.10502300
C	-0.23750500	4.16923800	1.47094400
C	0.70087600	3.98069800	-0.79599000
C	0.99007000	4.69871900	1.90549100
C	1.90048600	4.52782700	-0.31230000
C	2.06623200	4.89853700	1.03184500
H	1.10978700	4.97052700	2.95481600

H	2.72980500	4.66980400	-1.00326100
C	-1.36844000	3.97831300	2.48998700
C	-1.76412100	5.30784200	3.17761100
C	-1.00685500	2.89177900	3.53268200
H	-2.25625300	3.62641900	1.95155600
H	-2.03443800	6.07252400	2.43576200
H	-2.62960100	5.15276700	3.83811800
H	-0.94448000	5.70752400	3.79110300
H	-0.74065400	1.94932900	3.03811200
H	-0.15603800	3.20393900	4.15514800
H	-1.85957000	2.70002000	4.20042900
C	0.58954300	3.59363300	-2.27652800
C	1.85597500	2.88617000	-2.81553100
C	0.25678500	4.82951700	-3.15039000
H	-0.23934500	2.88150800	-2.36983800
H	2.16421300	2.06890100	-2.15718800
H	1.65402300	2.45869800	-3.80755100
H	2.70237600	3.57800600	-2.92493500
H	-0.67593200	5.31120200	-2.83137300
H	1.06069700	5.57781000	-3.08815400
H	0.14487500	4.53827200	-4.20528100
C	3.37180100	5.51991500	1.53082400
C	3.60709700	6.91394200	0.89878000
C	4.58638100	4.59189700	1.29374100
H	3.26894200	5.66084000	2.61788100
H	2.75660900	7.58319900	1.08975900
H	4.51133900	7.38330500	1.31330300
H	3.73708400	6.83744700	-0.19043200
H	4.42080500	3.60307000	1.74057000
H	4.77544400	4.45276200	0.22053500
H	5.49568800	5.02130000	1.73915300
C	1.01166400	-6.21954300	-1.02188100
C	1.21078300	-7.37144300	-0.01074700
C	2.31122500	-5.38795000	-1.17713500
H	0.78906200	-6.67236100	-2.00084900
H	0.28127300	-7.93860800	0.13791900
H	1.98036700	-8.06798400	-0.37308000
H	1.54129800	-7.00046100	0.96959500
H	2.20061100	-4.63120100	-1.96521000
H	2.55334200	-4.86662700	-0.23991100
H	3.16327100	-6.03191400	-1.44092600
C	-2.91853600	-3.41978100	-2.58204500
C	-3.78207000	-4.57837900	-3.13958700
C	-2.09905500	-2.74308400	-3.70739700

H	-3.61225700	-2.66654600	-2.18855800
H	-4.38745400	-5.03885200	-2.34610400
H	-4.46497800	-4.21024900	-3.91929900
H	-3.15604400	-5.36445500	-3.58539400
H	-1.48863200	-1.92420500	-3.30743600
H	-1.43005100	-3.46008400	-4.20408900
H	-2.77028900	-2.32792200	-4.47337800
C	-1.54148700	-3.44247300	2.39997800
C	-0.20618200	-3.19305600	3.14020800
C	-2.40313700	-4.46451500	3.18704600
H	-2.08332300	-2.48815800	2.38700700
H	0.44093500	-2.51378600	2.57869900
H	-0.40534500	-2.73799000	4.12155400
H	0.34100100	-4.12848400	3.32475400
H	-3.37615400	-4.63484200	2.70921800
H	-1.88651900	-5.43373900	3.24976300
H	-2.58445800	-4.10934800	4.21230500
4TRIP-ROAc			
Pd	2.50256900	-1.24421200	-0.73190700
H	4.40920200	-0.37711200	2.82560000
O	4.38934400	-2.05918100	-1.15514900
O	4.07277400	-4.17934000	1.69079200
C	1.75013300	-3.73901100	0.89663400
C	3.09675000	-4.39746600	0.60803000
C	4.05179500	-3.06815700	2.47453100
C	3.01338100	-1.93799000	2.25618300
N	2.03490600	-2.24737100	1.10960500
H	1.12375000	-1.80329100	1.35742900
C	1.08375400	-4.38640300	2.13725600
C	0.80374300	-3.91000200	-0.30801300
H	3.54501600	-4.02619900	-0.31801100
H	2.98828800	-5.48522500	0.54744900
O	4.88397400	-2.97344700	3.36176500
C	2.21772900	-1.69445000	3.56918300
C	3.80937600	-0.64390800	1.94922200
H	0.20245600	-3.81863100	2.44644000
H	1.76205500	-4.48370100	2.99063000
H	0.75594600	-5.39690900	1.86264200
H	-0.15246200	-3.40788500	-0.12156300
H	0.60279500	-4.97705300	-0.45942200
H	1.23573400	-3.50504000	-1.23198400
H	2.91841900	-1.42822700	4.36705800
H	1.64380500	-2.56529400	3.89139700
H	1.52495000	-0.85935000	3.41710800

