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(CH)2PF2+ HF OPT
1\1\LRZM-YMP\FOPT\RHF\6-31G(D)\C2H2F2P1(1+)\CLARK\09-FEB-92\1\#\ RHF/6-31G* OPT
NAME=CLARK SCF=DIRECT\3-Phosponia-cyclopropene-3,3-difluoride\1,1\P\X,1,r1\
C,2,r2,1,90.\C,2,r2,1,90.,3,180.,0\H,3,r3,2,a3,1,180.,0\H,4,r3,2,a3,1,180.,0\F,
1,r4,2,a4,3,90.,0\F,1,r4,2,a4,3,-90.,0\|r1=1.525334\r2=0.675643\r3=1.073025\r4=
1.512059\|a3=140.462236\|a4=129.026766\|Version=Cray-Y-MP/464-UniCOS-G90RevG\Stat
e=1-A1\HF=-616.1945612\RMSD=0.723E-08\RMSF=0.459E-04\Dipole=0.,0.,1.608793\PG=C
02V [C2(P1),SGV(C2H2),SGV'(F2)]\|
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```
(CH)2PF2+ HF Freq
FREQ RHF 6-31G(D) C2H2F2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-616.1945611 ZPE=26.2489336
*** 3-PHOSPHONIA-CYCLOPROPENE-3,3-DIFLUORIDE
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```
(CH)2PF2+ MP2 OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C2H2F2P1(1+)\GOELLER\19-Apr-1995\1\|
# RMP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\3-Phosponia-cyclopropen
e-3,3-difluoride\1,1\P\X,1,r1\C,2,r2,1,90.\C,2,r2,1,90.,3,180.,0\H,3,r3,2,a3,1
,180.,0\H,4,r3,2,a3,1,180.,0\F,1,r4,2,a4,3,90.,0\F,1,r4,2,a4,3,-90.,0\|r1=1.543
0481\r2=0.6902809\r3=1.08621925\r4=1.54981378\|a3=140.15773855\|a4=128.63521362\|
Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-616.1949993\MP2=-616.8991197\
RMSD=7.906e-09\RMSF=2.109e-05\Dipole=-0.,0.,1.6844767\PG=C02V [C2(P1),SGV(C2H2)
,SGV'(F2)]\|@
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```
(CH)2PF2+ MP4 SP
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H2F2P1(1+)\GOELLER\7-May-1995\0\|
\# RMP4/6-31+G* NAME=GOELLER SCF=DIRECT GEOM=CHECKPOINT GUESS=READ\3-Phosponi
a-cyclopropene-3,3-difluoride\1,1\P\X,1,1.5430480979\C,2,0.6902808979,1,90.\C,
2,0.6902808979,1,90.,3,180.,0\H,3,1.086219251,2,140.15773855,1,180.,0\H,4,1.086
219251,2,140.15773855,1,180.,0\F,1,1.5498137797,2,128.63521362,3,90.,0\F,1,1.54
98137797,2,128.63521362,3,-90.,0\|Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1
\HF=-616.1949993\MP2=-616.8991197\MP3=-616.9045561\MP4D=-616.9192881\MP4DQ=-616
.9085547\MP4SDQ=-616.920122\MP4SDTQ=-616.9478699\RMSD=8.432e-10\PG=C02V [C2(P1)
,SGV(C2H2),SGV'(F2)]\|@
```

(CH)2P(OH)2+ HF OPT
 1\1\FAU-CCC-DERIOC3\FOPT\RHF\6-31G(D)\C2H4O2P1(1+)\GOELLER\28-Feb-1995\1\#\ RHF
 /6-31G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2p(OH)2(1+)\1,1\p\X,1,PX\C
 ,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\O,1,Pn1,2,A21,3,90.,0\O,1,Pn2,2,A22,3,-90.,0\
 H,3,CH,2,HCC,1,hcxn,0\H,4,CH,2,HCC,1,-hcxn,0\H,5,nh21,1,hnp21,2,180.,0\H,6,nh22
 ,1,hnp22,2,0.,0\PX=1.54197039\Pn1=1.54646686\Pn2=1.55695309\CH=1.07258575\CX=0
 .67304089\nh21=0.95704665\nh22=0.95596078\A21=126.26389996\A22=130.55354081\HCC
 =139.675857\hnp21=119.39163294\hnp22=120.67135613\hcxn=182.15426608\Version=HP
 -PARisc-HPUX-G92/DFT-RevG.2\State=1-A'\HF=-568.2228274\RMSD=2.465e-09\RMSF=1.25
 2e-04\Dipole=0.,0.7955392,0.4954039\PG=CS [SG(H2O2P1),X(C2H2)]\@

(CH)2P(OH)2+ HF Freq
 FREQ RHF 6-31G(D) C2H4O2P1(1+) PG=CS DIP=0.000000 NIMAG=0
 STATE=1-A' HF=-568.2228274 ZPE=41.5948341
 *** (CH)2P(OH)2(1+)

(CH)2P(OH)2+ MP2 OPT
 1\1\FAU-CCC-DERIOC2\FOPT\RMP2-FC\6-31+G(D)\C2H4O2P1(1+)\GOELLER\03-May-1996\0\
 # RMP2/6-31+G* NAME=GOELLER FOPT GUESS=READ GEOM=CHECKPOINT\ (CH)2p(OH)2(1+) 1
 H to ring\1,1\p,0.0443848187,0.0956444289,0.\C,-0.6001152561,-1.3227561656,0.6
 87878229\C,-0.6001152561,-1.3227561656,-0.687878229\O,1.5951848704,0.3819087678
 ,0.\O,-0.6001152561,1.5490312385,0.\H,-0.863172847,-1.9791023119,1.5118774998\H
 ,-0.863172847,-1.9791023119,-1.5118774998\H,1.8806557083,1.3232737233,0.\H,-1.5
 792561359,1.6258184039,0.\Version=HP-PARisc-HPUX-G94RevC.3\State=1-A'\HF=-568.
 2232928\MP2=-568.9399573\RMSD=4.645e-09\RMSF=6.532e-05\Dipole=-0.9548144,-0.177
 0927,0.\PG=CS [SG(H2O2P1),X(C2H2)]\@

(CH)2P(OH)2+ MP4 SP
 1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4O2P1(1+)\GOELLER\03-May-1996\0
 \#\ RMP4/6-31+G* NAME=GOELLER GUESS=READ GEOM=CHECKPOINT\ (CH)2p(OH)2(1+) 1 H t
 o ring //MP2/6-31+G*\1,1\p,0.0443848187,0.0956444289,0.\C,-0.6001152561,-1.322
 7561656,0.687878229\C,-0.6001152561,-1.3227561656,-0.687878229\O,1.5951848704,0
 .3819087678,0.\O,-0.6001152561,1.5490312385,0.\H,-0.863172847,-1.9791023119,1.5
 118774998\H,-0.863172847,-1.9791023119,-1.5118774998\H,1.8806557083,1.323273723
 3,0.\H,-1.5792561359,1.6258184039,0.\Version=HP-PARisc-HPUX-G94RevC.3\State=1-
 A'\HF=-568.2232928\MP2=-568.9399573\MP3=-568.954818\MP4D=-568.9705233\MP4DQ=-56
 8.9579609\MP4SDQ=-568.9665382\MP4SDTQ=-568.993196\RMSD=7.081e-10\PG=CS [SG(H2O2

P1),X(C2H2)]\\@

(CH)2PC12+ HF OPT
1\\1\\FAU-CCC-DERIOC3\\FOPT\\RHF\\6-31G(D)\\C2H2CL2P1(1+)\\GOELLER\\30-Mar-1995\\1\\# RH
F/6-31G* FOPT OPTCYC=99 NAME=GOELLER SCF=DIRECT\\(CH)2Pc12(1+) C2v\\1,1\\P\\X,1,P
X\\C,2,CX,1,90.\\C,2,CX,1,90.,3,180.,0\\C1,1,PH,2,A2,3,90.,0\\C1,1,PH,2,A2,5,180.,0
\\H,3,CH,2,HCC,1,180.,0\\H,4,CH,2,HCC,1,180.,0\\PX=1.57006767\\PH=1.96138257\\CH=1.
