

Supplementary Material

PNP pincer osmium polyhydrides for catalytic dehydrogenation of primary alcohols.

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Computational Information

Basis set used for the calculations of the osmium complexes:

P Cl O
6-311+G(d)

C N O H O
6-31+G(d,p)

Hydride labels O
S 1 1.00 0.000000000000
0.3600000000D-01 0.1000000000D+01
P 1 1.00 0.000000000000
0.4400000000D+01 0.1000000000D+01
P 1 1.00 0.000000000000
0.2750000000D+00 0.1000000000D+01
D 1 1.00 0.000000000000
0.1000000000D+01 0.1000000000D+01

Os O
S 4 1.00
24.000000000 0.24559132972
18.204262749 -1.3020204925

	14.048192487	1.9114896000
	9.5166786954	-0.83098846799
S 1	1.00	
	4.2529406042	1.00000000
S 1	1.00	
	1.2999583502	1.00000000
S 1	1.00	
	0.61756850127	1.00000000
S 1	1.00	
	0.18785305474	1.00000000
S 1	1.00	
	0.87865523960E-01	1.00000000
S 1	1.00	
	0.37004242944E-01	1.00000000
P 4	1.00	
	15.5000000000	0.16016463376
	14.0000000000	-0.23201520402
	5.5458290420	0.29772587274
	1.4139502215	-0.54253238176
P 1	1.00	
	0.68136686765	1.00000000
P 1	1.00	
	0.30911452647	1.00000000
P 1	1.00	
	0.900000000000E-01	1.00000000
P 1	1.00	
	0.330000000000E-01	1.00000000
D 3	1.00	
	8.5557226523	0.55081304746E-01
	6.1927250845	-0.15041777374
	1.4916733698	0.55087247584
D 1	1.00	
	0.67423241512	1.00000000
D 1	1.00	
	0.28635737076	1.00000000
D 1	1.00	
	0.11074292707	1.00000000
F 1	1.00	
	1.3802600	1.00000000
F 1	1.00	
	0.5506500	1.00000000
F 1	1.00	
	0.2196800	1.00000000
F 1	1.00	
	0.0876400	1.00000000
G 1	1.00	
	1.2249700	1.00000000
G 1	1.00	
	0.4280300	1.00000000

OS	0	

OS-ECP 3 60
f-ul potential
1
2 2.76707510 18.90945701
s-ul potential
3
2 13.87575390 885.40571914
2 6.93787690 25.96704014
2 2.76707510 -18.90945701
p-ul potential
3
2 10.19379260 320.08390185
2 5.09689620 26.14876493
2 2.76707510 -18.90945701
d-ul potential
3
2 7.09923846 115.04484313
2 3.54961923 13.62257457
2 2.76707510 -18.90945701

Calculated PBE0 energies of the Os complexes (in THF, at P = 302 atm)

Complex	H, Hartree	G, Hartree
1	-1920.577500	-1920.663537
2	-1459.851270	-1459.932675
3	-1461.038211	-1461.118466
4	-1920.600875	-1920.694604

Calculated mPW1k energies of the Os complexes (in THF, at P = 302 atm)

Complex	H, Hartree	G, Hartree
1	-1921.744841	-1921.829022
1-ts2	-1921.737474	-1921.820623
1-ts1	-1921.725379	-1921.806864
2	-1460.838883	-1460.919402
3	-1462.036089	-1462.115390
Os(H ₂)H ₃ [N(C ₂ H ₄ P ⁱ Pr ₂) ₂]	-1462.001312	-1462.083710
3-ts2	-1461.985753	-1462.066054
3-ts1	-1461.988854	-1462.072142
OsH ₃ [N(C ₂ H ₄ P ⁱ Pr ₂) ₂]·HO ⁱ Pr	-1655.053371	-1655.153002
ts1	-1655.044172	-1655.134834
OsH ₃ [O ⁱ Pr][HN(C ₂ H ₄ P ⁱ Pr ₂) ₂]	-1655.041311	-1655.134545
ts2	-1655.040810	-1655.130033
OsH ₄ [HN(C ₂ H ₄ P ⁱ Pr ₂) ₂]·O=CMe ₂	-1655.061379	-1655.160862

Optimized geometries of the osmium complexes at the PBE0 level

Complex 1, E -1921.15150777:

O 1			
Os	0.04902000	-0.20899400	0.00000000
P	-0.07782100	0.04189200	2.30762300
H	0.89803700	-1.59411900	0.00000000
H	-1.55885300	-0.29338100	0.00000000
P	-0.07782100	0.04189200	-2.30762300
H	-0.65571900	-1.63710900	0.00000000
Cl	2.36644500	0.83305500	0.00000000
N	-0.48018200	1.93493100	0.00000000
C	-0.46963900	1.85963400	2.47423300
C	-1.42153600	-0.79484400	3.29607300
C	1.46993000	-0.08024300	3.34647600
C	-0.46963900	1.85963400	-2.47423300
C	1.46993000	-0.08024300	-3.34647600
C	-1.42153600	-0.79484400	-3.29607300
C	-1.17959300	2.37143000	1.22729000
C	-1.17959300	2.37143000	-1.22729000
H	0.45650000	2.34965400	0.00000000
H	-1.06651900	2.08038400	3.36608000
H	0.49017800	2.37830100	2.59190000
H	-1.29218200	-0.45513100	4.33241200
C	-2.81546000	-0.37609900	2.82998900
C	-1.27746700	-2.31592000	3.24807500
H	2.08281700	0.71034600	2.89228400
C	1.27267100	0.23967500	4.82699400
C	2.22625300	-1.39236900	3.14399100
H	0.49017800	2.37830100	-2.59190000
H	-1.06651900	2.08038400	-3.36608000
H	2.08281700	0.71034600	-2.89228400
C	2.22625300	-1.39236900	-3.14399100
C	1.27267100	0.23967500	-4.82699400
H	-1.29218200	-0.45513100	-4.33241200
C	-2.81546000	-0.37609900	-2.82998900
C	-1.27746700	-2.31592000	-3.24807500
H	-2.19796800	1.97501800	1.17088900
H	-1.24857300	3.46830000	1.24909800
H	-1.24857300	3.46830000	-1.24909800
H	-2.19796800	1.97501800	-1.17088900
H	-3.57284400	-0.89877200	3.42592200
H	-2.97524300	-0.63656300	1.77846000
H	-2.99174900	0.69731900	2.94877700
H	-2.09640100	-2.78557200	3.80563500
H	-0.33810300	-2.66153300	3.68692800
H	-1.31915000	-2.67763700	2.21487600
H	2.24785300	0.32810600	5.32059300
H	0.72130400	-0.55557400	5.34107000

H	0.73693200	1.18159200	4.98646100
H	3.22230100	-1.31590000	3.59611400
H	2.34820700	-1.61395000	2.08027500
H	1.71863700	-2.23865200	3.61781000
H	3.22230100	-1.31590000	-3.59611400
H	1.71863700	-2.23865200	-3.61781000
H	2.34820700	-1.61395000	-2.08027500
H	2.24785300	0.32810600	-5.32059300
H	0.73693200	1.18159200	-4.98646100
H	0.72130400	-0.55557400	-5.34107000
H	-3.57284400	-0.89877200	-3.42592200
H	-2.99174900	0.69731900	-2.94877700
H	-2.97524300	-0.63656300	-1.77846000
H	-2.09640100	-2.78557200	-3.80563500
H	-1.31915000	-2.67763700	-2.21487600
H	-0.33810300	-2.66153300	-3.68692800

Complex 2, E -1460.40744794:

O 1			
Os	0.22536700	0.00056400	0.00000000
P	0.02478900	-0.14564100	-2.29953500
P	0.02478900	-0.14564100	2.29953500
N	-1.29444300	-1.25511500	0.00000000
H	-0.05694400	1.58377600	0.00000000
H	1.75577500	-0.50905300	0.00000000
H	1.50695600	1.07076700	0.00000000
C	-1.16155500	-1.56662300	-2.46666400
C	-0.79677600	1.22917700	-3.25744800
C	1.45605900	-0.72685700	-3.35242500
C	-1.16155500	-1.56662300	2.46666400
C	1.45605900	-0.72685700	3.35242500
C	-0.79677600	1.22917700	3.25744800
C	-2.00654900	-1.70127400	-1.20236000
C	-2.00654900	-1.70127400	1.20236000
H	-1.79125900	-1.48491200	-3.35987400
H	-0.54061000	-2.46280000	-2.58476300
H	-0.91780100	0.86319600	-4.28607900
C	-2.18247600	1.52144500	-2.68087500
C	0.05112600	2.49990200	-3.27184300
H	1.63091900	-1.72876100	-2.93378400
C	2.73442100	0.08118500	-3.13251400
C	1.12753500	-0.87677900	-4.83700400
H	-0.54061000	-2.46280000	2.58476300
H	-1.79125900	-1.48491200	3.35987400
H	1.63091900	-1.72876100	2.93378400
C	1.12753500	-0.87677900	4.83700400
C	2.73442100	0.08118500	3.13251400
H	-0.91780100	0.86319600	4.28607900
C	-2.18247600	1.52144500	2.68087500
C	0.05112600	2.49990200	3.27184300
H	-2.94429700	-1.13110000	-1.30381800
H	-2.30734700	-2.75396700	-1.08080600

H	-2.94429700	-1.13110000	1.30381800
H	-2.30734700	-2.75396700	1.08080600
H	-2.85183900	0.65851600	-2.74495900
H	-2.11044400	1.82228200	-1.62969200
H	-2.64961200	2.34310900	-3.23661600
H	-0.48549000	3.29965400	-3.79614200
H	0.25325500	2.84112300	-2.25050900
H	1.00982000	2.35950700	-3.77787000
H	3.58540300	-0.44172600	-3.58488200
H	2.67733600	1.07096500	-3.59621800
H	2.93691300	0.21710500	-2.06637800
H	1.95192800	-1.38307100	-5.35304300
H	0.21983700	-1.46560800	-5.00694100
H	0.99443800	0.09880000	-5.31748900
H	1.95192800	-1.38307100	5.35304300
H	0.99443800	0.09880000	5.31748900
H	0.21983700	-1.46560800	5.00694100
H	2.67733600	1.07096500	3.59621800
H	3.58540300	-0.44172600	3.58488200
H	2.93691300	0.21710500	2.06637800
H	-2.11044400	1.82228200	1.62969200
H	-2.85183900	0.65851600	2.74495900
H	-2.64961200	2.34310900	3.23661600
H	0.25325500	2.84112300	2.25050900
H	-0.48549000	3.29965400	3.79614200
H	1.00982000	2.35950700	3.77787000

Complex 3, E -1461.61670036

O 1

Os	-0.22686300	0.08247800	0.00000000
H	-0.49006400	1.68130900	0.00000000
P	-0.03308600	-0.11720500	2.29224500
P	-0.03308600	-0.11720500	-2.29224500
H	-1.75237300	0.63125300	0.00000000
N	1.21148200	-1.60063900	0.00000000
H	-1.31080200	-1.21467800	0.00000000
H	1.23250400	0.91748200	0.00000000
C	0.75432800	1.21234800	3.34847000
C	-1.47397900	-0.74876400	3.31094500
C	1.15217500	-1.55253000	2.46580200
C	-1.47397900	-0.74876400	-3.31094500
C	0.75432800	1.21234800	-3.34847000
C	1.15217500	-1.55253000	-2.46580200
C	2.03170600	-1.65239800	1.22766700
C	2.03170600	-1.65239800	-1.22766700
H	0.60603800	-2.41939600	0.00000000
C	-0.04102500	2.51561600	3.27274600
C	2.20971900	1.46050300	2.95380600
H	0.73750900	0.83889300	4.38109000
C	-2.73647600	0.10033000	3.16591500
C	-1.15809700	-1.02999600	4.77917600
H	-1.66981300	-1.70676300	2.80747100

H	1.77131400	-1.47989200	3.36663400
H	0.54610900	-2.46249800	2.56545500
C	-2.73647600	0.10033000	-3.16591500
C	-1.15809700	-1.02999600	-4.77917600
H	-1.66981300	-1.70676300	-2.80747100
C	-0.04102500	2.51561600	-3.27274600
H	0.73750900	0.83889300	-4.38109000
C	2.20971900	1.46050300	-2.95380600
H	1.77131400	-1.47989200	-3.36663400
H	0.54610900	-2.46249800	-2.56545500
H	2.72522700	-0.80763500	1.17763500
H	2.62287100	-2.57963400	1.24563800
H	2.72522700	-0.80763500	-1.17763500
H	2.62287100	-2.57963400	-1.24563800
H	-1.06301400	2.40739600	3.64526400
H	-0.09750900	2.86990500	2.23767800
H	0.45104000	3.29043000	3.87292000
H	2.62193500	2.27519200	3.56118900
H	2.28353800	1.74902100	1.89980600
H	2.84288400	0.58210700	3.11424100
H	-2.93452000	0.34429200	2.11808800
H	-2.66237700	1.03689300	3.72806100
H	-3.60000000	-0.44710900	3.56242200
H	-1.02231600	-0.10193300	5.34539500
H	-1.99139500	-1.57144900	5.24313400
H	-0.25732500	-1.63970800	4.90668300
H	-3.60000000	-0.44710900	-3.56242200
H	-2.93452000	0.34429200	-2.11808800
H	-2.66237700	1.03689300	-3.72806100
H	-1.02231600	-0.10193300	-5.34539500
H	-1.99139500	-1.57144900	-5.24313400
H	-0.25732500	-1.63970800	-4.90668300
H	-1.06301400	2.40739600	-3.64526400
H	0.45104000	3.29043000	-3.87292000
H	-0.09750900	2.86990500	-2.23767800
H	2.62193500	2.27519200	-3.56118900
H	2.28353800	1.74902100	-1.89980600
H	2.84288400	0.58210700	-3.11424100

Complex 4, E -1921.28495231

O 1

Os	-0.06298700	-0.04862700	0.00000000
H	-0.27242000	1.64487800	0.00000000
H	-0.05071400	-1.75616300	0.00000000
P	-0.42154200	-0.03151300	2.30042000
P	-0.42154200	-0.03151300	-2.30042000
P	2.20886600	-0.04621300	0.00000000
N	-2.28841200	-0.20788300	0.00000000
C	-2.27086300	-0.21013900	2.45577200
C	-0.13339100	1.47947000	3.38533500

C	0.16875600	-1.39658400	3.46428600
C	-2.27086300	-0.21013900	-2.45577200
C	0.16875600	-1.39658400	-3.46428600
C	-0.13339100	1.47947000	-3.38533500
C	3.08946100	-0.89068300	-1.39094500
C	3.08946100	-0.89068300	1.39094500
C	3.17954300	1.53199500	0.00000000
C	-2.93421200	0.33565600	1.20803600
C	-2.93421200	0.33565600	-1.20803600
H	-2.43543400	-1.21649100	0.00000000
H	-2.65179200	0.29883500	3.34798900
H	-2.50393200	-1.27619900	2.56555200
C	-0.76286200	2.74157300	2.80200300
C	1.34790500	1.70501000	3.67763600
H	-0.64433800	1.25632100	4.33073900
C	-0.36005200	-1.29633100	4.89725700
C	-0.11565100	-2.78559600	2.89540200
H	1.25820400	-1.27323100	3.49196600
H	-2.65179200	0.29883500	-3.34798900
H	-2.50393200	-1.27619900	-2.56555200
C	-0.11565100	-2.78559600	-2.89540200
C	-0.36005200	-1.29633100	-4.89725700
H	1.25820400	-1.27323100	-3.49196600
C	-0.76286200	2.74157300	-2.80200300
C	1.34790500	1.70501000	-3.67763600
H	-0.64433800	1.25632100	-4.33073900
H	4.17051500	-0.91826900	-1.21429500
H	2.71467400	-1.91345600	-1.49100600
H	2.90394900	-0.35801900	-2.32700200
H	2.90394900	-0.35801900	2.32700200
H	4.17051500	-0.91826900	1.21429500
H	2.71467400	-1.91345600	1.49100600
H	2.92184900	2.12416500	0.88217400
H	2.92184900	2.12416500	-0.88217400
H	4.25864500	1.33983600	0.00000000
H	-2.82812200	1.42353700	1.15662100
H	-4.00887700	0.09872200	1.19953300
H	-2.82812200	1.42353700	-1.15662100
H	-4.00887700	0.09872200	-1.19953300
H	-0.38162000	2.93626100	1.79421700
H	-1.85336700	2.66655200	2.73917700
H	-0.53096400	3.60121900	3.44307900
H	1.47246300	2.56598400	4.34547600
H	1.89808700	1.92183300	2.75668200
H	1.81939300	0.84383500	4.16259800
H	-0.01138700	-2.15898600	5.47819900
H	-0.01781900	-0.39786900	5.41795900
H	-1.45584300	-1.30958900	4.92641200
H	-1.18856400	-3.01415200	2.90984800
H	0.38421600	-3.54623000	3.50719100
H	0.22964700	-2.87281900	1.86247500