H	3.11885600	0.17859800	1.73989900
H	4.48567200	-0.77080400	1.09927600
C	4.49232100	-1.41373500	-2.28231000
O	3.51103800	-0.66290100	-2.61237400
C	5.70918700	-1.57845100	-3.13750000
H	6.61031400	-1.60305400	-2.51273700
H	5.77546100	-0.76412400	-3.86679200
H	5.64071800	-2.53505300	-3.67613400
P	-0.40024500	0.02225700	0.28973300
O	-0.44798500	-0.97721000	1.43587500
O	0.72267500	-0.12812800	-0.78465000
O	-0.37366600	1.53959600	0.98794200
O	-1.78174600	0.13315300	-0.63902300
C	-2.97435200	0.49354100	0.02104400
C	-3.16343300	1.81479800	0.42560500
C	-3.95417900	-0.53249400	0.17416300
C	-4.34848500	2.11739900	1.19321000
C	-5.14801600	-0.18992300	0.78670300
C	-4.55066500	3.36862700	1.84792400
C	-5.36202600	1.10179800	1.34168900
H	-5.92712400	-0.94334100	0.89621000
C	-5.70577900	3.62137400	2.56754700
H	-3.77960600	4.13262800	1.78560800
C	-6.54962800	1.40275500	2.07313700
C	-6.72359400	2.63754300	2.67063500
H	-5.83178600	4.58235900	3.06590100
H	-7.31330800	0.62993100	2.16706400
H	-7.63135600	2.85278300	3.23385200
C	-0.80956400	2.68745400	0.31095800
C	-2.16885500	2.86736400	0.05467800
C	0.18891500	3.65419900	-0.01080100
C	-2.57310600	4.07456900	-0.63070900
C	-0.23240500	4.86899400	-0.52271100
C	-3.89435900	4.28854700	-1.12605600
C	-1.59326400	5.10957100	-0.85614300
H	0.50760200	5.63470000	-0.75253000
C	-4.24373400	5.47380200	-1.75030700
H	-4.63919800	3.50479000	-1.01771200
C	-1.99213800	6.32765100	-1.48307000
C	-3.29226400	6.51353200	-1.91496600
H	-5.25882200	5.60672900	-2.12406500
H	-1.24203100	7.10479900	-1.63364600
H	-3.58334400	7.44509400	-2.39969600
C	1.64503300	3.30271200	0.08443400

C	2.29699000	3.19506000	1.33692700
C	2.35887600	3.04288000	-1.11776500
C	3.65542400	2.84066500	1.36338900
C	3.71358200	2.68057600	-1.03376900
C	4.38252600	2.57462100	0.19400200
H	4.16479100	2.76007600	2.32437200
H	4.25580700	2.47807100	-1.95535000
C	-3.66025900	-1.92976900	-0.28864000
C	-3.51505900	-2.20744000	-1.67393000
C	-3.48769400	-2.96893500	0.66538800
C	-3.17989300	-3.50915400	-2.07729500
C	-3.14237000	-4.25180600	0.20639300
C	-2.97364100	-4.54446300	-1.15409400
H	-3.07963100	-3.71667400	-3.14152700
H	-2.99655100	-5.05235000	0.93243900
C	-3.76029800	-1.14115000	-2.74914700
C	-5.03131400	-1.47113900	-3.57152000
C	-2.53448200	-0.93672500	-3.67085300
H	-3.94975900	-0.18561300	-2.24681400
H	-5.90784400	-1.58361300	-2.91787700
H	-5.24386400	-0.66776200	-4.29213000
H	-4.91012400	-2.40665200	-4.13619500
H	-1.63863200	-0.70663000	-3.08199900
H	-2.32990400	-1.83043100	-4.27739700
H	-2.71396700	-0.10003100	-4.36172500
C	-3.68742200	-2.74943200	2.17184900
C	-2.48260000	-3.21854300	3.01722800
C	-4.99945400	-3.41974700	2.65106900
H	-3.78685200	-1.67320100	2.34815400
H	-1.57544600	-2.69682900	2.69460800
H	-2.65397700	-2.98559500	4.07856200
H	-2.31812800	-4.30228200	2.94029100
H	-5.86383800	-3.06754100	2.07167700
H	-4.94805600	-4.51302700	2.54265800
H	-5.18477000	-3.19337800	3.71148900
C	-2.62148300	-5.96562400	-1.59886900
C	-1.54651600	-6.01227000	-2.70957700
C	-3.89457000	-6.73353500	-2.03801800
H	-2.21141600	-6.48351300	-0.71723300
H	-0.65929500	-5.42618100	-2.43649200
H	-1.23087200	-7.04972100	-2.89098400
H	-1.92932600	-5.61611400	-3.66058900
H	-4.64585600	-6.74765100	-1.23619300
H	-4.35074600	-6.25776900	-2.91857400