07272466\\CX=0.66402258\\A2=125.73997955\\HCC=142.8085635\\Version=HP-PARisc-HPUX-
G92/DFT-RevG.2\\State=1-A1\\HF=-1336.2676297\\RMSD=9.571e-09\\RMSF=7.553e-05\\Dipole
=0.,0.,1.609216\\PG=C02V [C2(P1),SGV(C2H2),SGV'(C12)]\\@

(CH)2PC12+ HF Freq
FREQ RHF 6-31G(D) C2H2CL2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-1336.2676297 ZPE=24.185523
*** (CH)2PCL2(1+) C2V

(CH)2PC12+ MP2 OPT
1\\1\\FAU-CCC-DERIOC4\\FOPT\\RMP2-FC\\6-31+G(D)\\C2H2CL2P1(1+)\\GOELLER\\2-Apr-1995\\1\\
RMP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\(CH)2Pc
12(1+) C2v\\1,1\\P\\X,1,PX\\C,2,CX,1,90.\\C,2,CX,1,90.,3,180.,0\\C1,1,PH,2,A2,3,90.,
0\\C1,1,PH,2,A2,5,180.,0\\H,3,CH,2,HCC,1,180.,0\\H,4,CH,2,HCC,1,180.,0\\PX=1.58427
023\\PH=1.96570383\\CH=1.08610233\\CX=0.67806527\\A2=125.36998808\\HCC=142.45448201\\
\\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\\State=1-A1\\HF=-1336.2687697\\MP2=-1336.88
50775\\RMSD=5.494e-09\\RMSF=5.057e-05\\Dipole=0.,0.,1.4837199\\PG=C02V [C2(P1),SGV(
C2H2),SGV'(C12)]\\@

(CH)2PC12+ MP4 SP
1\\1\\FAU-CCC-DERIOC2\\SP\\RMP4SDTQ-FC\\6-31+G(D)\\C2H2CL2P1(1+)\\GOELLER\\4-May-1995\\0
\\# RMP4/6-31+G* NAME=GOELLER SCF=DIRECT\\(CH)2Pc12(1+) C2v\\1,1\\P\\X,1,1.584270
23\\C,2,0.67806527,1,90.\\C,2,0.67806527,1,90.,3,180.,0\\C1,1,1.96570383,2,125.369
98808,3,90.,0\\C1,1,1.96570383,2,125.36998808,5,180.,0\\H,3,1.08610233,2,142.4544
8201,1,180.,0\\H,4,1.08610233,2,142.45448201,1,180.,0\\Version=HP-PARisc-HPUX-G9
2/DFT-RevG.2\\State=1-A1\\HF=-1336.2687697\\MP2=-1336.8850775\\MP3=-1336.9208738\\MP
4D=-1336.9353856\\MP4DQ=-1336.9205159\\MP4SDQ=-1336.9265518\\MP4SDTQ=-1336.9530268
\\RMSD=4.689e-09\\PG=C02V [C2(P1),SGV(C2H2),SGV'(C12)]\\@

(CH)2P(NH2)2+ HF OPT 90859

1\1\FAU-CCC-HP106\FOPT\RHF\6-31G(D)\C2H6N2P1(1+)\GOELLER\11-Apr-1995\1\#\ RHF/6-31G* FOPT NAME=GOELLER SCF=DIRECT\(\CH)2P(NH2)2(1+)\1,1\P\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\N,1,Pn,2,A2,3,D1,0\N,1,Pn,2,A2,4,D1,0\H,3,CH,2,HCC,1,D2,0\H,4,CH,2,HCC,1,D2,0\H,5,nh1,1,hnp1,6,hnp1,0\H,5,nh2,1,hnp2,6,hnp2,0\H,6,nh1,1,hnp1,5,hnp1,0\H,6,nh2,1,hnp2,5,hnp2,0\PX=1.56522902\Pn=1.62016721\CH=1.07262189\CX=0.66850258\nh1=0.99991505\nh2=1.00085398\A2=127.8121069\HCC=139.74622451\hnp2=120.47223571\hnp1=120.66603221\hnp2=-38.72008054\hnp1=164.62759888\D1=80.54451174\D2=179.88632868\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A\HF=-528.5712828\RMSD=5.597e-09\RMSF=3.684e-05\Dipole=0.,0.,-0.0568786\PG=C02 [C2(P1),X(C2H6N2)]\@

(CH)2P(NH2)2+ HF Freq
FREQ RHF 6-31G(D) C2H6N2P1(1+) PG=C02 DIP=0.000000 NIMAG=0
STATE=1-A HF=-528.5712828 ZPE=58.3063296
*** (CH)2P(NH2)2(1+)

(CH)2P(NH2)2+ MP2 OPT
1\1\FAU-CCC-DERIOC2\FOPT\RMP2-FC\6-31+G(D)\C2H6N2P1(1+)\GOELLER\21-Apr-1995\1\#\ RMP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT\(\CH)2P(NH2)2(1+)\1,1\P\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\N,1,Pn,2,A2,3,D1,0\N,1,Pn,2,A2,4,D1,0\H,3,CH,2,HCC,1,D2,0\H,4,CH,2,HCC,1,D2,0\H,5,nh1,1,hnp1,6,hnp1,0\H,5,nh2,1,hnp2,6,hnp2,0\H,6,nh1,1,hnp1,5,hnp1,0\H,6,nh2,1,hnp2,5,hnp2,0\PX=1.58298849\Pn=1.63565339\CH=1.08581559\CX=0.68218582\nh1=1.01716758\nh2=1.01817128\A2=128.0207772\HCC=139.62727903\hnp2=119.9743527\hnp1=119.94222903\hnp2=-43.21667862\hnp1=164.08466283\D1=78.65910305\D2=179.96227682\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A\HF=-528.5727951\MP2=-529.257727\RMSD=9.055e-09\RMSF=2.174e-05\Dipole=0.,0.,-0.0011038\PG=C02 [C2(P1),X(C2H6N2)]\@

(CH)2P(NH2)2+ MP4 SP
1\1\FAU-CCC-DERIOC3\SP\RMP4SDTQ-FC\6-31+G(D)\C2H6N2P1(1+)\GOELLER\3-May-1995\0\#\ RMP4/6-31+G* NAME=GOELLER SCF=DIRECT GEOM=CHECKPOINT GUESS=READ\(\CH)2P(NH2)2(1+)\1,1\P\X,1,1.5829884851\C,2,0.6821858158,1,90.\C,2,0.6821858158,1,90.,3,180.,0\N,1,1.6356533898,2,128.0207772,3,78.65910305,0\N,1,1.6356533898,2,128.0207772,4,78.65910305,0\H,3,1.0858155933,2,139.62727903,1,179.96227682,0\H,4,1.0858155933,2,139.62727903,1,179.96227682,0\H,5,1.0171675791,1,119.94222903,6,164.08466283,0\H,5,1.0181712819,1,119.9743527,6,-43.21667862,0\H,6,1.0171675791,1,119.94222903,5,164.08466283,0\H,6,1.0181712819,1,119.9743527,5,-43.21667862,0\Ve

rsion=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A\HF=-528.5727951\MP2=-529.257727\M
P3=-529.2866773\MP4D=-529.3023011\MP4DQ=-529.2886697\MP4SDQ=-529.295314\MP4SDTQ
=-529.3212305\RMSD=6.182e-10\PG=C02 [C2(P1),X(C2H6N2)]\@

(CH)2PBr2+ HF OPT
1\1\FAU-CCC-DERIOC2\FOPT\RHF\GEN\C2H2BR2P1(1+)\GOELLER\24-Feb-1995\1\#\ RHF/GEN
FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2Pbr2(1+) SHASv+d\1,1\P\X,1,PX\C,
2,CX,1,90.\C,2,CX,1,90.,3,180.,0\Br,1,PH,2,A2,3,90.,0\Br,1,PH,2,A2,5,180.,0\H,3
,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.59365813\PH=2.1511142\CH=1.08484
604\CX=0.66453654\A2=125.39712864\HCC=143.18031372\Version=HP-PARisc-HPUX-G92/
DFT-RevG.2\State=1-A1\HF=-5561.3495315\RMSD=1.508e-09\RMSF=6.788e-05\Dipole=0.,
0.,2.0076218\PG=C02V [C2(P1),SGV(C2H2),SGV'(Br2)]\@

(CH)2PBr2+ HF Freq
FREQ RHF GEN C2H2BR2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-5561.3495315 ZPE=23.0538038
*** (CH)2PBR2(1+) SHASV+D

(CH)2PBr2+ MP2 OPT
1\1\LRZM-YMP\FOPT\RMP2-FC\GEN\C2H2BR2P1(1+)\GOELLER\11-May-1995\1\#\ RMP2/GEN F
OPT=CALCHFFC NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2Pbr2(1+) SHASv+d/631+G*-ba
sis\1,1\P\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\Br,1,PH,2,A2,3,90.,0\Br,1,
PH,2,A2,5,180.,0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.59779521\PH=
2.14461335\CH=1.08632806\CX=0.6757349\A2=124.72374335\HCC=143.15227335\Version
=CrayYMP-Unicos-G92RevC\State=1-A1\HF=-5561.5149056\MP2=-5562.3337585\RMSD=8.97
8e-09\RMSF=4.162e-05\Dipole=0.,0.,1.9375623\PG=C02V [C2(P1),SGV(C2H2),SGV'(Br2)
]\@

(CH)2PBr2+ MP4 SP
1\1\LRZM-YMP\SP\RMP4SDTQ-FC\GEN\C2H2BR2P1(1+)\GOELLER\14-Jun-1995\0\#\ RMP4/GEN
NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2Pbr2(1+) SHASv+d/631+
G*-basis\1,1\P\X,1,1.5977952093\C,2,0.6757348972,1,90.\C,2,0.6757348972,1,90.,
3,180.,0\Br,1,2.1446133533,2,124.72374335,3,90.,0\Br,1,2.1446133533,2,124.72374
335,5,180.,0\H,3,1.0863280581,2,143.15227335,1,180.,0\H,4,1.0863280581,2,143.15
227335,1,180.,0\Version=CrayYMP-Unicos-G92RevC\State=1-A1\HF=-5561.5149056\MP2
=-5562.3337585\MP3=-5562.3442451\MP4D=-5562.3618114\MP4DQ=-5562.3475872\MP4SDQ=
-5562.3555647\MP4SDTQ=-5562.3868321\RMSD=5.795e-09\PG=C02V [C2(P1),SGV(C2H2),SG

V'(Br2)]\\

```
(CH)2PI2+ HF OPT
1\1\FAU-CCC-HP102\FOPT\RHF\GEN\C2H2I2P1(1+)\GOELLER\2-Oct-1994\1\\# RHF/GEN OPT
OPTCY=99 NAME=GOELLER SCF=DIRECT PSEUDO=CARDS\\(CH)2Pi2(1+) c,h,p:6-31G*,i(7ve
-mwb-ecp'93,dzp)\\1,1\P\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\I,1,PH,2,A2,3
,90.,0\I,1,PH,2,A2,5,180.,0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\\PX=1.6
0246285\PH=2.39229423\CH=1.07183024\CX=0.65671666\A2=123.67412911\HCC=144.18262
92\\Version=HP-PARisc-HPUX-G92\DFT-RevF.2\State=1-A1\HF=-439.6511888\RMSD=2.657
e-09\RMSF=7.895e-05\Dipole=0.,0.,1.885709\PG=C02V [C2(P1),SGV(C2H2),SGV'(I2)]\\
@
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```
(CH)2PI2+ HF Freq
FREQ RHF GEN C2H2I2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-439.6511892 ZPE=22.806893
*** (CH)2PI2(1+) C,H,P:6-31G*,I(7VE-MWB-ECP'93,DZP)
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```
(CH)2PI2+ MP2 OPT
1\1\FAU-CCC-DERIOC3\FOPT\RMP2-FC\GEN\C2H2I2P1(1+)\GOELLER\12-Jul-1995\0\\# RMP2
/GEN FOPT OPTCYC=100 NAME=GOELLER SCF=(QC,DIRECT) PSEUDO=CARDS\\(CH)2Pi2(1+) c,
h,p:6-31G*,i(7ve-mwb-ecp'93,dzp)\\1,1\P,0.,0.,0.8584102078\C,0.6711967374,0.,2.