H	0.22964700	-2.87281900	-1.86247500
H	-1.18856400	-3.01415200	-2.90984800
H	0.38421600	-3.54623000	-3.50719100
H	-0.01781900	-0.39786900	-5.41795900
H	-0.01138700	-2.15898600	-5.47819900
H	-1.45584300	-1.30958900	-4.92641200
H	-0.38162000	2.93626100	-1.79421700
H	-1.85336700	2.66655200	-2.73917700
H	-0.53096400	3.60121900	-3.44307900
H	1.81939300	0.84383500	-4.16259800
H	1.47246300	2.56598400	-4.34547600
H	1.89808700	1.92183300	-2.75668200

Optimized geometries of the osmium complexes at the mPW1k level

Complex 1, E -1922.33089146

O 1			
Os	0.04794900	-0.20868700	0.00000000
P	-0.07801500	0.04363100	2.30691400
H	0.89653100	-1.58537000	0.00000000
H	-1.55209400	-0.30173100	0.00000000
P	-0.07801500	0.04363100	-2.30691400
H	-0.64780500	-1.63091400	0.00000000
Cl	2.35022100	0.84091400	0.00000000
N	-0.49068500	1.92447000	0.00000000
C	-0.47589500	1.84920200	2.46210900
C	-1.40838800	-0.79191800	3.29163600
C	1.46426900	-0.07261700	3.33210900
C	-0.47589500	1.84920200	-2.46210900
C	1.46426900	-0.07261700	-3.33210900
C	-1.40838800	-0.79191800	-3.29163600
C	-1.19113800	2.34975600	1.22002100
C	-1.19113800	2.34975600	-1.22002100
H	0.43321100	2.34821400	0.00000000
H	-1.06588100	2.07216700	3.35027000
H	0.47574700	2.37158300	2.57060300
H	-1.28691100	-0.44635600	4.32013200
C	-2.80000400	-0.39058900	2.82219400
C	-1.25395300	-2.30654900	3.25710000
H	2.07103500	0.71595700	2.88230900
C	1.27137000	0.24222800	4.80853000
C	2.22341300	-1.37639400	3.12817400
H	0.47574700	2.37158300	-2.57060300
H	-1.06588100	2.07216700	-3.35027000
H	2.07103500	0.71595700	-2.88230900
C	2.22341300	-1.37639400	-3.12817400
C	1.27137000	0.24222800	-4.80853000

H	-1.28691100	-0.44635600	-4.32013200
C	-2.80000400	-0.39058900	-2.82219400
C	-1.25395300	-2.30654900	-3.25710000
H	-2.19875800	1.94373000	1.16592100
H	-1.27323900	3.43907900	1.24355300
H	-1.27323900	3.43907900	-1.24355300
H	-2.19875800	1.94373000	-1.16592100
H	-3.54883200	-0.90909900	3.42087300
H	-2.95713900	-0.66206700	1.77989800
H	-2.98307100	0.67653300	2.92933700
H	-2.06970400	-2.77444000	3.80817600
H	-0.32212600	-2.63947100	3.70584800
H	-1.28304800	-2.67578500	2.23301400
H	2.24217000	0.33302100	5.29598700
H	0.72756400	-0.55122500	5.31977900
H	0.73588400	1.17660700	4.97020700
H	3.21518300	-1.29433700	3.57316700
H	2.34134400	-1.59755600	2.07051200
H	1.72549500	-2.21991900	3.60229900
H	3.21518300	-1.29433700	-3.57316700
H	1.72549500	-2.21991900	-3.60229900
H	2.34134400	-1.59755600	-2.07051200
H	2.24217000	0.33302100	-5.29598700
H	0.73588400	1.17660700	-4.97020700
H	0.72756400	-0.55122500	-5.31977900
H	-3.54883200	-0.90909900	-3.42087300
H	-2.98307100	0.67653300	-2.92933700
H	-2.95713900	-0.66206700	-1.77989800
H	-2.06970400	-2.77444000	-3.80817600
H	-1.28304800	-2.67578500	-2.23301400
H	-0.32212600	-2.63947100	-3.70584800

Complex 2, E -1461.40666467

O 1

Os	-0.22430900	0.00633300	0.00000000
P	-0.02465200	-0.14626500	2.29911100
P	-0.02465200	-0.14626500	-2.29911100
N	1.28813000	-1.24734400	0.00000000
H	0.05777500	1.58159600	0.00000000
H	-1.74469300	-0.50688000	0.00000000
H	-1.50013900	1.07040400	0.00000000
C	1.14832000	-1.56465700	2.45326800
C	0.79596500	1.21511200	3.25291800
C	-1.45317400	-0.72152800	3.33642900
C	1.14832000	-1.56465700	-2.45326800
C	-1.45317400	-0.72152800	-3.33642900
C	0.79596500	1.21511200	-3.25291800
C	1.99516400	-1.69126500	1.19563400
C	1.99516400	-1.69126500	-1.19563400
H	1.77147800	-1.49853200	3.34468100

H	0.52708900	-2.45475700	2.55670300
H	0.91120200	0.85352400	4.27683100
C	2.18058600	1.49839700	2.68473300
C	-0.03937000	2.48722900	3.26336300
H	-1.63419000	-1.71431000	2.91587200
C	-2.72243800	0.09141900	3.12153000
C	-1.13094100	-0.88072000	4.81554900
H	0.52708900	-2.45475700	-2.55670300
H	1.77147800	-1.49853200	-3.34468100
H	-1.63419000	-1.71431000	-2.91587200
C	-1.13094100	-0.88072000	-4.81554900
C	-2.72243800	0.09141900	-3.12153000
H	0.91120200	0.85352400	-4.27683100
C	2.18058600	1.49839700	-2.68473300
C	-0.03937000	2.48722900	-3.26336300
H	2.92547400	-1.12303000	1.30317900
H	2.29701300	-2.73693200	1.07583300
H	2.92547400	-1.12303000	-1.30317900
H	2.29701300	-2.73693200	-1.07583300
H	2.84147100	0.63759200	2.75586000
H	2.11688600	1.79447900	1.63840400
H	2.64549400	2.31485200	3.23741900
H	0.49632100	3.27703000	3.79026600
H	-0.23049600	2.82986200	2.24736300
H	-0.99679500	2.35380400	3.75982200
H	-3.57082200	-0.42751000	3.56789400
H	-2.66154600	1.07221300	3.58854500
H	-2.92314600	0.23321700	2.06244200
H	-1.95448400	-1.38309100	5.32306100
H	-0.23193500	-1.47172000	4.98352100
H	-0.99507500	0.08582600	5.29894100
H	-1.95448400	-1.38309100	-5.32306100
H	-0.99507500	0.08582600	-5.29894100
H	-0.23193500	-1.47172000	-4.98352100
H	-2.66154600	1.07221300	-3.58854500
H	-3.57082200	-0.42751000	-3.56789400
H	-2.92314600	0.23321700	-2.06244200
H	2.11688600	1.79447900	-1.63840400
H	2.84147100	0.63759200	-2.75586000
H	2.64549400	2.31485200	-3.23741900
H	-0.23049600	2.82986200	-2.24736300
H	0.49632100	3.27703000	-3.79026600
H	-0.99679500	2.35380400	-3.75982200