H	-3.65316600	-7.77426700	-2.30044100
C	1.56874700	3.47672800	2.65629200
C	2.15488300	4.71994000	3.36966600
C	1.56497200	2.24305800	3.58981600
H	0.52240000	3.70709000	2.42083400
H	2.12686800	5.60219200	2.71460300
H	1.57822100	4.95171300	4.27713700
H	3.19985100	4.55545700	3.66891200
H	1.09966500	1.38616000	3.09061100
H	2.58239800	1.95943700	3.89333100
H	0.99040700	2.45482200	4.50359300
C	1.70812900	3.18297500	-2.50239700
C	1.86771500	1.92500800	-3.38308600
C	2.24422900	4.44307300	-3.22737200
H	0.63203200	3.32644500	-2.35862100
H	1.45360400	1.04535700	-2.88030200
H	1.33355300	2.06742300	-4.33459500
H	2.91777400	1.70993800	-3.61581200
H	2.10463100	5.34598900	-2.61696100
H	3.31848900	4.34767700	-3.44306900
H	1.71973300	4.59231300	-4.18266800
C	5.87437900	2.24279800	0.28103600
C	6.72617000	3.51273000	0.02511100
C	6.30914600	1.09478900	-0.65630200
H	6.06891200	1.91479700	1.31434300
H	6.45734500	4.31812700	0.72259200
H	7.79805500	3.29755800	0.14724200
H	6.56803200	3.88599700	-0.99734800
H	5.70966100	0.19515400	-0.48012500
H	6.20813800	1.37004600	-1.71499500
H	7.36363300	0.83752400	-0.48193800

4TRIP-ROAc-TS

Pd	-2.39681600	-1.45370100	0.55690600
H	-4.75373900	-3.17753900	-0.22385900
O	-4.66767600	-2.26461900	2.24136600
O	-3.25381000	-5.02777200	-1.72276200
C	-1.17754800	-3.90986700	-0.93392300
C	-2.29880000	-4.90063300	-0.60945900
C	-3.66427700	-3.88572100	-2.33976100
C	-3.23364200	-2.53901600	-1.70744900
N	-1.82924500	-2.54053200	-1.11511300
H	-1.16840300	-1.94549700	-1.64408900
C	-0.46960100	-4.27344200	-2.25913900
C	-0.16431500	-3.88972000	0.22386000