4763433246\C,-0.6711967374,0.,2.4763433246\I,0.,-1.996244482,-0.4605328057\I,0.
,1.996244482,-0.4605328057\H,1.5516641901,0.,3.1121021956\H,-1.5516641901,0.,3.
1121021956\\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-439.6517438\MP2=-44
0.1992309\RMSD=0.000e+00\RMSF=1.787e-04\Dipole=0.,0.,1.8630727\PG=C02V [C2(P1),
SGV(C2H2),SGV'(I2)]\\@
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```
(CH)2PI2+ MP4 SP
1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\GEN\C2H2I2P1(1+)\GOELLER\14-Jul-1995\0\\# RM
P4/GEN SCF=DIRECT PSEUDO=CARDS\\(CH)2Pi2(1+) c,h,p:6-31G*,i(7ve-mwb-ecp'93,dzp)
\\1,1\P\X,1,1.60246285\C,2,0.65671666,1,90.\C,2,0.65671666,1,90.,3,180.,0\I,1,2
.39229423,2,123.67412911,3,90.,0\I,1,2.39229423,2,123.67412911,5,180.,0\H,3,1.0
7183024,2,144.1826292,1,180.,0\H,4,1.07183024,2,144.1826292,1,180.,0\\Version=H
P-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-439.6533462\MP2=-440.1977173\MP3=-440.22
44011\MP4D=-440.2390503\MP4DQ=-440.2250128\MP4SDQ=-440.2308787\MP4SDTQ=-440.255
7402\RMSD=4.759e-09\PG=C02V [C2(P1),SGV(C2H2),SGV'(I2)]\\@
```


.,0\H,3,1.0841865058,2,143.62900805,1,180.,0\H,4,1.0841865058,2,143.62900805,1,180.,0\H,5,1.0943052802,1,109.80462021,2,120.10840687,0\H,5,1.0943052802,1,109.80462021,2,-120.10840687,0\H,6,1.0943052802,1,109.80462021,2,120.10840687,0\H,6,1.0943052802,1,109.80462021,2,-120.10840687,0\H,5,1.0926972992,1,109.33002909,2,0.,0\H,6,1.0926972992,1,109.33002909,2,0.,0\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A1\HF=-496.5610641\MP2=-497.1798809\MP3=-497.2219175\MP4D=-497.2382659\MP4DQ=-497.2247491\MP4SDQ=-497.2309283\MP4SDTQ=-497.2559767\RMSE=1.281e-09\PG=C02V [C2(P1),SGV(C2H2),SGV'(C2H2),X(H4)]\@

(CH)2PH2+ HF OPT
1\0\FAU-ERLG\FOPT\RHF\6-31G(D)\C2H4P1(1+)\SCHLEYER\85/01/06\1\#\ RHF/6-31G* OPT
NAME=SCHLEYER\ (CH)2PH2(1+) CS\1,1\PX,1,1\CX,1,90.\C,2,CX,1,90.,3,180.,
0\H,1,PH,2,A2,3,90.,0\H,1,PH,2,A2,5,180.,0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,
180.,0\PX=1.61213\PH=1.37879\CH=1.07148\CX=0.65243\A2=124.37331\HCC=145.29939
\Version=CYBER-NOS-G82RevH\HF=-418.4400799\RMSE=0.648D-09\RMSF=0.967D-04\PG=C0
2V\

(CH)2PH2+ HF Freq
FREQ RHF 6-31G(D) C2H4P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-418.4400799 ZPE=33.7250866
*** (CH)2PH2(1+) C2V

(CH)2PH2+ MP2 OPT
1\1\FAU-CCC-DERIOC4\FOPT\RMP2-FC\6-31+G(D)\C2H4P1(1+)\GOELLER\18-Apr-1995\1\#\
RMP2/6-31+G* NAME=GOELLER FOPT OPTCYC=99 SCF=DIRECT\ (CH)2PH2(1+) C2v\1,1\PX,
1,1\CX,1,90.\C,2,CX,1,90.,3,180.,0\H,1,PH,2,A2,3,90.,0\H,1,PH,2,A2,5,180.,
0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.63018012\PH=1.39504655\CH=1.
.08395306\CX=0.66327992\A2=123.67865498\HCC=146.03045761\Version=HP-PARisc-HPU
X-G92/DFT-RevG.2\State=1-A1\HF=-418.4391531\MP2=-418.7895609\RMSE=3.042e-09\RMS
F=4.608e-05\Dipole=0.,0.,-0.3100179\PG=C02V [C2(P1),SGV(C2H2),SGV'(H2)]\@

(CH)2PH2+ MP4 SP
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4P1(1+)\GOELLER\7-May-1995\0\#\
RMP4/6-31+G* NAME=GOELLER SCF=DIRECT GEOM=CHECKPOINT GUESS=READ\ (CH)2PH2(1+)
C2v\1,1\PX,1,1.6301801212\C,2,0.6632799167,1,90.\C,2,0.6632799167,1,90.,3,180
.,0\H,1,1.3950465488,2,123.67865498,3,90.,0\H,1,1.3950465488,2,123.67865498,5,1

80.,0\H,3,1.0839530596,2,146.03045761,1,180.,0\H,4,1.0839530596,2,146.03045761,
1,180.,0\\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-418.4391531\MP2=-41
8.7895609\MP3=-418.8141531\MP4D=-418.8246914\MP4DQ=-418.8162196\MP4SDQ=-418.819
9795\MP4SDTQ=-418.8356008\RMSD=4.643e-10\PG=C02V [C2(P1),SGV(C2H2),SGV'(H2)]\\@

(CH2)2PF2+ HF OPT
1\1\LRZM-YMP\FOPT\RHF\6-31G(D)\C2H4F2P1(1+)\CLARK\09-FEB-92\1\\# RHF/6-31G* OPT
NAME=CLARK SCF=DIRECT\\3-Phosphonia-cyclopropane-3,3-difluoride\\1,1\P\X,1,r1\
C,2,r2,1,90.\C,2,r2,1,90.,3,180.,0\H,3,r3,2,a3,1,d3,0\H,3,r3,2,a3,1,-d3,0\H,4,r
3,2,a3,1,d3,0\H,4,r3,2,a3,1,-d3,0\F,1,r4,2,a4,3,90.,0\F,1,r4,2,a4,3,-90.,0\\r1=
1.524116\r2=0.808748\r3=1.078451\r4=1.512281\ a3=116.157066\ a4=126.815358\d3=110
.3811\\Version=Cray-Y-MP/464-UniCOS-G90RevG\State=1-A1\HF=-617.3921909\RMSD=0.6
47E-08\RMSF=0.519E-04\Dipole=0.,0.,1.2944619\PG=C02V [C2(P1),SGV(C2),SGV'(F2),X
(H4)]\\

(CH2)2PF2+ HF Freq
FREQ RHF 6-31G(D) C2H4F2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-617.3921909 ZPE=41.3639419
*** 3-PHOSPHONIA-CYCLOPROPANE-3,3-DIFLUORIDE

(CH2)2PF2+ MP2 OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C2H4F2P1(1+)\GOELLER\27-May-1995\1\\
RMP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT\\3-Phosphonia-cyclopropane-3,3-difl
uoride\\1,1\P\X,1,r1\C,2,r2,1,90.\C,2,r2,1,90.,3,180.,0\H,3,r3,2,a3,1,d3,0\H,3,
r3,2,a3,1,-d3,0\H,4,r3,2,a3,1,d3,0\H,4,r3,2,a3,1,-d3,0\F,1,r4,2,a4,3,90.,0\F,1,
r4,2,a4,3,-90.,0\\r1=1.52917558\r2=0.81525474\r3=1.09048032\r4=1.55022055\ a3=11
6.07305125\ a4=126.33300282\d3=110.31154035\\Version=Convex-Unix-G92/DFT-RevG.2\
State=1-A1\HF=-617.3940284\MP2=-618.1108142\RMSD=7.256e-09\RMSF=2.927e-05\Dipol
e=-0.,-0.,1.3931165\PG=C02V [C2(P1),SGV(C2),SGV'(F2),X(H4)]\\@

(CH2)2PF2+ MP4 SP
1\1\LRZM-YMP\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4F2P1(1+)\GOELLER\23-Jun-1995\0\\# RMP
4/6-31+G* NAME=GOELLER SCF=DIRECT\\3-Phosphonia-cyclopropane-3,3-difluoride //M
P2/6-31+G*\\1,1\P\X,1,1.52917558\C,2,0.81525474,1,90.\C,2,0.81525474,1,90.,3,18
0.,0\H,3,1.09048032,2,116.07305125,1,110.31154035,0\H,3,1.09048032,2,116.073051
25,1,-110.31154035,0\H,4,1.09048032,2,116.07305125,1,110.31154035,0\H,4,1.09048
032,2,116.07305125,1,-110.31154035,0\F,1,1.55022055,2,126.33300282,3,90.,0\F,1,

1.55022055,2,126.33300282,3,-90.,0\\Version=CrayYMP-Unicos-G92RevC\\State=1-A1\\HF=-617.3940284\\MP2=-618.1108142\\MP3=-618.1240477\\MP4D=-618.1392945\\MP4DQ=-618.1299348\\MP4SDQ=-618.141151\\MP4SDTQ=-618.1657184\\RMSD=6.911e-09\\PG=C02V [C2(P1),SGV(C2),SGV'(F2),X(H4)]\\