Complex 3, E -1462.62673075

O 1

Os	0.22652200	0.08321200	0.00000000
P	0.03263900	-0.11748900	2.29080100
P	0.03263900	-0.11748900	-2.29080100
H	-1.22933500	0.90971900	0.00000000

H	0.49269700	1.67314300	0.00000000
H	1.74258000	0.63379900	0.00000000
H	1.30591500	-1.20881300	0.00000000
H	-0.60558400	-2.40837800	0.00000000
N	-1.20469500	-1.59382600	0.00000000
C	-0.75146600	1.20312600	3.33864700
C	1.46754600	-0.74345700	3.29770000
C	-1.14359800	-1.54603800	2.45401000
C	-0.75146600	1.20312600	-3.33864700
C	1.46754600	-0.74345700	-3.29770000
C	-1.14359800	-1.54603800	-2.45401000
C	-2.02060200	-1.64211400	1.22018400
C	-2.02060200	-1.64211400	-1.22018400
C	-2.20290800	1.44664700	2.94866300
C	0.03477800	2.50504100	3.26124900
H	-0.73320500	0.83556500	4.36647500
C	1.15542300	-1.02924200	4.75996800
C	2.72310500	0.10659700	3.15786600
H	1.66780000	-1.69376300	2.79579400
H	-1.75916700	-1.48197800	3.35025600
H	-0.54018700	-2.45086500	2.54651300
C	-2.20290800	1.44664700	-2.94866300
C	0.03477800	2.50504100	-3.26124900
H	-0.73320500	0.83556500	-4.36647500
C	1.15542300	-1.02924200	-4.75996800
C	2.72310500	0.10659700	-3.15786600
H	1.66780000	-1.69376300	-2.79579400
H	-1.75916700	-1.48197800	-3.35025600
H	-0.54018700	-2.45086500	-2.54651300
H	-2.70826400	-0.80094100	1.17189600
H	-2.61100500	-2.56195600	1.24008600
H	-2.70826400	-0.80094100	-1.17189600
H	-2.61100500	-2.56195600	-1.24008600
H	-2.27988400	1.73529100	1.90174700
H	-2.61360600	2.25414500	3.55519800
H	-2.82913500	0.57111600	3.10868500
H	0.08203400	2.86133600	2.23333400
H	-0.45327900	3.27089700	3.86451500
H	1.05378400	2.40061100	3.62417700
H	1.01966900	-0.10888200	5.32634500
H	1.98541200	-1.56813300	5.21761400
H	0.26107100	-1.63749500	4.88558500
H	2.64782500	1.03399800	3.72244400
H	3.58255000	-0.43855200	3.54872900
H	2.91979700	0.35516300	2.11759800
H	-2.27988400	1.73529100	-1.90174700
H	-2.61360600	2.25414500	-3.55519800
H	-2.82913500	0.57111600	-3.10868500
H	0.08203400	2.86133600	-2.23333400
H	-0.45327900	3.27089700	-3.86451500
H	1.05378400	2.40061100	-3.62417700

H	1.01966900	-0.10888200	-5.32634500
H	1.98541200	-1.56813300	-5.21761400
H	0.26107100	-1.63749500	-4.88558500
H	2.64782500	1.03399800	-3.72244400
H	3.58255000	-0.43855200	-3.54872900
H	2.91979700	0.35516300	-2.11759800

1-ts1, E -1922.31070147

O 1

Os	0.00000100	0.00148000	-0.27052500
H	0.52504200	-1.41658600	-0.86707400
P	-2.32391700	-0.03770600	0.05676200
H	-0.00000400	0.53140500	-1.82258000
P	2.32392800	-0.03777000	0.05678700
H	-0.52505800	-1.41655300	-0.86713700
N	0.00000200	-0.57910500	1.88306600
Cl	0.00004200	2.28857800	0.70283700
C	-2.44241400	-0.48680900	1.85112600
C	-3.31042900	1.53211700	0.01562700
C	-3.36295100	-1.30616600	-0.81282300
C	2.44242400	-0.48710200	1.85110000
C	3.36294500	-1.30616500	-0.81290500
C	3.31047400	1.53204000	0.01587600
C	1.22187400	-1.27354300	2.29402200
C	-1.22195100	-1.27335800	2.29409400
H	0.00008100	0.33515600	2.32736100
H	-2.48137000	0.45504800	2.40142700
H	-3.35572400	-1.03054800	2.08698000
H	-2.72856800	2.16233400	0.69024700
C	-3.30802000	2.21192800	-1.34628500
C	-4.72543700	1.40527800	0.56386300
H	-4.39768700	-1.07028000	-0.55849700
C	-3.07476600	-2.72343000	-0.33536600
C	-3.19457000	-1.22539000	-2.32500000
H	3.35566800	-1.03100300	2.08684300
H	2.48153900	0.45467400	2.40152900
H	4.39767100	-1.07047600	-0.55835900
C	3.07449900	-2.72349300	-0.33579500
C	3.19479600	-1.22501300	-2.32508200
H	2.72874200	2.16209500	0.69075900
C	4.72556900	1.40501400	0.56384300
C	3.30784500	2.21222800	-1.34584800
H	1.20680700	-2.26064200	1.83599300
H	1.23928900	-1.41203900	3.37875300
H	-1.23936400	-1.41176400	3.37883700
H	-1.20701300	-2.26049600	1.83614800
H	-3.68231200	3.23038700	-1.24412100
H	-3.95904300	1.70050200	-2.05323700
H	-2.30816100	2.26113900	-1.76979900
H	-5.16888300	2.39680200	0.65613900

H	-4.75663600	0.94275500	1.54833600
H	-5.36697900	0.82901700	-0.10144100
H	-3.69744000	-3.42501500	-0.88989000
H	-3.28980300	-2.86313000	0.72133900
H	-2.03625300	-3.00167800	-0.51318100
H	-3.88073300	-1.92102300	-2.80796700
H	-2.18113500	-1.49780200	-2.61415200
H	-3.39253300	-0.23347200	-2.72018600
H	3.69722900	-3.42503200	-0.89031500
H	2.03600000	-3.00160300	-0.51389800
H	3.28928200	-2.86342200	0.72093100
H	3.88070000	-1.92086000	-2.80810900
H	3.39327600	-0.23310600	-2.72003500
H	2.18126500	-1.49688400	-2.61440900
H	5.16902700	2.39650600	0.65640700
H	5.36700300	0.82899800	-0.10177500
H	4.75692900	0.94213200	1.54814400
H	3.68212900	3.23066800	-1.24345700
H	2.30792200	2.26152500	-1.76918900
H	3.95877000	1.70101500	-2.05304400

1-ts2, E -1922.32288394

O 1

Os	-0.06642700	-0.21554600	0.00000000
H	1.46804900	-0.72280600	0.00000000
P	0.08894900	0.05971500	2.30525000
P	0.08894900	0.05971500	-2.30525000
N	0.45806800	1.88701100	0.00000000
H	-0.51394500	-1.74098100	0.48786000
H	-0.51394500	-1.74098100	-0.48786000
Cl	-2.45780500	0.75737600	0.00000000
C	0.45840300	1.86236400	2.45881800
C	-1.44316500	-0.08286900	3.34033300
C	1.43611400	-0.79004400	3.25333800
C	0.45840300	1.86236400	-2.45881800
C	1.43611400	-0.79004400	-3.25333800
C	-1.44316500	-0.08286900	-3.34033300
C	1.16534000	2.34011800	-1.20804700
C	1.16534000	2.34011800	1.20804700
H	-0.46454100	2.31738100	0.00000000
H	-0.49987700	2.37387700	2.55969100
H	1.04600300	2.10020200	3.34400100
H	-2.08768300	0.64935800	2.84937400
C	-2.13906800	-1.43099600	3.22050700
C	-1.26178600	0.32014200	4.79715800
H	1.26789500	-0.55415500	4.30576700
C	2.81575700	-0.27755000	2.86303100
C	1.36966500	-2.29965300	3.06259700
H	1.04600300	2.10020200	-3.34400100
H	-0.49987700	2.37387700	-2.55969100