H	-2.84518000	-4.60834900	0.29651400
H	-1.89493000	-5.90696700	-0.47194400
O	-4.41679300	-3.95799300	-3.29389800
C	-3.34113600	-1.40157800	-2.72880400
C	-4.15536100	-2.28422900	-0.45204300
H	0.35581900	-3.57893400	-2.43925900
H	-1.14449100	-4.23758900	-3.12288100
H	-0.06008800	-5.28934100	-2.19231000
H	-0.65225000	-3.69069100	1.18603400
H	0.59864700	-3.12509300	0.05313600
H	0.33602100	-4.86411400	0.27944800
H	-4.36903400	-1.31788000	-3.09436900
H	-2.68054900	-1.58615100	-3.58465200
H	-3.06036600	-0.45427800	-2.25678300
H	-4.83368900	-1.44708800	-0.62262600
H	-3.99458400	-2.30022700	0.94315300
C	-4.15892500	-1.23350500	2.79567800
O	-3.17430700	-0.57562800	2.29019800
C	-4.74743700	-0.71986900	4.09158600
H	-4.04485200	-0.06267300	4.61152100
H	-5.03180700	-1.56072400	4.73430300
H	-5.65877000	-0.15236500	3.85493500
P	0.40423500	-0.05089800	-0.23801400
O	-0.59020800	-0.41003700	0.90935200
O	0.54358900	-0.98788400	-1.42798100
O	1.80222400	0.26136900	0.62222200
O	0.09473600	1.45760700	-0.90107300
C	0.36484500	2.66753000	-0.25787200
C	1.68341400	3.05037700	-0.01379800
C	-0.76116000	3.50894200	0.01028600
C	1.90619500	4.30836000	0.66364200
C	-0.51412900	4.78303900	0.48889600
C	3.17973700	4.70890700	1.16697200
C	0.79332100	5.20498000	0.85518700
H	-1.34850700	5.46571700	0.64742800
C	3.35684500	5.94031500	1.77468500
H	4.02491500	4.03151300	1.07865200
C	1.01450800	6.47673800	1.46270000
C	2.27112100	6.84388700	1.90846700
H	4.33931500	6.21644100	2.15723100
H	0.16502500	7.14932500	1.58736200
H	2.42617300	7.81418000	2.37974100
C	2.88976000	0.84318500	-0.05129200
C	2.83176100	2.18576000	-0.42489800

C	4.04274700	0.02120800	-0.23556100
C	3.92479000	2.71072700	-1.21151700
C	5.14397800	0.58868100	-0.85476300
C	3.88037000	3.98558200	-1.85050000
C	5.10621200	1.90391900	-1.39307400
H	6.04715200	-0.00680400	-0.98492600
C	4.95249200	4.45468400	-2.58988300
H	2.98362800	4.59351300	-1.76457000
C	6.20257600	2.42700000	-2.14174300
C	6.13280500	3.67848800	-2.72555900
H	4.88693200	5.42705700	-3.07767100
H	7.09401900	1.80996200	-2.26032200
H	6.97273600	4.06365100	-3.30328600
C	4.04134000	-1.41123300	0.21101700
C	4.10367900	-2.45148400	-0.75404900
C	3.97103800	-1.73100600	1.59455400
C	4.07315700	-3.78617600	-0.31055900
C	3.95038400	-3.07885700	1.98090900
C	3.99058000	-4.12453900	1.04593300
H	4.11196200	-4.58913900	-1.04765500
H	3.90711200	-3.31897300	3.04250900
C	-2.15293500	2.97558700	-0.16090400
C	-2.65279800	2.67613900	-1.45391400
C	-2.94777100	2.71783500	0.99284700
C	-3.92202800	2.09134700	-1.57183600
C	-4.20612100	2.11684400	0.81396900
C	-4.71220400	1.79156600	-0.45246000
H	-4.31108300	1.86593000	-2.56537100
H	-4.80151100	1.88679800	1.69052400
C	4.20249900	-2.17978900	-2.26224400
C	3.03318900	-2.81380000	-3.04901000
C	5.57433400	-2.63163600	-2.82032500
H	4.12753800	-1.09885500	-2.41965000
H	2.08088400	-2.41972500	-2.67683300
H	3.11398500	-2.56495100	-4.11763600
H	3.02126500	-3.90935700	-2.96223800
H	6.40165200	-2.15237200	-2.27831900
H	5.70282800	-3.72020000	-2.73280200
H	5.66518900	-2.36667000	-3.88386300
C	3.97144600	-0.65204800	2.68518100
C	5.29037800	-0.68800500	3.49737600
C	2.73758700	-0.75395200	3.61293500
H	3.92890800	0.32885000	2.19903400
H	6.16336900	-0.57321200	2.83936500