(CH2)2P(OH)2+ HF OPT
1\\1\\FAU-CCC-HP109\\FOPT\\RHF\\6-31G(D)\\C2H6O2P1(1+)\\GOELLER\\21-Jun-1995\\1\\#RHF/6-31G* NAME=GOELLER SCF=DIRECT FOPT OPTCYC=99\\(Ch2)2P(OH)2+ planar\\1,1\\P\\X,1,PX\\C,2,PC,1,90.\\C,2,PC,1,90.,3,180.,0\\O,1,PCL,2,HPCL,3,D4,0\\O,1,PCL,2,HPCL,4,D4,0\\H,3,HC1,2,HCP1,1,D21,0\\H,3,HC2,2,HCP2,1,-D22,0\\H,4,HC2,2,HCP2,1,-D22,0\\H,4,HC1,2,HCP1,1,D21,0\\H,5,HO,1,HON,2,D3,0\\H,6,HO,1,HON,2,D3,0\\PX=1.54635136\\PC=0.79716749\\PCL=1.55532396\\HPCL=123.35380629\\HC1=1.07696339\\HC2=1.07702549\\HO=0.95748866\\HCP1=115.95340911\\HCP2=116.31948587\\HON=119.97160636\\D21=110.58617324\\D22=110.07210669\\D3=116.95421347\\D4=84.38282272\\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\\State=1-A\\HF=-569.4205854\\RMSD=5.262e-09\\RMSF=6.142e-05\\Dipole=0.,0.,-0.2416797\\PG=C02 [C2(P1),X(C2H6O2)]\\@

(CH2)2P(OH)2+ HF Freq
FREQ RHF 6-31G(D) C2H6O2P1(1+) PG=C02 DIP=0.000000 NIMAG=0
STATE=1-A HF=-569.4205854 ZPE=56.9167919
*** (CH2)2P(OH)2+ PLANAR

(CH2)2P(OH)2+ MP2 OPT
1\\1\\FAU-CCC-DERIOC1\\FOPT\\RMP2-FC\\6-31+G(D)\\C2H6O2P1(1+)\\GOELLER\\03-Jul-1995\\0\\#RMP2/6-31+G* NAME=GOELLER SCF=DIRECT FOPT\\(Ch2)2P(OH)2+ lower energy C2 form//HF/6-31G*\\1,1\\P,0.,0.,-0.1998709107\\C,0.8008475,-0.0070340174,1.354690338\\C,-0.8008475,0.0070340174,1.354690338\\O,0.1522674119,-1.3329627804,-1.0479838029\\O,-0.1522674119,1.3329627804,-1.0479838029\\H,1.2825639071,0.9078453914,1.6948766169\\H,1.2768889522,-0.9281606548,1.6866081923\\H,-1.2768889522,0.9281606548,1.6866081923\\H,-1.2825639071,-0.9078453914,1.6948766169\\H,-0.59655748,-1.6001298579,-1.626724584\\H,0.59655748,1.6001298579,-1.626724584\\Version=Convex-Unix-G94RevB.1\\State=1-A\\HF=-569.4216376\\MP2=-570.1521447\\RMSD=3.528e-09\\RMSF=2.651e-05\\Dipole=0.,0.,-0.1558952\\PG=C02 [C2(P1),X(C2H6O2)]\\@

(CH2)2P(OH)2+ MP4 SP
1\\1\\FAU-CCC-DERIOC3\\SP\\RMP4SDTQ-FC\\6-31+G(D)\\C2H6O2P1(1+)\\GOELLER\\7-Jul-1995\\0\\#RMP4/6-31+G* SCF=DIRECT GEOM=CHECKPOINT GUESS=READ\\(Ch2)2P(OH)2+ lower energy

y C2 form //MP2/6-31+G*\1,1\P,0.,0.,-0.1998709107\C,0.8008475,-0.0070340174,1.354690338\C,-0.8008475,0.0070340174,1.354690338\O,0.1522674119,-1.3329627804,-1.0479838029\O,-0.1522674119,1.3329627804,-1.0479838029\H,1.2825639071,0.9078453914,1.6948766169\H,1.2768889522,-0.9281606548,1.6866081923\H,-1.2768889522,0.9281606548,1.6866081923\H,-1.2825639071,-0.9078453914,1.6948766169\H,-0.59655748,-1.6001298579,-1.626724584\H,0.59655748,1.6001298579,-1.626724584\\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A\HF=-569.4216376\MP2=-570.1521447\MP3=-570.1748056\MP4D=-570.1910859\MP4DQ=-570.179771\MP4SDQ=-570.1879276\MP4SDTQ=-570.2116351\RMSD=6.926e-10\PG=C02 [C2(P1),X(C2H6O2)]\@

(CH2)2PCl2+ HF OPT
1\1\FAU-CCC-HP101\FOPT\RHf\6-31G(D)\C2H4CL2P1(1+)\GOELLER\30-Sep-1994\1\#\RHf/6-31G* OPTCYC=99 OPT NAME=GOELLER SCF=DIRECT\PHOSPHIRANE, (Ch2)2Pcl+\1,1\P\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\C1,1,PCL,2,HPCL,3,90.,0\C1,1,PCL,2,HPCL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\PX=1.58636125\PC=0.78111405\PCL=1.95828705\HPCL=123.83842656\HC=1.07752672\HCP=117.12967119\D2=108.92702824\\Version=HP-PARisc-HPUX-G92/DFT-RevF.2\State=1-A1\HF=-1337.4719986\RMSD=3.056e-09\RMSF=6.118e-05\Dipole=0.,0.,1.3345016\PG=C02V [C2(P1),SGV(C2),SGV'(C12),X(H4)]\@

(CH2)2PCl2+ HF Freq
FREQ RHf 6-31G(D) C2H4CL2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-1337.4719987 ZPE=39.8176724
*** PHOSPHIRANE, (CH2)2PCL+

(CH2)2PCl2+ MP2 OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C2H4CL2P1(1+)\GOELLER\22-Jun-1995\1\#\RMP2/6-31+G* OPTCYC=99 OPT NAME=GOELLER SCF=DIRECT\PHOSPHIRANE, (Ch2)2Pcl+//6-31G*\1,1\P\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\C1,1,PCL,2,HPCL,3,90.,0\C1,1,PCL,2,HPCL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\PX=1.58536123\PC=0.78660068\PCL=1.96229863\HPCL=123.40933135\HC=1.08974752\HCP=117.0084519\D2=109.07005156\\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-1337.4742216\MP2=-1338.1020152\RMSD=7.570e-09\RMSF=4.413e-05\Dipole=-0.,0.,1.2149031\PG=C02V [C2(P1),SGV(C2),SGV'(C12),X(H4)]\@

(CH2)2PCl2+ MP4 SP
1\1\FAU-CCC-DERIOC2\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4CL2P1(1+)\GOELLER\27-Jul-1995\

0\\#RMP4/6-31+G* SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\PHOSPHIRANE, (Ch2)2Pc1+/
 /6-31G*\\1,1\\P\\X,1,1.5853612299\\C,2,0.7866006799,1,90.\\C,2,0.7866006799,1,90.,3
 ,180.,0\\C1,1,1.962298634,2,123.40933135,3,90.,0\\C1,1,1.962298634,2,123.40933135
 ,3,-90.,0\\H,3,1.0897475247,2,117.0084519,1,109.07005156,0\\H,3,1.0897475247,2,11
 7.0084519,1,-109.07005156,0\\H,4,1.0897475247,2,117.0084519,1,-109.07005156,0\\H,
 4,1.0897475247,2,117.0084519,1,109.07005156,0\\Version=HP-PARisc-HPUX-G94RevB.1
 \\State=1-A1\\HF=-1337.4742216\\MP2=-1338.1020152\\MP3=-1338.1460049\\MP4D=-1338.160
 7723\\MP4DQ=-1338.1474171\\MP4SDQ=-1338.1529296\\MP4SDTQ=-1338.1759167\\RMSD=1.328e
 -09\\PG=C02V [C2(P1),SGV(C2),SGV'(C12),X(H4)]\\@

(CH2)2P(NH)2+ HF OPT
 1\\1\\FAU-CCC-HP110\\FOPT\\RHF\\6-31G(D)\\C2H8N2P1(1+)\\GOELLER\\19-Apr-1995\\1\\#RHF/6-
 31G* FOPT OPTCYC=99 NAME=GOELLER SCF=DIRECT\\(Ch2)2P(NH2)2+\\1,1\\P\\X,1,PX\\C,2,P
 C,1,90.\\C,2,PC,1,90.,3,180.,0\\N,1,Pn,2,HPCL,3,90.,0\\N,1,Pn,2,HPCL,3,-90.,0\\H,3,
 HC,2,HCP,1,D2,0\\H,3,HC,2,HCP,1,-D2,0\\H,4,HC,2,HCP,1,-D2,0\\H,4,HC,2,HCP,1,D2,0\\H
 ,5,hn,2,hcn,1,hcnx,0\\H,5,hn,2,hcn,1,-hcnx,0\\H,6,hn,2,hcn,1,hcnx,0\\H,6,hn,2,hcn,
 1,-hcnx,0\\PX=1.59129779\\PC=0.77559741\\Pn=1.63146962\\hn=1.00097444\\HPCL=118.758
 40609\\hcn=122.66742353\\HC=1.07548587\\HCP=116.60895752\\D2=109.21935746\\hcnx=95.1