H	1.26789500	-0.55415500	-4.30576700
C	2.81575700	-0.27755000	-2.86303100
C	1.36966500	-2.29965300	-3.06259700
H	-2.08768300	0.64935800	-2.84937400
C	-1.26178600	0.32014200	-4.79715800
C	-2.13906800	-1.43099600	-3.22050700
H	2.17345400	1.93558100	-1.15692300
H	1.24185300	3.42985900	-1.20368800
H	1.24185300	3.42985900	1.20368800
H	2.17345400	1.93558100	1.15692300
H	-3.13032500	-1.36965500	3.66956900
H	-1.59767000	-2.21785800	3.74262300
H	-2.26122400	-1.72375900	2.18051300
H	-2.23536100	0.39281000	5.28201800
H	-0.77011400	1.28524900	4.90702000
H	-0.68240500	-0.41886600	5.34905100
H	3.57746900	-0.82836000	3.41479900
H	2.94982800	0.77748300	3.09235500
H	2.99661000	-0.42727300	1.79976200
H	2.15314800	-2.78113300	3.64782600
H	1.52272900	-2.55401600	2.01517400
H	0.41838500	-2.72192900	3.37500000
H	3.57746900	-0.82836000	-3.41479900
H	2.99661000	-0.42727300	-1.79976200
H	2.94982800	0.77748300	-3.09235500
H	2.15314800	-2.78113300	-3.64782600
H	0.41838500	-2.72192900	-3.37500000
H	1.52272900	-2.55401600	-2.01517400
H	-2.23536100	0.39281000	-5.28201800
H	-0.68240500	-0.41886600	-5.34905100
H	-0.77011400	1.28524900	-4.90702000
H	-3.13032500	-1.36965500	-3.66956900
H	-2.26122400	-1.72375900	-2.18051300
H	-1.59767000	-2.21785800	-3.74262300

Os(H₂)H₃[N(C₂H₄PⁱPr₂)₂], E -1462.58636482

O 1

Os	0.29820000	-0.01571100	0.00000000
P	-0.00697900	-0.12622800	2.30935600
P	-0.00697900	-0.12622800	-2.30935600
H	-1.08173900	0.85079000	0.00000000
H	0.55992800	1.56608300	0.00000000
H	1.75425300	0.73257200	0.00000000
H	1.45818100	-1.26787000	0.43838700
H	1.45818100	-1.26787000	-0.43838700
N	-1.06040300	-1.64178600	0.00000000
C	-0.87848000	1.23624300	3.21341000
C	1.42805700	-0.61045200	3.38628000
C	-1.10733300	-1.59506000	2.45672500
C	-0.87848000	1.23624300	-3.21341000

C	1.42805700	-0.61045200	-3.38628000
C	-1.10733300	-1.59506000	-2.45672500
C	-1.89840200	-1.74677900	1.16820000
C	-1.89840200	-1.74677900	-1.16820000
C	-2.32062600	1.39993500	2.75415000
C	-0.13296100	2.55808000	3.08909900
H	-0.89188000	0.93239200	4.26192500
C	1.07528100	-0.79545800	4.85564100
C	2.65886500	0.26944600	3.21774500
H	1.67393600	-1.59194300	2.97065700
H	-1.76085300	-1.53905700	3.32694100
H	-0.45442800	-2.45903000	2.58923100
C	-2.32062600	1.39993500	-2.75415000
C	-0.13296100	2.55808000	-3.08909900
H	-0.89188000	0.93239200	-4.26192500
C	1.07528100	-0.79545800	-4.85564100
C	2.65886500	0.26944600	-3.21774500
H	1.67393600	-1.59194300	-2.97065700
H	-1.76085300	-1.53905700	-3.32694100
H	-0.45442800	-2.45903000	-2.58923100
H	-2.70373700	-0.99115800	1.15361800
H	-2.40866500	-2.72111300	1.18697800
H	-2.70373700	-0.99115800	-1.15361800
H	-2.40866500	-2.72111300	-1.18697800
H	-2.36904800	1.64927300	1.69584700
H	-2.78751000	2.21059600	3.31379500
H	-2.91294000	0.50288500	2.91789100
H	-0.06592400	2.86344300	2.04620900
H	-0.66694400	3.33544000	3.63555800
H	0.87633500	2.50970600	3.48848900
H	0.89270400	0.16032800	5.34471100
H	1.90555100	-1.27070900	5.37782500
H	0.19624500	-1.42206200	4.99634500
H	2.53237900	1.23836200	3.69628400
H	3.51873000	-0.21049500	3.68497200
H	2.88973500	0.43724800	2.16840000
H	-2.36904800	1.64927300	-1.69584700
H	-2.78751000	2.21059600	-3.31379500
H	-2.91294000	0.50288500	-2.91789100
H	-0.06592400	2.86344300	-2.04620900
H	-0.66694400	3.33544000	-3.63555800
H	0.87633500	2.50970600	-3.48848900
H	0.89270400	0.16032800	-5.34471100
H	1.90555100	-1.27070900	-5.37782500
H	0.19624500	-1.42206200	-4.99634500
H	2.53237900	1.23836200	-3.69628400
H	3.51873000	-0.21049500	-3.68497200
H	2.88973500	0.43724800	-2.16840000

3-ts1, E -1462.57189712

O 1			
Os	-0.55219900	0.56250400	-0.00089500
P	-0.80704000	0.43005400	2.30176300
P	-0.80969900	0.42939000	-2.30310000
H	-1.62756600	1.71624500	-0.00214700
H	0.01244300	2.07871400	-0.00164400
H	1.05061400	0.90591700	-0.00707000
N	-1.98645300	-0.86156900	0.00022000
C	-1.66814700	1.80745600	3.19809600
C	0.61399100	-0.07165600	3.38909000
C	-1.91850400	-1.03399900	2.45122700
C	-1.66742600	1.80892100	-3.19942300
C	0.60940200	-0.07699800	-3.39060000
C	-1.92577700	-1.03140100	-2.45108400
C	-2.75277400	-1.17471500	1.18790000
C	-2.75725300	-1.17054900	-1.18565200
C	-3.14060300	1.88914700	2.81600700
C	-0.98983800	3.14650900	2.93815300
H	-1.60443600	1.57482100	4.26280200
C	0.22659200	-0.43169700	4.81695700
C	1.77154400	0.91695700	3.36679800
H	0.95201500	-0.98314800	2.88798300
H	-2.54240400	-1.00478800	3.34379500
H	-1.25731200	-1.89696700	2.54391700
C	-3.13948300	1.89484700	-2.81669200
C	-0.98548000	3.14624900	-2.94002800
H	-1.60473100	1.57586300	-4.26411000
C	0.21986600	-0.43959000	-4.81724400
C	1.76832700	0.91005700	-3.37196600
H	0.94698200	-0.98739900	-2.88727400
H	-2.55165200	-0.99999100	-3.34220000
H	-1.26743200	-1.89641800	-2.54593900
H	-3.64739900	-0.53945800	1.26082700
H	-3.12737600	-2.20520800	1.12893100
H	-3.64974800	-0.53197600	-1.25556500
H	-3.13537000	-2.19976000	-1.12690700
H	-3.25797400	2.04397500	1.74433500
H	-3.60370300	2.73329200	3.32720700
H	-3.69281300	0.99456900	3.09336200
H	-1.04288900	3.39768700	1.88051700
H	-1.49388300	3.93134200	3.50261300
H	0.05783100	3.15160600	3.22598300
H	-0.08284500	0.44714500	5.38085800
H	1.08461000	-0.86010800	5.33541000
H	-0.57954500	-1.16134900	4.85863000
H	1.55185200	1.80120100	3.96251200
H	2.66072500	0.45438300	3.79502100
H	2.00801200	1.23588100	2.35394400
H	-3.25578300	2.05109800	-1.74511200
H	-3.60060100	2.73973100	-3.32846300
H	-3.69429900	1.00149200	-3.09278200