H	5.30958200	0.12718700	4.23561900
H	5.40032300	-1.63709500	4.04129100
H	1.80941400	-0.72427900	3.02979000
H	2.74841200	-1.68311500	4.20065400
H	2.72313300	0.08664400	4.32199200
C	3.97246500	-5.58851000	1.48895600
C	2.75864800	-5.91575600	2.39149100
C	5.29745300	-5.98046900	2.18912000
H	3.88457500	-6.20056000	0.57779300
H	1.81495500	-5.62780900	1.90953000
H	2.71964700	-6.99291900	2.60947300
H	2.81861000	-5.38442400	3.35176800
H	6.16253700	-5.78588300	1.54010700
H	5.43586500	-5.40595900	3.11636100
H	5.29902200	-7.04902300	2.45026900
C	-6.10433300	1.18393100	-0.66186700
C	-7.09122300	2.25759700	-1.19226000
C	-6.69311500	0.48864400	0.58280900
H	-6.00014600	0.42065000	-1.45133200
H	-6.72326200	2.72062300	-2.11755300
H	-8.07574700	1.81386800	-1.40129700
H	-7.22745300	3.05565600	-0.44754700
H	-6.00642400	-0.25624200	1.00094300
H	-6.93115100	1.21296800	1.37459400
H	-7.62649700	-0.02844200	0.32041700
C	-1.87711300	3.03731500	-2.72723000
C	-2.57153100	4.20518900	-3.47278300
C	-1.66337900	1.82665400	-3.66469700
H	-0.88408500	3.39495500	-2.43176200
H	-2.69255500	5.07801900	-2.81590900
H	-1.97810000	4.51448000	-4.34582500
H	-3.56927400	3.91210700	-3.82997900
H	-1.15101300	1.01232700	-3.13981200
H	-2.61533900	1.44493600	-4.05946200
H	-1.04244800	2.11783600	-4.52454500
C	-2.45714400	3.07794200	2.41072700
C	-1.35927100	2.11327000	2.92726300
C	-3.58997000	3.19270500	3.45486400
H	-2.00097900	4.07394700	2.34743600
H	-0.48954700	2.08686600	2.26342800
H	-1.01352800	2.44043200	3.91956000
H	-1.74605200	1.09309500	2.99958300
H	-4.38684600	3.87380200	3.12397500
H	-4.04278300	2.21804200	3.67983100

H	-3.18171000	3.58704600	4.39616000
4TRIP-RPA			
Pd	-2.18702100	0.20253700	-0.63897400
O	-5.40425100	-0.62805700	-1.02639400
O	-3.37810400	-0.61278700	-2.06614500
H	-2.71765900	4.37391300	-0.07791700
O	-4.35990600	3.02464300	2.56283400
C	-3.88242900	0.66908900	1.94240200
C	-3.48243400	1.87053100	2.79959000
C	-4.68777700	3.31631200	1.27381900
C	-3.91714300	2.57205300	0.14574500
N	-3.75297400	1.07310700	0.45595000
H	-4.53317300	0.57466200	-0.02366200
C	-5.35959400	0.27668200	2.18776500
C	-2.95543300	-0.50916100	2.29830900
H	-2.44256400	2.16464200	2.62573600
H	-3.60687500	1.63738700	3.86106900
O	-5.49517700	4.20055600	1.05409600
C	-4.68779300	2.69670500	-1.18077500
C	-2.54727300	3.29642000	0.03080500
H	-5.61084300	-0.62394900	1.61765300
H	-6.05688500	1.07042400	1.89160700
H	-5.51424300	0.07105000	3.25466400
H	-3.10376000	-1.34877100	1.61205800
H	-3.19105400	-0.85666900	3.31265000
H	-1.90187400	-0.21668100	2.26913400
H	-4.76564300	3.74984200	-1.46782900
H	-5.69977400	2.28407400	-1.09791900
H	-4.15084400	2.16099800	-1.97263900
H	-2.01379300	2.93884200	-0.85657100
H	-1.90060500	3.13118100	0.89369500
C	-4.63995800	-0.94875100	-1.96208900
C	-5.12229800	-1.83566500	-3.10413600
H	-5.06106900	-2.88044900	-2.76641800
H	-4.50095300	-1.72479700	-3.99851300
H	-6.17006100	-1.61034600	-3.33374100
P	0.43830100	-0.05934400	-0.31320600
O	-0.48531800	0.85059100	0.55469500
O	-0.35271700	-0.58154100	-1.54460600
O	1.02297100	-1.23079900	0.69292800
O	1.81841200	0.62920500	-0.87962100
C	2.94196700	0.79717700	-0.03212400