 8250297\\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\\State=1-A1\\HF=-529.7696339\\RMSD=
 2.148e-09\\RMSF=1.922e-05\\Dipole=0.,0.,-0.7724829\\PG=C02V [C2(P1),SGV(C2),SGV'(N
 2),X(H8)]\\@

(CH2)2P(NH)2+ HF Freq
 FREQ RHF 6-31G(D) C2H8N2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
 STATE=1-A1 HF=-529.7696339 ZPE=73.5159952
 *** (CH2)2P(NH2)2+

(CH2)2P(NH)2+ MP2 OPT
 1\\1\\FAU-CCC-DERIOC1\\FOPT\\RMP2-FC\\6-31+G(D)\\C2H8N2P1(1+)\\GOELLER\\15-Jun-1995\\1\\
 #RMP2/6-31+G* FOPT OPTCYC=99 NAME=GOELLER SCF=DIRECT\\(Ch2)2P(NH2)2+ //6-31G*\\
 1,1\\P\\X,1,PX\\C,2,PC,1,90.\\C,2,PC,1,90.,3,180.,0\\N,1,Pn,2,HPCL,3,90.,0\\N,1,Pn,2,
 HPCL,3,-90.,0\\H,3,HC,2,HCP,1,D2,0\\H,3,HC,2,HCP,1,-D2,0\\H,4,HC,2,HCP,1,-D2,0\\H,4
 ,HC,2,HCP,1,D2,0\\H,5,hn,2,hcn,1,hcnx,0\\H,5,hn,2,hcn,1,-hcnx,0\\H,6,hn,2,hcn,1,hc
 nx,0\\H,6,hn,2,hcn,1,-hcnx,0\\PX=1.60382487\\PC=0.77547076\\Pn=1.64847873\\hn=1.018
 51949\\HPCL=117.06021224\\hcn=123.27586194\\HC=1.0870572\\HCP=116.72335399\\D2=108.6
 6950625\\hcnx=92.94442523\\Version=Convex-Unix-G92/DFT-RevG.2\\State=1-A1\\HF=-529
 .7711846\\MP2=-530.4705409\\RMSD=4.971e-09\\RMSF=9.873e-05\\Dipole=-0.,0.,-0.764359

1\PG=C02V [C2(P1),SGV(C2),SGV'(N2),X(H8)]\@

(CH2)2P(NH)2+ MP4 SP

1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\6-31+G(D)\C2H8N2P1(1+)\GOELLER\20-Jul-1995\0
\\#RMP4/6-31+G* SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\(Ch2)2P(NH2)2+ //MP2/6-3
1+G*\\1,1\P\X,1,1.6038248653\C,2,0.7754707619,1,90.\C,2,0.7754707619,1,90.,3,18
0.,0\N,1,1.6484787327,2,117.06021224,3,90.,0\N,1,1.6484787327,2,117.06021224,3,
-90.,0\H,3,1.0870572022,2,116.72335399,1,108.66950625,0\H,3,1.0870572022,2,116.
72335399,1,-108.66950625,0\H,4,1.0870572022,2,116.72335399,1,-108.66950625,0\H,
4,1.0870572022,2,116.72335399,1,108.66950625,0\H,5,1.0185194916,2,123.27586194,
1,92.94442523,0\H,5,1.0185194916,2,123.27586194,1,-92.94442523,0\H,6,1.01851949
16,2,123.27586194,1,92.94442523,0\H,6,1.0185194916,2,123.27586194,1,-92.9444252
3,0\\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-529.7711846\MP2=-530.47054
09\MP3=-530.5075888\MP4D=-530.5237961\MP4DQ=-530.5112957\MP4SDQ=-530.5174247\MP
4SDTQ=-530.5405411\RMDS=1.143e-09\PG=C02V [C2(P1),SGV(C2),SGV'(N2),X(H8)]\@

(CH2)2PBr2+ HF OPT

1\1\FAU-CCC-HP106\FOPT\RHF\GEN\C2H4BR2P1(1+)\GOELLER\12-Dec-1994\1\\#RHF/GEN OP
TCYC=99 FOPT NAME=GOELLER SCF=DIRECT\\PHOSPHIRANE, (Ch2)2Pbr+ SHASv+d\\1,1\P\X,1
,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\Br,1,PCL,2,HPCL,3,90.,0\Br,1,PCL,2,HPCL,
3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2
,HCP,1,D2,0\\PX=1.62088185\PC=0.77224827\PCL=2.14668994\HPCL=123.11856891\HC=1.
08944885\HCP=117.75831277\D2=108.05177343\\Version=HP-PARisc-HPUX-G92/DFT-RevF.
2\State=1-A1\HF=-5562.5482322\RMDS=5.178e-09\RMSF=2.082e-05\PG=C02V [C2(P1),SGV
(C2),SGV'(Br2),X(H4)]\@

(CH2)2PBr2+ HF Freq

FREQ RHF GEN C2H4BR2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-5562.5482322 ZPE=38.2032622
*** PHOSPHIRANE, (CH2)2PBR+ SHASV+D

(CH2)2PBr2+ MP2 OPT

1\1\FAU-CCC-DERIOC4\FOPT\RMP2-FC\GEN\C2H4BR2P1(1+)\GOELLER\24-Jun-1995\1\\#RMP2
/GEN OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\\PHOSPHIRANE, (Ch2)2Pbr+ SHASv+d//6-
31G*\\1,1\P\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\Br,1,PCL,2,HPCL,3,90.,0\B
r,1,PCL,2,HPCL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1
, -D2,0\H,4,HC,2,HCP,1,D2,0\\PX=1.60481744\PC=0.779974\PCL=2.13847752\HPCL=122.5

592869\HC=1.08982897\HCP=117.27232925\D2=108.58365906\\Version=HP-PARisc-HPUX-G
92/DFT-RevG.2\State=1-A1\HF=-5562.7216148\MP2=-5563.5517121\RMSE=6.137e-09\RMSE
=2.514e-05\Dipole=0.,0.,1.6648025\PG=C02V [C2(P1),SGV(C2),SGV'(Br2),X(H4)]\\@

(CH2)2PBr2+ MP4 SP
1\1\FAU-CCC-DERIOC2\SP\RMP4SDTQ-FC\GEN\C2H4BR2P1(1+)\GOELLER\28-Jun-1995\0\\#RM
P4/GEN NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\PHOSPHIRANE, (Ch2)2Pb
r+ SHASv+d//MP2/6-31+G*\\1,1\PX,1,1.6048174444\C,2,0.7799740011,1,90.\C,2,0.77
99740011,1,90.,3,180.,0\Br,1,2.1384775211,2,122.5592869,3,90.,0\Br,1,2.13847752
11,2,122.5592869,3,-90.,0\H,3,1.089828969,2,117.27232925,1,108.58365906,0\H,3,1
.089828969,2,117.27232925,1,-108.58365906,0\H,4,1.089828969,2,117.27232925,1,-1
08.58365906,0\H,4,1.089828969,2,117.27232925,1,108.58365906,0\\Version=HP-PARisc-
HPUX-G92/DFT-RevG.2\State=1-A1\HF=-5562.7216148\MP2=-5563.5517121\MP3=-5563.5
704654\MP4D=-5563.5882159\MP4DQ=-5563.5755774\MP4SDQ=-5563.5830315\MP4SDTQ=-556
3.6107505\RMSE=5.574e-10\PG=C02V [C2(P1),SGV(C2),SGV'(Br2),X(H4)]\\@

(CH2)2PI2+ HF OPT
1\1\FAU-CCC-DERIOC4\FOPT\RHF\GEN\C2H4I2P1(1+)\GOELLER\17-Nov-1994\1\\#RHF/GEN F
OPT OPTCYC=99 NAME=GOELLER SCF=DIRECT PSEUDO=CARDS\\PHOSPHIRANE, (Ch2)2PI+ c,h,p
:6-31G*,i(7ve-mwb-ecp'93,dzp)\\1,1\PX,1,PC,1,90.\C,2,PC,1,90.,3,180.,0\
I,1,PCL,2,HPCL,3,90.,0\I,1,PCL,2,HPCL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP
,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\\PX=1.63180287\PC=0.76447062\
PCL=2.38310851\HPCL=121.7473222\HC=1.07656162\HCP=117.72314866\D2=108.08089655\
\Version=HP-PARisc-HPUX-G92/DFT-RevF.2\State=1-A1\HF=-440.8593058\RMSE=5.716e-0
9\RMSE=1.381e-04\Dipole=0.,0.,1.6542895\PG=C02V [C2(P1),SGV(C2),SGV'(I2),X(H4)]
\\@

(CH2)2PI2+ HF Freq
FREQ RHF GEN C2H4I2P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-440.8593064 ZPE=38.7347648
*** PHOSPHIRANE, (CH2)2PI+ C,H,P:6-31G*,I(7VE-MWB-ECP'93,DZP)

(CH2)2PI2+ MP2 OPT
1\1\FAU-CCC-DERIOC4\FOPT\RMP2-FC\GEN\C2H4I2P1(1+)\GOELLER\19-Jul-1995\0\\#RMP2/
GEN FOPT OPTCYC=99 NAME=GOELLER SCF=DIRECT PSEUDO=READ\\PHOSPHIRANE, (Ch2)2PI+ c
,h,p:6-31G*,i(7ve-mwb-ecp'93,dzp) //6-31G*\\1,1\P,0.,0.,0.7632788455\C,0.770938