H	-1.03773300	3.39783900	-1.88245000
H	-1.48756700	3.93224100	-3.50462100
H	0.06215300	3.14851400	-3.22798200
H	-0.08956500	0.43840200	-5.38248800
H	1.07688500	-0.86970200	-5.33594300
H	-0.58695900	-1.16860400	-4.85655200
H	1.54906300	1.79338300	-3.96921100
H	2.65618300	0.44525800	-3.80052600
H	2.00672800	1.23038700	-2.36005400
H	1.13801400	-1.17250700	0.14866600
H	0.59782400	-1.62505300	-0.10779700

3-ts2, E -1462.56866367

O 1

Os	0.23906700	0.05661200	0.00000000
P	0.01566600	-0.11876200	2.30625400
P	0.01566600	-0.11876200	-2.30625400
H	-1.04648700	1.05467400	0.00000000
H	0.57512400	1.63044600	0.00000000
H	1.77483000	0.59648800	0.00000000
H	1.25902100	-1.45745900	0.00000000
H	0.39792400	-1.76682300	0.00000000
N	-1.14128900	-1.58975600	0.00000000
C	-0.80816100	1.21315100	3.29771500
C	1.47531000	-0.67745300	3.31278400
C	-1.09900300	-1.58667500	2.45333900
C	-0.80816100	1.21315100	-3.29771500
C	1.47531000	-0.67745300	-3.31278400
C	-1.09900300	-1.58667500	-2.45333900
C	-1.93916900	-1.72170800	1.19361100
C	-1.93916900	-1.72170800	-1.19361100
C	-2.26691300	1.39221000	2.89946800
C	-0.06612300	2.53729300	3.17429100
H	-0.77798200	0.88143500	4.33744600
C	1.15893100	-0.98578900	4.76978700
C	2.69210400	0.22955800	3.19202200
H	1.72253300	-1.61698500	2.81031800
H	-1.72684500	-1.54628500	3.34263700
H	-0.44988600	-2.45812600	2.55350400
C	-2.26691300	1.39221000	-2.89946800
C	-0.06612300	2.53729300	-3.17429100
H	-0.77798200	0.88143500	-4.33744600
C	1.15893100	-0.98578900	-4.76978700
C	2.69210400	0.22955800	-3.19202200
H	1.72253300	-1.61698500	-2.81031800
H	-1.72684500	-1.54628500	-3.34263700
H	-0.44988600	-2.45812600	-2.55350400
H	-2.73699900	-0.96365300	1.20707000
H	-2.44222400	-2.69782700	1.20821700
H	-2.73699900	-0.96365300	-1.20707000

H	-2.44222400	-2.69782700	-1.20821700
H	-2.35332900	1.66869700	1.85013600
H	-2.71054700	2.18961800	3.49586400
H	-2.85665100	0.49321100	3.06341700
H	-0.04785100	2.86870500	2.13738500
H	-0.57191600	3.30076900	3.76556900
H	0.96097700	2.47737800	3.52345200
H	0.96607400	-0.07596500	5.33650000
H	2.01047100	-1.48096300	5.23669600
H	0.29711000	-1.64164800	4.87921200
H	2.57098800	1.14515600	3.76752800
H	3.57145300	-0.28175600	3.58378600
H	2.88754000	0.50039200	2.15706300
H	-2.35332900	1.66869700	-1.85013600
H	-2.71054700	2.18961800	-3.49586400
H	-2.85665100	0.49321100	-3.06341700
H	-0.04785100	2.86870500	-2.13738500
H	-0.57191600	3.30076900	-3.76556900
H	0.96097700	2.47737800	-3.52345200
H	0.96607400	-0.07596500	-5.33650000
H	2.01047100	-1.48096300	-5.23669600
H	0.29711000	-1.64164800	-4.87921200
H	2.57098800	1.14515600	-3.76752800
H	3.57145300	-0.28175600	-3.58378600
H	2.88754000	0.50039200	-2.15706300

ts1, E -1655.72546844

O 1

Os	-0.00003400	-0.11790900	-.30597300
P	2.29970100	-0.29484200	-0.00367800
P	-2.29976900	-0.29482700	-0.00361700
H	-0.00004300	-1.64439900	0.14741500
C	2.47041200	0.33901400	1.72094300
C	3.02676900	-2.00753000	0.00086700
C	3.54466400	0.71654900	-0.93774700
C	-2.47045300	0.33907100	1.72099400
C	-3.54470000	0.71664300	-0.93763400
C	-3.02684100	-2.00750200	0.00108900
H	3.34363400	-0.05404200	2.23937100
H	2.60224600	1.41814600	1.63278400
C	1.20195000	0.05437700	2.50784700
H	4.10941300	-1.87040500	-0.02414700
C	2.68275500	-2.79518100	1.25790100
C	2.60504700	-2.80122200	-1.23035500
H	3.11382400	1.71610100	-0.88794900
C	4.93040900	0.76591300	-0.30797100
C	3.62407400	0.33188700	-2.40919200
C	-1.20196700	0.05451000	2.50789300
H	-2.60236900	1.41819200	1.63280600
H	-3.34363300	-0.05403600	2.23945800

H	-3.11401100	1.71623400	-0.88730800
C	-3.62366900	0.33261000	-2.40927000
C	-4.93061600	0.76557700	-0.30821000
H	-4.10949100	-1.87037600	-0.02351200
C	-2.68237400	-2.79517400	1.25798800
C	-2.60557800	-2.80114600	-1.23031700
N	-0.00000400	0.39476000	1.73858000
H	1.15858800	-0.99844900	2.78976100
H	1.21558500	0.63229600	3.43706900
H	3.12304600	-3.79020000	1.19295200
H	1.60540600	-2.91918800	1.35998900
H	3.06368200	-2.32895000	2.16331400
H	3.14128000	-3.75013700	-1.25488700
H	2.80588300	-2.28031900	-2.16207600
H	1.53876300	-3.01387500	-1.19619500
H	5.55864000	1.46323100	-0.86246600
H	5.42508800	-0.20386200	-0.33803800
H	4.90569500	1.10080200	0.72662400
H	4.17503400	1.09492500	-2.95843200
H	2.63691500	0.24104600	-2.85848200
H	4.15371100	-0.60931000	-2.54731200
H	-1.21557100	0.63253600	3.43704900
H	-1.15862300	-0.99828300	2.78993300
H	-4.17448000	1.09587300	-2.95834900
H	-4.15324400	-0.60853700	-2.54795600
H	-2.63638200	0.24197100	-2.85831000
H	-5.55865300	1.46336000	-0.86234300
H	-4.90619100	1.09964600	0.72665900
H	-5.42533400	-0.20414500	-0.33921100
H	-3.12264600	-3.79020800	1.19315800
H	-3.06303700	-2.32897900	2.16353200
H	-1.60498600	-2.91912700	1.35973500
H	-3.14166400	-3.75015000	-1.25457800
H	-1.53924100	-3.01362300	-1.19668300
H	-2.80697900	-2.28029100	-2.16194400
H	0.00006400	1.59722200	1.66996400
H	1.22019600	4.69713500	-0.12529600
C	1.24977900	3.64031900	-0.39290700
H	2.13901100	3.21342600	0.06108300
H	1.32431100	3.56133500	-1.47675500
C	0.00010300	2.96428200	0.15035400
O	0.00009600	2.84478800	1.48593500
C	-1.24944000	3.64060100	-0.39285100
H	-0.00006200	1.89085600	-0.35986300
H	-2.13876100	3.21367900	0.06093400
H	-1.21976500	4.69733200	-0.12491600
H	-1.32387400	3.56194000	-1.47672800
H	-0.00004000	-1.17791700	-1.50102900
H	-0.00001400	0.25442300	-1.88951300