C	3.67523700	-0.31627500	0.37044900
C	3.27123500	2.14221800	0.29952700
C	4.79395200	-0.08982200	1.25648800
C	4.42033700	2.35078100	1.04204300
C	5.50942500	-1.14850700	1.89083600
C	5.19065700	1.26737900	1.54813800
H	4.71129700	3.36957400	1.29479600
C	6.58787400	-0.88815000	2.71853100
H	5.19865200	-2.17675500	1.72644100
C	6.31997600	1.49845900	2.38927900
C	7.01107300	0.44488500	2.95814400
H	7.11329500	-1.71519100	3.19542500
H	6.61728200	2.52814300	2.59012600
H	7.86806500	0.63472700	3.60382200
C	1.96404000	-2.12527500	0.12082600
C	3.27300100	-1.68991100	-0.06696500
C	1.49141400	-3.43302100	-0.18888900
C	4.19045300	-2.59767200	-0.71226000
C	2.42134400	-4.33441500	-0.67886600
C	5.49806400	-2.21433800	-1.13291000
C	3.75879600	-3.94945400	-0.97507100
H	2.11317700	-5.35713500	-0.88700500
C	6.35193100	-3.12532200	-1.73013200
H	5.82520400	-1.18800900	-0.98797400
C	4.67285200	-4.86787300	-1.57258900
C	5.94542200	-4.46908800	-1.93751200
H	7.34395600	-2.80640200	-2.04914700
H	4.34045800	-5.89054600	-1.75376000
H	6.63161200	-5.17791700	-2.40015200
C	0.04049400	-3.78585700	-0.00605000
C	-0.49830000	-3.92700900	1.29988500
C	-0.79878300	-3.94742200	-1.14187500
C	-1.85867300	-4.24038600	1.44667200
C	-2.15029200	-4.27359300	-0.93658900
C	-2.70309000	-4.42377200	0.34166500
H	-2.26821700	-4.34727600	2.45051100
H	-2.79917900	-4.40540900	-1.80168100
C	2.34777900	3.25998500	-0.09078900
C	2.24665600	3.67056600	-1.44464800
C	1.53332500	3.86703100	0.90119000
C	1.33373700	4.68118200	-1.78259700
C	0.63314900	4.87198000	0.50815600
C	0.50813000	5.28840600	-0.82423600
H	1.26580200	4.99847400	-2.82210200

H	-0.00049300	5.34013500	1.26160200
C	3.12269300	3.05652600	-2.54268100
C	4.15130500	4.08513600	-3.07447200
C	2.28231500	2.45603000	-3.69430200
H	3.69703700	2.23414800	-2.09961000
H	4.77668100	4.47661100	-2.25973600
H	4.81363900	3.61930800	-3.81895900
H	3.65115300	4.93790900	-3.55561000
H	1.55208500	1.73332400	-3.30978500
H	1.73728700	3.23485000	-4.24611100
H	2.93402500	1.93594600	-4.41134800
C	-0.47616200	6.39827400	-1.19855000
C	-1.32734600	6.06107900	-2.44531500
C	0.26338300	7.74738500	-1.38628800
H	-1.16615300	6.51502800	-0.34825800
H	-1.82355700	5.08730500	-2.34266100
H	-2.10353700	6.82508000	-2.59553000
H	-0.71527800	6.03175100	-3.35779800
H	0.82392200	8.02136000	-0.48155600
H	0.97822600	7.68706000	-2.21991200
H	-0.44815800	8.55683300	-1.60621100
C	1.61314100	3.47153700	2.38267500
C	0.23212500	3.13307100	2.98990000
C	2.33256400	4.56878200	3.20540300
H	2.21787300	2.56044300	2.45720600
H	-0.24757800	2.33640200	2.41087800
H	0.34952200	2.78338400	4.02602500
H	-0.43610200	4.00513400	3.01070300
H	3.33423200	4.77480900	2.80373900
H	1.76417600	5.51018300	3.18955700
H	2.44316700	4.25704600	4.25441100
C	0.36819900	-3.77962400	2.55692600
C	0.50724500	-5.13004000	3.30287700
C	-0.15727300	-2.66886200	3.49625800
H	1.37752700	-3.48592200	2.24541400
H	0.91788500	-5.90587700	2.64146400
H	1.18125900	-5.02615100	4.16587900
H	-0.46472700	-5.48398000	3.67479400
H	-0.22679800	-1.71423500	2.96307500
H	-1.15092000	-2.91382000	3.89646000
H	0.52333700	-2.53637900	4.35009000
C	-4.18549600	-4.75981600	0.51401500
C	-4.96995800	-3.56551900	1.10960000
C	-4.40251500	-6.04137300	1.35372100