7092,0.,2.3927215015\C,-0.7709387092,0.,2.3927215015\I,0.,-2.0330259432,-0.4805

273639\I,0.,2.0330259432,-0.4805273639\H,1.2756964784,0.9173477883,2.693514967\H,1.2756964784,-0.9173477883,2.693514967\H,-1.2756964784,0.9173477883,2.693514967\H,-1.2756964784,-0.9173477883,2.693514967\\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-440.8608142\MP2=-441.4189794\RMSD=2.244e-09\RMSF=1.578e-04\Dipole=0.,0.,1.5968782\PG=C02V [C2(P1),SGV(C2),SGV'(I2),X(H4)]\\@

(CH2)2PI2+ MP4 SP
1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\GEN\C2H4I2P1(1+)\GOELLER\19-Jul-1995\0\#\RMP4/GEN NAME=GOELLER SCF=DIRECT PSEUDO=READ GUESS=READ GEOM=CHECKPOINT\PHOSPHIRANE,(Ch2)2PI+ c,h,p://MP2/6-31+G*,i(7ve-mwb-ecp'93,dzp)\\1,1\PC,0.,0.,0.7632788455\C,0.7709387092,0.,2.3927215015\C,-0.7709387092,0.,2.3927215015\I,0.,-2.0330259432,-0.4805273639\I,0.,2.0330259432,-0.4805273639\H,1.2756964784,0.9173477883,2.693514967\H,1.2756964784,-0.9173477883,2.693514967\H,-1.2756964784,0.9173477883,2.693514967\H,-1.2756964784,-0.9173477883,2.693514967\\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-440.8608142\MP2=-441.4189794\MP3=-441.4532272\MP4D=-441.4683352\MP4DQ=-441.4556924\MP4SDQ=-441.461236\MP4SDTQ=-441.4832571\RMSD=3.358e-10\PG=C02V [C2(P1),SGV(C2),SGV'(I2),X(H4)]\\@

(CH2)2P(CH3)2+ HF OPT
1\1\FAU-CCC-HP110\FOPT\RHF\6-31G(D)\C4H10P1(1+)\GOELLER\18-Apr-1995\1\#\RHF/6-31G* OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\\1,1-Dimethyl-PHOSPHIRANE,(Ch2)2P(CH3)2+\\1,1\PC,0.,0.,0.7632788455\C,0.7709387092,0.,2.3927215015\C,-0.7709387092,0.,2.3927215015\I,0.,-2.0330259432,-0.4805273639\I,0.,2.0330259432,-0.4805273639\H,1.2756964784,0.9173477883,2.693514967\H,1.2756964784,-0.9173477883,2.693514967\H,-1.2756964784,0.9173477883,2.693514967\H,-1.2756964784,-0.9173477883,2.693514967\\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A1\HF=-497.7699562\RMSD=4.415e-09\RMSF=2.674e-05\Dipole=0.,0.,-0.2049823\PG=C02V [C2(P1),SGV(C2H2),SGV'(C2),X(H8)]\\@

(CH2)2P(CH3)2+ HF Freq
FREQ RHF 6-31G(D) C4H10P1(1+) PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-497.7699562 ZPE=88.2094309
*** 1,1-DIMETHYL-PHOSPHIRANE, (CH2)2P(CH3)2+

(CH2)2P(CH3)2+ MP2 OPT

1\1\FAU-CCC-DERIOC3\FOPT\RMP2-FC\6-31+G(D)\C4H10P1(1+)\GOELLER\7-Jun-1995\1\1\#RMP2/6-31+G* OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\1,1-Dimethyl-PHOSPHIRANE, (Ch2)2P(CH3)2+//6-31G*\1,1\X,P,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\C,1,PC2,2,HPC,3,90.,0\C,1,PC2,2,HPC,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\H,5,HC2,1,HCP2,2,0.,0\H,6,HC2,1,HCP2,2,0.,0\H,5,HC3,1,HCP3,2,D3,0\H,5,HC3,1,HCP3,2,-D3,0\H,6,HC3,1,HCP3,2,D3,0\H,6,HC3,1,HCP3,2,-D3,0\X=1.62172268\PC=0.76890798\PC2=1.80327721\HPC=121.98056592\HC=1.08809894\HC2=1.09341525\HC3=1.09352572\HCP=117.43663888\HCP2=109.04274336\HCP3=109.95297479\D2=108.89379593\D3=119.67492605\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A1\HF=-497.7702316\MP2=-498.4004331\RMSE=8.408e-09\RMSEF=4.204e-05\Dipole=0.,0.,-0.2131681\PG=C02V [C2(P1),SGV(C2H2),SGV'(C2),X(H8)]\@

(CH2)2P(CH3)2+ MP4 SP

1\1\LRZM-YMP\SP\RMP4SDTQ-FC\6-31+G(D)\C4H10P1(1+)\GOELLER\23-Jun-1995\0\1\#RMP4/6-31+G* NAME=GOELLER SCF=DIRECT\1,1-Dimethyl-PHOSPHIRANE, (Ch2)2P(CH3)2+//MP2/6-31+G*\1,1\X,P,1,1.62172268\C,2,0.76890798,1,90.\C,2,0.76890798,1,90.,3,180.,0\C,1,1.80327721,2,121.98056592,3,90.,0\C,1,1.80327721,2,121.98056592,3,-90.,0\H,3,1.08809894,2,117.43663888,1,108.89379593,0\H,3,1.08809894,2,117.43663888,1,-108.89379593,0\H,4,1.08809894,2,117.43663888,1,-108.89379593,0\H,4,1.08809894,2,117.43663888,1,108.89379593,0\H,5,1.09341525,1,109.04274336,2,0.,0\H,6,1.09341525,1,109.04274336,2,0.,0\H,5,1.09352572,1,109.95297479,2,119.67492605,0\H,5,1.09352572,1,109.95297479,2,-119.67492605,0\H,6,1.09352572,1,109.95297479,2,119.67492605,0\H,6,1.09352572,1,109.95297479,2,-119.67492605,0\Version=CrayYMP-Unicos-G92RevC\State=1-A1\HF=-497.7702316\MP2=-498.4004331\MP3=-498.4503408\MP4D=-498.4667475\MP4DQ=-498.4546725\MP4SDQ=-498.460265\MP4SDTQ=-498.4820634\RMSE=4.868e-09\PG=C02V [C2(P1),SGV(C2H2),SGV'(C2),X(H8)]\@

(CH2)2PH2+ HF OPT

1\0\FAU ERLG\FOPT\RFH\6-31G*\C2H6P1(1+)\STOUT\86/05/23\1\1\# RFH/6-31G* OPT\PROTONATED PHOSPHIRANE\1,1\X,P,1,PX\C,1,CX,2,90.\C,1,CX,2,90.,3,180.,0\H,2,PH,1,A1,3,90.,0\H,2,PH,1,A1,3,-90.,0\H,3,CH,2,A2,1,D,0\H,3,CH,2,A2,1,-D,0\H,4,CH,2,A2,1,D,0\H,4,CH,2,A2,1,-D,0\X=1.63573\CX=.75834\PH=1.37669\CH=1.07659\A1=122.82393\A2=116.07499\D=110.3897\Version=CYBER-NOS-G82RevH\HF=-419.6508216\RMSE=.601E-07\RMSEF=.922E-04\PG=C02V\@

(CH2)2PH2+ HF Freq
FREQ RFH 6-31G(D)

C2H6P1(1+) PG=C02V[C2(P1),SGV(C2),SGV'(H2),

X(H4)] DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-419.6508216 ZPE=49.4436471

(CH2)2PH2+ MP2 OPT
1\1\FAU-CCC-DERIOC3\FOPT\RMP2-FC\6-31+G(D)\C2H6P1(1+)\GOELLER\1-Jun-1995\1\#\ R
MP2/6-31+G* FOPT SCF=DIRECT NAME=GOELLER\PROTONATED PHOSPHIRANE\1,1\X\P,1,PX\
C,1,CX,2,90.\C,1,CX,2,90.,3,180.,0\H,2,PH,1,A1,3,90.,0\H,2,PH,1,A1,3,-90.,0\H,3
,CH,2,A2,1,D,0\H,3,CH,2,A2,1,-D,0\H,4,CH,2,A2,1,D,0\H,4,CH,2,A2,1,-D,0\PX=1.63
748097\CX=0.7603382\PH=1.39194612\CH=1.08802109\A1=122.31018318\A2=115.88016388
\D=110.5081607\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A1\HF=-419.650920
1\MP2=-420.0126552\RMSD=1.781e-09\RMSF=1.181e-05\Dipole=0.,0.,0.4802663\PG=C02V
[C2(P1),SGV(C2),SGV'(H2),X(H4)]\@

(CH2)2PH2+ MP4 SP
1\1\LRZM-YMP\SP\RMP4SDTQ-FC\6-31+G(D)\C2H6P1(1+)\GOELLER\3-Jun-1995\0\#\ RMP4/6
-31+G* SCF=DIRECT NAME=GOELLER\PROTONATED PHOSPHIRANE//MP2/6-31+G*\1,1\X\P,1,
1.63748097\C,1,0.7603382,2,90.\C,1,0.7603382,2,90.,3,180.,0\H,2,1.39194612,1,12
2.31018318,3,90.,0\H,2,1.39194612,1,122.31018318,3,-90.,0\H,3,1.08802109,2,115.