ts2, E -1655.72399607

O 1			
Os	-0.00001900	-0.10745300	-.30615000
P	2.29204900	-0.29894700	-0.00621000
P	-2.29213900	-0.29882400	-0.00624700
H	-0.00018300	-1.63472100	0.26430100
C	2.46876400	0.27808700	1.74116800
C	3.04002600	-2.00508000	-0.04855900
C	3.54967400	0.73738800	-0.89706000
C	-2.46887400	0.27806300	1.74118100
C	-3.54984700	0.73765700	-0.89682900
C	-3.04011900	-2.00495700	-0.04867200
H	3.34599700	-0.12759100	2.24281900
H	2.59424800	1.36077600	1.69453500
C	1.21212600	-0.04887900	2.52826600
H	4.12065400	-1.85449100	-0.08042600
C	2.72025600	-2.83422900	1.18775600
C	2.61602000	-2.77141200	-1.29597500
H	3.12133400	1.73510100	-0.81825400
C	4.93454800	0.76539300	-0.26425700
C	3.63061400	0.39807900	-2.37961500
C	-1.21224000	-0.04892300	2.52827100
H	-2.59441700	1.36075100	1.69463400
H	-3.34610600	-0.12768400	2.24278000
H	-3.12160100	1.73538900	-0.81768200
C	-3.63077300	0.39884100	-2.37949200
C	-4.93472800	0.76533000	-0.26402100
H	-4.12075000	-1.85438900	-0.08034700
C	-2.72016300	-2.83422400	1.18751900
C	-2.61628600	-2.77113300	-1.29624600
N	-0.00006600	0.36192200	1.80289900
H	1.14312000	-1.11946600	2.70837900
H	1.24176900	0.44741100	3.50152300
H	3.17730200	-3.81918200	1.09085300
H	1.64589600	-2.97970500	1.29212700
H	3.10077700	-2.38898100	2.10425800
H	3.15800600	-3.71618300	-1.34741300
H	2.80707500	-2.22643700	-2.21603400
H	1.55106700	-2.98949900	-1.25879200
H	5.56400800	1.48064100	-0.79428900
H	5.43012900	-0.20245500	-0.32529100
H	4.90887100	1.06594300	0.78092900
H	4.18395500	1.17556500	-2.90599500
H	2.64294500	0.32266100	-2.83103500
H	4.15762500	-0.54021500	-2.54553500
H	-1.24188100	0.44734600	3.50153900
H	-1.14322700	-1.11951300	2.70836100
H	-4.18436600	1.17634900	-2.90557500
H	-4.15749500	-0.53955900	-2.54572100
H	-2.64311900	0.32388800	-2.83099400
H	-5.56417100	1.48089000	-0.79365100

H	-4.90906300	1.06527800	0.78134100
H	-5.43031700	-0.20247600	-0.32562300
H	-3.17710800	-3.81921400	1.09052300
H	-3.10068800	-2.38912600	2.10409400
H	-1.64578200	-2.97959100	1.29181800
H	-3.15805800	-3.71603100	-1.34757800
H	-1.55126800	-2.98896700	-1.25938400
H	-2.80775600	-2.22615600	-2.21621700
H	-0.00013000	1.40340100	1.78223100
H	1.27130000	4.69213100	-0.33651300
C	1.26388100	3.60344600	-0.42415000
H	2.13621800	3.22528500	0.09725700
H	1.31228600	3.34212200	-1.47763000
C	0.00036000	3.10759000	0.24363600
O	0.00063900	3.02211900	1.50653000
C	-1.26337100	3.60343800	-0.42375400
H	0.00011800	1.69979500	-0.32369700
H	-2.13556100	3.22526200	0.09789300
H	-1.27079900	4.69212800	-0.33617600
H	-1.31204700	3.34206100	-1.47721400
H	0.00014100	-1.22754700	-1.44605800
H	-0.00003400	0.28472300	-1.88234100

OsH₃[N(C₂H₄PⁱPr₂)₂] $\cdot$ HOⁱPr, E -1655.74032104

O 1

Os	0.11288100	0.11576200	0.24011900
P	2.40402500	0.44047500	0.13717400
P	-2.19436500	0.22505700	0.05552400
H	0.06263500	0.56101800	1.77075100
C	2.54007400	1.50285200	-1.36819800
C	3.24846600	1.43274200	1.45577100
C	3.55513800	-0.95717000	-0.27354200
C	-2.38243900	1.30679000	-1.42972000
C	-3.19005700	-1.26481500	-0.43108300
C	-3.17291400	1.09871400	1.36519000
H	3.39154000	2.18129300	-1.32448100
H	2.71227900	0.82175700	-2.20219400
C	1.24358500	2.26382100	-1.60179000
H	4.27233500	1.59336400	1.11182600
C	2.57820400	2.79175400	1.61104900
C	3.28194300	0.70235300	2.79061800
H	3.20076500	-1.24178500	-1.26732700
C	5.01796100	-0.55274300	-0.39022100
C	3.37575200	-2.17204600	0.62648700
C	-1.14811700	2.17587400	-1.61623800
H	-2.47321500	0.63503000	-2.28323500
H	-3.28794000	1.91160100	-1.39174900
H	-2.77749700	-1.48396600	-1.41943700
C	-2.92534200	-2.48318200	0.44251700
C	-4.68036900	-0.99715500	-0.58802200

H	-4.19685400	1.16643200	0.99196800
C	-2.64401000	2.51259200	1.56938000
C	-3.17209400	0.33758500	2.68287200
N	0.07138500	1.51682000	-1.15400000
H	1.27167400	3.23265700	-1.09247300
H	1.14974600	2.48967500	-2.66923200
H	3.06960500	3.35520600	2.40423000
H	1.52834100	2.68019100	1.87904800
H	2.63719100	3.38747400	0.70315600
H	3.74192700	1.33821100	3.54713800
H	3.85534000	-0.21974900	2.74671300
H	2.27456700	0.45829800	3.12470600
H	5.59904800	-1.37854900	-0.80058800
H	5.44299700	-0.31071500	0.58289100
H	5.16005900	0.30594200	-1.04451400
H	3.91037300	-3.02298800	0.20424400
H	2.32635800	-2.43887700	0.72329600
H	3.77441400	-2.00265100	1.62441800
H	-1.04989900	2.42849000	-2.67685700
H	-1.26489400	3.12801100	-1.08857600
H	-3.36988300	-3.36656700	-0.01604900
H	-3.36299100	-2.37801200	1.43304600
H	-1.85890500	-2.65758200	0.56211200
H	-5.16657800	-1.86094400	-1.04134900
H	-4.88249600	-0.13561600	-1.22248700
H	-5.15765600	-0.82663300	0.37602000
H	-3.21751500	3.00999200	2.35156100
H	-2.72472500	3.11849700	0.66984400
H	-1.59945800	2.49659700	1.87760500
H	-3.71465200	0.90585500	3.43848400
H	-2.15437500	0.18792100	3.04039600
H	-3.64774400	-0.63624600	2.60182700
H	0.03537800	0.13932300	-2.79296900
H	1.52026800	-1.85200600	-4.95519900
C	1.18873300	-2.17046900	-3.96716100
H	1.91684300	-1.82487100	-3.23614800
H	1.17374600	-3.25931700	-3.94282900
C	-0.18406700	-1.60110400	-3.66710900
O	-0.15242300	-0.18720700	-3.68206300
C	-1.21402800	-2.05308000	-4.67871000
H	-0.49224400	-1.93766100	-2.67280100
H	-2.19657900	-1.65583200	-4.43231600
H	-0.94335800	-1.69942500	-5.67338200
H	-1.27739200	-3.13934000	-4.70883700
H	0.14536500	-1.02086400	1.44301800
H	0.19240500	-1.45933100	-0.04979100