H	-4.59112500	-4.95122600	-0.49142600
H	-4.85269000	-2.66734700	0.49123600
H	-6.04396800	-3.79632500	1.16730100
H	-4.62115100	-3.33089200	2.12507300
H	-3.85770500	-6.89508900	0.92670600
H	-4.05738600	-5.90599500	2.38873800
H	-5.47041000	-6.30167500	1.39003000
C	-0.27987900	-3.79909900	-2.57863500
C	-1.25371000	-3.03026900	-3.50415700
C	0.04334100	-5.18567800	-3.19407400
H	0.65064200	-3.21960100	-2.53725200
H	-1.58990200	-2.09636500	-3.04590500
H	-0.75040800	-2.79115500	-4.45244000
H	-2.13987900	-3.63240800	-3.75107300
H	0.76377100	-5.74901200	-2.58821400
H	-0.87134700	-5.79155900	-3.27465300
H	0.46394300	-5.07131200	-4.20412200

4TRIP-RPA-TS

Pd	-2.30753500	-1.12613300	-0.47879800
O	-4.32402700	-3.24898300	-1.80769500
O	-2.13751600	-3.07008200	-1.17806700
H	-2.82803200	1.62175100	0.72871200
O	-4.98184500	0.49882700	2.42179500
C	-4.65078800	-1.77301900	1.46275400
C	-4.24344400	-0.76788000	2.54301900
C	-5.16655700	1.02318400	1.18079800
C	-4.46774000	0.34425500	-0.02277500
N	-4.26401100	-1.16445300	0.12531900
H	-4.70092900	-1.71021800	-0.64022800
C	-6.17863700	-2.01784700	1.44780400
C	-3.89897100	-3.09450800	1.69440500
H	-3.16692100	-0.55550800	2.50552800
H	-4.49773400	-1.14472300	3.53726900
O	-5.79499500	2.06048600	1.06311300
C	-5.24625800	0.62222800	-1.31368500
C	-2.99561400	0.89474900	-0.07622600
H	-6.42604900	-2.78022400	0.69842200
H	-6.75054200	-1.11197400	1.21345800
H	-6.50560200	-2.37905400	2.43108900
H	-4.11280600	-3.80023500	0.88574200
H	-4.23267600	-3.54408200	2.63833300
H	-2.81574900	-2.93862500	1.74150300
H	-5.34331600	1.69982400	-1.46656400
H	-6.25146100	0.18455300	-1.26060900

H	-4.71250300	0.19132600	-2.16988900
H	-2.77640300	1.40540000	-1.01825700
H	-1.73906500	0.41476900	0.57815700
C	-3.15439800	-3.69105700	-1.71661200
C	-2.82298900	-5.08992300	-2.23439100
H	-3.27736600	-5.23089100	-3.22301800
H	-3.26686800	-5.82949900	-1.55309500
H	-1.74405000	-5.25982000	-2.28742900
P	0.43155500	0.12418300	0.00236300
O	-0.53485600	0.60737600	1.12754300
O	-0.23311600	-0.77112300	-1.06801800
O	1.71883500	-0.54333000	0.79360200
O	1.13672500	1.38138900	-0.81118400
C	1.93588700	2.25995500	-0.03803500
C	3.20911800	1.84413400	0.34064500
C	1.38043900	3.53708500	0.26723300
C	3.98222200	2.72856900	1.17873400
C	2.18607900	4.42287700	0.96344200
C	5.21944900	2.35008300	1.77937200
C	3.46852000	4.04918300	1.45235000
H	1.81127100	5.42043700	1.18604500
C	5.93370900	3.23833700	2.56469900
H	5.60436500	1.34587000	1.62154100
C	4.24102800	4.94570900	2.24987900
C	5.45132500	4.55370000	2.79112800
H	6.87341800	2.92282400	3.01740800
H	3.84788300	5.94511300	2.43887900
H	6.02855500	5.24499100	3.40462400
C	2.96869600	-0.64517900	0.13589400
C	3.71739500	0.50694100	-0.09744200
C	3.40346000	-1.96157100	-0.18986800
C	4.96676800	0.36188900	-0.80609200
C	4.66115200	-2.09488900	-0.75292500
C	5.73485600	1.47320500	-1.26556500
C	5.45380100	-0.96524100	-1.09500900
H	5.03616100	-3.09028600	-0.98516200
C	6.93681500	1.28786200	-1.92623800
H	5.36627600	2.48221700	-1.10040400
C	6.70584700	-1.11962700	-1.76180000
C	7.43816000	-0.01832400	-2.16422500
H	7.50088600	2.15374900	-2.27223300
H	7.06695100	-2.12852700	-1.96360500
H	8.38960500	-0.14911900	-2.67905900
C	2.50182600	-3.14192100	0.03084400