88016388,1,110.5081607,0\H,3,1.08802109,2,115.88016388,1,-110.5081607,0\H,4,1.0
8802109,2,115.88016388,1,110.5081607,0\H,4,1.08802109,2,115.88016388,1,-110.508
1607,0\Version=CrayYMP-Unicos-G92RevC\State=1-A1\HF=-419.6509201\MP2=-420.0126
552\MP3=-420.0449747\MP4D=-420.0556567\MP4DQ=-420.0485229\MP4SDQ=-420.0517017\M
P4SDTQ=-420.0641959\RMSD=9.291e-09\PG=C02V [C2(P1),SGV(C2),SGV'(H2),X(H4)]\@

(CH)2SiF2+ HF OPT
1\1\RRZE-ERYMPEL\FOPT\RHF\6-31G(D)\C2H2F2SI1\GOELLER\27-Sep-1994\1\#\ RHF/6-31G
* OPT NAME=GOELLER SCF=DIRECT\ (CH)2sif2(1+)\0,1\Si\X,1,PX\C,2,CX,1,90.\C,2,CX
,1,90.,3,180.,0\F,1,PH,2,A2,3,90.,0\F,1,PH,2,A2,5,180.,0\H,3,CH,2,HCC,1,180.,0\
H,4,CH,2,HCC,1,180.,0\PX=1.61910307\PH=1.57744019\CH=1.07413591\CX=0.67630462\
A2=128.3723679\HCC=132.59783381\Version=CrayYMP-Unicos-G92RevC\State=1-A1\HF=-
564.7519513\RMSD=8.322e-09\RMSF=1.821e-05\Dipole=0.,0.,0.8458295\PG=C02V [C2(Si
1),SGV(C2H2),SGV'(F2)]\@

(CH)2SiF2+ HF Freq
FREQ RHF 6-31G(D) C2H2F2SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-564.7519513 ZPE=25.2380196

*** (CH)2SIF2(1+)

(CH)2SiF2+ MP2 OPT
1\1\FAU-CCC-DERIOC4\FOPT\RMP2-FC\6-31+G(D)\C2H2F2SI1\GOELLER\18-Apr-1995\1\#\ R
MP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2sif2(1+)\0,1\Si\X,1,P
X\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\F,1,PH,2,A2,3,90.,0\F,1,PH,2,A2,5,180.,0\H
,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.63180294\PH=1.61506702\CH=1.08
647378\CX=0.68991012\A2=128.16498726\HCC=132.51917993\Version=HP-PARisc-HPUX-G
92/DFT-RevG.2\State=1-A1\HF=-564.7602063\MP2=-565.4472779\RMSD=5.408e-09\RMSF=2
.186e-05\Dipole=0.,0.,0.9676417\PG=C02V [C2(Si1),SGV(C2H2),SGV'(F2)]\@

(CH)2SiF2+ MP4 SP
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H2F2SI1\GOELLER\13-May-1995\0\#\ R
RMP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2sif2(1+)\
\0,1\Si\X,1,1.631802935\C,2,0.6899101177,1,90.\C,2,0.6899101177,1,90.,3,180.,0
\F,1,1.6150670159,2,128.16498726,3,90.,0\F,1,1.6150670159,2,128.16498726,5,180.
,0\H,3,1.0864737772,2,132.51917993,1,180.,0\H,4,1.0864737772,2,132.51917993,1,1
80.,0\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-564.7602063\MP2=-565.4
472779\MP3=-565.453223\MP4D=-565.4671003\MP4DQ=-565.4580911\MP4SDQ=-565.4685037
\MP4SDTQ=-565.4930741\RMSD=6.512e-10\PG=C02V [C2(Si1),SGV(C2H2),SGV'(F2)]\@

(CH)2Si(OH)2+ HF OPT
1\1\FAU-CCC-HP110\FOPT\RHF\6-31G(D)\C2H4O2SI1\GOELLER\03-May-1996\1\#\ RHF/6-31
G* FOPT=Z-MATRIX NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2Si(OH)2 1 H to ring\0
,1\Si\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\O,1,Pn1,2,A21,3,90.,0\O,1,Pn2,2
,A22,3,-90.,0\H,3,CH,2,HCC,1,hcxn,0\H,4,CH,2,HCC,1,-hcxn,0\H,5,nh21,1,hnp21,2,1
80.,0\H,6,nh22,1,hnp22,2,0.,0\PX=1.63580641\Pn1=1.62844491\Pn2=1.63900507\CH=1
.07579412\CX=0.67554407\nh21=0.9474249\nh22=0.94657194\A21=127.78438245\A22=128
.89506531\HCC=131.89608894\hnp21=116.18730501\hnp22=117.45901682\hcxn=181.66360
128\Version=HP-PARisc-HPUX-G94RevC.3\State=1-A'\HF=-516.7222715\RMSD=4.517e-09
\RMSF=1.223e-04\Dipole=0.,0.7371302,0.1045476\PG=CS [SG(H2O2Si1),X(C2H2)]\@

(CH)2Si(OH)2+ HF Freq
FREQ RHF 6-31G(D) C2H4O2SI1 PG=CS DIP=0.000000 NIMAG=0
STATE=1-A' HF=-516.7222715
*** (CH)2SI(OH)2 1 H TO RING

(CH)2Si(OH)2+ MP2 OPT

1\1\FAU-CCC-DERIOC3\FOPT\RMP2-FC\6-31+G(D)\C2H4O2SI1\GOELLER\14-May-1996\0\#\# R
MP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99 GUESS=READ GEOM=CHECK\((CH)2
Si(OH)2 1 H to ring //HF/6-31G*\0,1\Si,0.0149451693,0.1199951407,0.\C,0.014945
1693,-1.5274662941,0.6891955222\C,0.0149451693,-1.5274662941,-0.6891955222\O,1.
3386710264,1.1190425254,0.\O,-1.2702067588,1.1889175766,0.\H,0.0467635944,-2.33
75158676,1.4153435337\H,0.0467635944,-2.3375158676,-1.4153435337\H,1.1278254417
,2.0691764412,0.\H,-2.1576411733,0.7918380385,0.\Version=HP-PARisc-HPUX-G94Rev
C.3\State=1-A'\HF=-516.7290626\MP2=-517.4312772\RMSD=4.710e-09\RMSF=1.047e-04\D
ipole=0.,0.7399234,0.2065869\PG=CS [SG(H2O2Si1),X(C2H2)]\@

(CH)2Si(OH)2+ MP4 SP

1\1\FAU-CCC-DERIOC2\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4O2SI1\GOELLER\16-May-1996\0\#\#
RMP4/6-31+G* NAME=GOELLER GUESS=READ GEOM=CHECK\((CH)2Si(OH)2 1 H to ring //MP
2/6-31+G*\0,1\Si,0.0147780217,0.1200781957,0.\C,0.0147780217,-1.5273968043,0.6
89279\C,0.0147780217,-1.5273968043,-0.689279\O,1.3393410217,1.1181191957,0.\O,-
1.2701249783,1.1895421957,0.\H,0.0447180217,-2.3374038043,1.415527\H,0.04471802
17,-2.3374038043,-1.415527\H,1.1302310217,2.0686211957,0.\H,-2.1576239783,0.792
5621957,0.\Version=HP-PARisc-HPUX-G94RevC.3\State=1-A'\HF=-516.7290433\MP2=-51
7.4312764\MP3=-517.4460866\MP4D=-517.4613936\MP4DQ=-517.4503277\MP4SDQ=-517.458
2971\MP4SDTQ=-517.4824323\RMSD=2.894e-09\PG=CS [SG(H2O2Si1),X(C2H2)]\@

(CH)2SiCl2+ HF OPT

1\1\RRZE-ERYMPEL\FOPT\RHF\6-31G(D)\C2H2CL2SI1\GOELLER\8-Sep-1994\1\#\# RHF/6-31G
* FOPT NAME=GOELLER SCF=DIRECT PUNCH=(COORD,MO)\(CH)2SiCl2(1) CS\0,1\Si\X,1,P
X\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\Cl,1,PH,2,A2,3,90.,0\Cl,1,PH,2,A2,5,180.,0
\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.63438502\PH=2.04513249\CH=1.
0736752\CX=0.6715324\A2=126.69752774\HCC=134.16496189\Version=CrayYMP-Unicos-G
92RevC\State=1-A1\HF=-1284.811574\RMSD=3.933e-09\RMSF=2.017e-05\Dipole=0.,0.,0.
9764919\PG=C02V [C2(Si1),SGV(C2H2),SGV'(Cl2)]\@

(CH)2SiCl2+ HF Freq

FREQ RHF 6-31G(D) C2H2CL2SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-1284.811574 ZPE=23.5087146
*** (CH)2SiCl2(1) CS

(CH)2SiCl2+ MP2 OPT
 1\1\FAU-CCC-DERIOC4\FOPT\RMP2-FC\6-31+G(D)\C2H2CL2SI1\GOELLER\20-Apr-1995\1\#\
 RMP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\(\CH)2SiCl2(1)\0,1\Si\X,1,
 PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\C1,1,PH,2,A2,3,90.,0\C1,1,PH,2,A2,5,180.,
 0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.64914078\PH=2.04071839\CH=1
 .08671459\CX=0.68420871\A2=126.13412561\HCC=134.10166444\Version=HP-PARisc-HPU
 X-G92/DFT-RevG.2\State=1-A1\HF=-1284.8132293\MP2=-1285.4047321\RMSD=5.852e-09\R
 MSF=2.885e-05\Dipole=0.,0.,0.821062\PG=C02V [C2(Si1),SGV(C2H2),SGV'(C12)]\@

(CH)2SiCl2+ MP4 SP
 1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H2CL2SI1\GOELLER\15-May-1995\0\#\
 # RMP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\(\CH)2SiCl2(1
)\0,1\Si\X,1,1.6491407806\C,2,0.6842087075,1,90.\C,2,0.6842087075,1,90.,3,180.