OsH₃(OⁱPr)[HN(C₂H₄PⁱPr₂)₂], E -1655.72574379

O 1

Os	0.00180400	-0.27647500	0.09103900
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P	2.30149000	0.01103600	0.30037200
P	-2.29790000	0.01139100	0.29968000
H	0.00160600	0.08507000	1.64874900
C	2.47908000	1.79431800	-0.15067800
C	3.04023900	-0.11839700	2.00085200
C	3.55289900	-0.80882200	-0.80435800
C	-2.47508700	1.79468300	-0.15148700
C	-3.54908600	-0.80832600	-0.80540100
C	-3.03716900	-0.11787300	1.99994700
H	3.34171400	2.26612300	0.31878900
H	2.63573700	1.82763900	-1.22908700
C	1.20840900	2.55153600	0.19790200
H	4.10879800	0.05648300	1.86824000
C	2.52095400	0.94003300	2.96366300
C	2.83995000	-1.50942200	2.58724700
H	3.31644700	-0.36609900	-1.77103000
C	5.00610400	-0.48076000	-0.49009600
C	3.33546000	-2.31002500	-0.94013200
C	-1.20442100	2.55172300	0.19749200
H	-2.63138200	1.82799700	-1.22995000
H	-3.33780600	2.26662800	0.31768100
H	-3.31220100	-0.36574800	-1.77203300
C	-3.33191000	-2.30958900	-0.94094800
C	-5.00233600	-0.47994400	-0.49167800
H	-4.10567800	0.05706000	1.86700300
C	-2.51810100	0.94060200	2.96282700
C	-2.83713600	-1.50886400	2.58651100
N	0.00201400	1.83387100	-0.24233400
H	1.13797700	2.70079800	1.27399800
H	1.23179700	3.54123200	-0.26570300
H	2.98270100	0.79462400	3.94031700
H	1.44260800	0.86684300	3.09286000
H	2.76217000	1.94975100	2.63951400
H	3.31498100	-1.56925500	3.56648500
H	3.26870000	-2.29128700	1.96590300
H	1.78014400	-1.72455300	2.71080500
H	5.64283500	-0.82721700	-1.30402600
H	5.34409800	-0.97980900	0.41677600
H	5.17664200	0.58839300	-0.37383800
H	3.93956100	-2.69555800	-1.76139000
H	2.29287100	-2.54330800	-1.14324700
H	3.63267400	-2.84709100	-0.04150100
H	-1.22751000	3.54141000	-0.26614800
H	-1.13432200	2.70100600	1.27360500
H	-3.93579000	-2.69507500	-1.76239100
H	-3.62957100	-2.84650200	-0.04237500
H	-2.28929600	-2.54311400	-1.14365900
H	-5.63885000	-0.82633200	-1.30580800
H	-5.17270100	0.58925200	-0.37555800
H	-5.34075200	-0.97885900	0.41510900
H	-2.98007600	0.79524700	3.93938100

H	-2.75923400	1.95030400	2.63856900
H	-1.43978600	0.86741000	3.09227900
H	-3.31251500	-1.56861000	3.56558500
H	-1.77738200	-1.72402400	2.71045800
H	-3.26569200	-2.29075900	1.96507000
H	0.00218400	1.86648200	-1.33185200
H	1.22053100	0.08919300	-4.65876000
C	1.25350400	-0.15489600	-3.59594600
H	2.13828800	0.31597500	-3.18012100
H	1.33216300	-1.23579100	-3.49087100
C	0.00226800	0.40843700	-2.93595700
O	0.00232400	1.71689300	-2.79334400
C	-1.24881400	-0.15475100	-3.59636700
H	0.00203600	-0.15616300	-1.83328400
H	-2.13368000	0.31626300	-3.18087700
H	-1.21543200	0.08928600	-4.65918100
H	-1.32765800	-1.23563000	-3.49127000
H	0.00156500	-1.53239600	1.07545100
H	0.00174900	-1.83001500	-0.37401000

OsH₄[HN(C₂H₄PⁱPr₂)₂]₂·O=CMe₂, E -1655.74616474

O 1			
Os	0.29990100	0.15952600	0.37211600
P	2.60583800	0.11659200	0.43740900
P	-1.91663400	0.55787100	-0.12206300
H	0.35362400	1.66251600	1.10360600
C	3.05534000	1.18515100	-1.01125700
C	3.56685000	0.85548700	1.84751300
C	3.51709500	-1.44610900	0.00058800
C	-1.79292700	1.66719800	-1.60618500
C	-2.97498000	-0.80909400	-0.81350500
C	-3.04006500	1.50026700	1.02155200
H	3.99691600	1.71356500	-0.86800400
H	3.18265400	0.52516100	-1.87026300
C	1.93514100	2.16657000	-1.29723500
H	4.62319400	0.68680200	1.62929300
C	3.34030700	2.35663700	1.96448200
C	3.21218300	0.17436000	3.16284300
H	3.08404000	-1.66131700	-0.97975800
C	5.02335100	-1.29566000	-0.16083500
C	3.17606500	-2.61947900	0.90852100
C	-0.46636200	2.40282500	-1.59593200
H	-1.85036200	1.03021100	-2.48997000
H	-2.61840300	2.37516800	-1.66991700
H	-2.38898800	-1.09091000	-1.69202500
C	-3.04668900	-2.03652900	0.08399900
C	-4.36082800	-0.38286200	-1.27748200
H	-4.00819000	1.56526100	0.52106400
C	-2.53870700	2.91662400	1.26717900
C	-3.21239800	0.77176000	2.34778100

N	0.64376100	1.47086300	-1.36391800	H	-5.01304500	-0.16060400	-0.43387400
H	1.86000500	2.90655300	-0.50317800	H	-3.21043500	3.42750700	1.95755900
H	2.12235100	2.69346000	-2.23677700	H	-2.49962900	3.50854100	0.35485400
H	3.89672900	2.74449100	2.81819500	H	-1.54357300	2.90479200	1.70796700
H	2.28574000	2.57869600	2.11951100	H	-3.85769700	1.35016600	3.00952700
H	3.67782400	2.89924900	1.08367500	H	-2.24932500	0.64378800	2.83992600
H	3.77254300	0.62775900	3.98100200	H	-3.65911700	-0.21194800	2.22980100
H	3.43680200	-0.88889600	3.15841000	H	0.68691400	0.84717500	-2.16392500
H	2.14964600	0.28844200	3.37229100	H	2.21702500	-1.81741200	-6.17210500
H	5.44223600	-2.20298400	-0.59718500	C	2.35433500	-1.76009200	-5.09244100
H	5.51488700	-1.14622500	0.79961600	H	3.26678600	-1.21639400	-4.87376500
H	5.29348200	-0.46476100	-0.81043900	H	2.42910400	-2.78328600	-4.72853800
H	3.51092300	-3.55116800	0.45173900	C	1.17206300	-1.07316300	-4.48257200
H	2.10417400	-2.68754700	1.07981900	O	1.27277700	0.02339600	-3.97172600
H	3.67300500	-2.53940300	1.87361900	C	-0.13452300	-1.80166800	-4.52812200
H	-0.31703800	2.93183500	-2.54128300	H	0.34691900	-1.00268500	-0.84512400
H	-0.44156600	3.13579100	-0.79224300	H	-0.94994000	-1.14113900	-4.25545600
H	-3.45359900	-2.87973000	-0.47491600	H	-0.30673800	-2.22754400	-5.51449900
H	-3.69902800	-1.87418900	0.94002000	H	-0.09707400	-2.63167800	-3.82262500
H	-2.06176100	-2.31209900	0.45344900	H	0.09478100	0.02791400	1.96603600
H	-4.82896400	-1.19075500	-1.84063900	H	0.06956000	-1.30547000	1.01529500
H	-4.33450400	0.49397500	-1.92266300				