C	2.25812600	-3.62498000	1.34190900
C	1.87325400	-3.75506400	-1.08455900
C	1.39025900	-4.71468400	1.51369200
C	1.03077600	-4.85506400	-0.85815100
C	0.76281900	-5.34270100	0.42673400
H	1.19263600	-5.07430500	2.52284100
H	0.53704500	-5.32641700	-1.70664500
C	-0.03194000	3.86822300	-0.12320800
C	-0.37569000	4.01656500	-1.49060400
C	-1.03649100	3.99960200	0.87837500
C	-1.71448400	4.26911300	-1.83854800
C	-2.35374200	4.26270200	0.47440900
C	-2.72355100	4.38403800	-0.87489100
H	-1.96350700	4.37554600	-2.89208800
H	-3.13031900	4.35454600	1.23339300
C	0.67546700	3.95698100	-2.60599600
C	0.86966200	5.35226700	-3.25195400
C	0.34801600	2.88756500	-3.67472500
H	1.63646200	3.68114900	-2.15688600
H	1.13906800	6.10374700	-2.49633600
H	1.67104300	5.32097700	-4.00467700
H	-0.04851200	5.69154300	-3.75254500
H	0.20321600	1.90362100	-3.21261100
H	-0.56109000	3.14139600	-4.23811900
H	1.17336200	2.80719700	-4.39711700
C	-0.73169100	3.89022500	2.38024300
C	-1.72076300	2.98405600	3.15130700
C	-0.68877900	5.30035500	3.02449400
H	0.26181600	3.44090500	2.49281300
H	-1.73164300	1.97138000	2.73552200
H	-1.41211100	2.90989900	4.20420300
H	-2.74576600	3.37897600	3.13859000
H	0.02859000	5.95640300	2.51458300
H	-1.67634200	5.78163300	2.97238400
H	-0.39832200	5.23520300	4.08334700
C	-4.19233800	4.63974500	-1.22653900
C	-4.57375900	4.25145300	-2.67042900
C	-4.57203400	6.11752800	-0.94646100
H	-4.78863600	4.01187600	-0.54535000
H	-4.25655600	3.22950800	-2.91754700
H	-5.66366300	4.30564700	-2.79915600
H	-4.12268700	4.93161800	-3.40722000
H	-4.37151800	6.39151300	0.09814000
H	-3.99173300	6.79475100	-1.59072800

H	-5.64023900	6.28957600	-1.14429400
C	-0.26017800	-6.46164100	0.62663900
C	-1.57309700	-5.88066600	1.21045000
C	0.26901000	-7.63044400	1.48860900
H	-0.49490100	-6.86392900	-0.37106900
H	-1.92345300	-5.03900100	0.60322200
H	-2.36271000	-6.64595300	1.24123700
H	-1.41606700	-5.51338600	2.23505000
H	1.19445900	-8.04910700	1.06876400
H	0.48161300	-7.30936400	2.51827100
H	-0.47671800	-8.43709600	1.54112600
C	2.93007600	-3.00137800	2.57122400
C	3.92899300	-3.98932000	3.22301000
C	1.89855000	-2.48296000	3.60131900
H	3.51304400	-2.13432600	2.23770700
H	4.68005200	-4.32739700	2.49503100
H	4.45688400	-3.51019400	4.06075500
H	3.41365200	-4.87878700	3.61299400
H	1.19791600	-1.78161300	3.13105400
H	1.31849300	-3.30561200	4.04332300
H	2.40845200	-1.95727000	4.42198400
C	2.06534000	-3.24180900	-2.51789200
C	0.73183100	-3.12213200	-3.29572100
C	3.07138600	-4.12449900	-3.29822900
H	2.49106100	-2.23271600	-2.45506800
H	-0.02453900	-2.59946800	-2.70201100
H	0.89535400	-2.56495200	-4.23005000
H	0.33167400	-4.10843600	-3.57088400
H	4.04493300	-4.17351000	-2.79328000
H	2.69154000	-5.15231700	-3.39535900
H	3.23198500	-3.72562400	-4.31085000

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