 ,0\C1,1,2.0407183854,2,126.13412561,3,90.,0\C1,1,2.0407183854,2,126.13412561,5,
 180.,0\H,3,1.0867145909,2,134.10166444,1,180.,0\H,4,1.0867145909,2,134.10166444
 ,1,180.,0\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-1284.8132293\MP2=-
 1285.4047321\MP3=-1285.4416347\MP4D=-1285.4546007\MP4DQ=-1285.4415084\MP4SDQ=-1
 285.446646\MP4SDTQ=-1285.4695159\RMSD=1.796e-09\PG=C02V [C2(Si1),SGV(C2H2),SGV'
 (C12)]\@

(CH)2Si(NH2)2+ HF OPT
 1\1\FAU-CCC-DERIOC3\FOPT\RHF\6-31G(D)\C2H6N2SI1\GOELLER\3-Apr-1995\1\#\ RHF/6-3
 1G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\(\CH)2Si(NH2)2(1+)\0,1\Si\X,1,PX\C,
 2,CX,1,90.\C,2,CX,1,90.,3,180.,0\N,1,Pn,2,A2,3,D1,0\N,1,Pn,2,A2,4,D1,0\H,3,CH,2
 ,HCC,1,D2,0\H,4,CH,2,HCC,1,D2,0\H,5,nh1,1,hnp1,6,hnp1,0\H,5,nh2,1,hnp2,6,hnp2,
 0\H,6,nh1,1,hnp1,5,hnp1,0\H,6,nh2,1,hnp2,5,hnp2,0\PX=1.65449093\Pn=1.709290
 66\CH=1.07694609\CX=0.67317552\nh1=0.9969538\nh2=0.99767143\A2=127.98397696\HCC
 =131.81139596\hnp2=120.60981275\hnp1=120.92595335\hnp2=-38.39119893\hnp1=171.
 95708412\D1=81.08843551\D2=179.94017213\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\
 State=1-A\HF=-477.0277872\RMSD=8.999e-09\RMSF=5.542e-05\Dipole=0.,0.,-0.3455502
 \PG=C02 [C2(Si1),X(C2H6N2)]\@

(CH)2Si(NH2)2+ HF Freq
 FREQ RHF 6-31G(D) C2H6N2SI1 PG=C02 DIP=0.000000 NIMAG=0
 STATE=1-A HF=-477.0277872 ZPE=56.3675605
 *** (CH)2Si(NH2)2(1+)

(CH)2Si(NH2)2+ MP2 OPT
 1\1\FAU-CCC-DERIOC2\FOPT\RMP2-FC\6-31+G(D)\C2H6N2SI1\GOELLER\23-Apr-1995\1\#\ R
 MP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2si(NH2)2(1+)\0,1\Si\X
 ,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\N,1,Pn,2,A2,3,D1,0\N,1,Pn,2,A2,4,D1,0\
 H,3,CH,2,HCC,1,D2,0\H,4,CH,2,HCC,1,D2,0\H,5,nh1,1,hnp1,6,hnp1,0\H,5,nh2,1,hnp2
 ,6,hnp2,0\H,6,nh1,1,hnp1,5,hnp1,0\H,6,nh2,1,hnp2,5,hnp2,0\PX=1.66649566\Pn=
 1.72388169\CH=1.08960164\CX=0.68633774\nh1=1.01394422\nh2=1.01476751\A2=128.151
 43801\HCC=131.943372\hnp2=120.23945195\hnp1=120.26083829\hnp1,0\H,5,nh2,1,hnp2
 x1=171.79018691\D1=79.63570054\D2=180.05109883\Version=HP-PARisc-HPUX-G92/DFT-
 RevG.2\State=1-A\HF=-477.0367153\MP2=-477.7060415\RMSD=3.871e-09\RMSF=4.051e-05
 \Dipole=0.,0.,-0.2396356\PG=C02 [C2(Si1),X(C2H6N2)]\@

(CH)2Si(NH2)2+ MP4 SP
 1\1\FAU-CCC-DERIOC3\SP\RMP4SDTQ-FC\6-31+G(D)\C2H6N2SI1\GOELLER\13-May-1995\0\#\ R
 MP4/6-31+G* NAME=GOELLER SCF=DIRECT GEOM=CHECKPOINT GUESS=READ\ (CH)2si(NH2)2
 (1+)\0,1\Si\X,1,1.6664956639\C,2,0.6863377446,1,90.\C,2,0.6863377446,1,90.,3,1
 80.,0\N,1,1.723881694,2,128.15143801,3,79.63570054,0\N,1,1.723881694,2,128.1514
 3801,4,79.63570054,0\H,3,1.0896016394,2,131.943372,1,180.05109883,0\H,4,1.08960
 16394,2,131.943372,1,180.05109883,0\H,5,1.0139442249,1,120.26083829,6,171.79018
 691,0\H,5,1.014767512,1,120.23945195,6,-41.38047875,0\H,6,1.0139442249,1,120.26
 083829,5,171.79018691,0\H,6,1.014767512,1,120.23945195,5,-41.38047875,0\Versio
 n=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A\HF=-477.0367153\MP2=-477.7060415\MP3=
 -477.7351823\MP4D=-477.7504511\MP4DQ=-477.7381027\MP4SDQ=-477.7444918\MP4SDTQ=-
 477.7684197\RMSD=9.621e-11\PG=C02 [C2(Si1),X(C2H6N2)]\@

(CH)2SiBr2+ HF OPT
 1\1\FAU-CCC-DERIOC4\FOPT\RHF\GEN\C2H2BR2SI1\GOELLER\20-Mar-1995\1\#\ RHF/GEN FO
 PT OPTCYC=99 NAME=GOELLER SCF=DIRECT\ (CH)2sibr2(1+) SHAsv+d\0,1\Si\X,1,PX\C,2
 ,CX,1,90.\C,2,CX,1,90.,3,180.,0\Br,1,PH,2,A2,3,90.,0\Br,1,PH,2,A2,5,180.,0\H,3,
 CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.65227243\PH=2.22825134\CH=1.08551
 126\CX=0.67249889\A2=126.55669728\HCC=134.3829455\Version=HP-PARisc-HPUX-G92/D
 FT-RevG.2\State=1-A1\HF=-5509.8948429\RMSD=4.228e-09\RMSF=2.253e-05\Dipole=0.,0
 .,0.8209844\PG=C02V [C2(Si1),SGV(C2H2),SGV'(Br2)]\@

(CH)2SiBr2+	HF	Freq			
FREQ	RHF	GEN	C2H2BR2SI1	PG=C02V	DIP=0.000000
STATE=1-A1		HF=-5509.8948429		ZPE=22.577443	NIMAG=0

*** (CH)2SIBR2(1+) SHASV+D

(CH)2SiBr2+ MP2 OPT
1\1\LRZM-YMP\FOPT\RMP2-FC\GEN\C2H2BR2SI1\GOELLER\12-May-1995\1\#\# RMP2/GEN FOPT
=CALCHFRC OPTCYC=99 NAME=GOELLER SCF=DIRECT\ (CH)2sibr2(1+) SHASv+d/631+G*\0,1
\Si\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\Br,1,PH,2,A2,3,90.,0\Br,1,PH,2,A2
,5,180.,0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.65485933\PH=2.21634
308\CH=1.08692418\CX=0.68321099\A2=125.82796778\HCC=134.72016179\Version=CrayY
MP-Unicos-G92RevC\State=1-A1\HF=-5510.048438\MP2=-5510.8451585\RMSD=1.656e-09\R
MSF=4.611e-05\Dipole=0.,0.,0.8313757\PG=C02V [C2(Si1),SGV(C2H2),SGV'(Br2)]\

(CH)2SiBr2+ MP4 SP
1\1\LRZM-YMP\SP\RMP4SDTQ-FC\GEN\C2H2BR2SI1\GOELLER\14-Jun-1995\0\#\# RMP4/GEN NA
ME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2sibr2(1+) SHASv+d/631+G*
\0,1\Si\X,1,1.6548593274\C,2,0.6832109946,1,90.\C,2,0.6832109946,1,90.,3,180.,
0\Br,1,2.2163430815,2,125.82796778,3,90.,0\Br,1,2.2163430815,2,125.82796778,5,1
80.,0\H,3,1.0869241829,2,134.72016179,1,180.,0\H,4,1.0869241829,2,134.72016179,
1,180.,0\Version=CrayYMP-Unicos-G92RevC\State=1-A1\HF=-5510.048438\MP2=-5510.8
451585\MP3=-5510.8566256\MP4D=-5510.8723828\MP4DQ=-5510.8598476\MP4SDQ=-5510.86
6896\MP4SDTQ=-5510.8945262\RMSD=6.198e-09\PG=C02V [C2(Si1),SGV(C2H2),SGV'(Br2)]
\

(CH)2SiI2+ HF OPT
1\1\FAU-CCC-HP111\FOPT\RHF\GEN\C2H2I2SI1\GOELLER\8-Oct-1994\1\#\# RHF/GEN OPT OP
TCYC=99 NAME=GOELLER SCF=DIRECT PSEUDO=CARDS\ (CH)2sii2(1+) c,h,si:6-31G*,i(7ve
-mwb-ecp'93,dzp)\0,1\Si\X,1,PX\C,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\I,1,PH,2,A2,
3,90.,0\I,1,PH,2,A2,5,180.,0\H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.
64853775\PH=2.45753645\CH=1.07341719\CX=0.66802488\A2=125.40691146\HCC=135.1897
5128\Version=HP-PARisc-HPUX-G92/DFT-RevF.2\State=1-A1\HF=-388.1628521\RMSD=7.9
97e-09\RMSF=1.621e-05\Dipole=0.,0.,0.8103005\PG=C02V [C2(Si1),SGV(C2H2),SGV'(I2
)]\@

(CH)2SiI2+ HF Freq
FREQ RHF GEN C2H2I2SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-388.1628521 ZPE=22.4444841
*** (CH)2SII2(1+) C,H,SI:6-31G*,I(7VE-MWB-ECP'93,DZP)

(CH)2SiI2+ MP2 OPT
 1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\GEN\C2H2I2SI1\GOELLER\10-Jul-1995\0\#\# RMP2/GE
 N FOPT OPTCYC=100 NAME=GOELLER SCF=(QC,DIRECT) PSEUDO=CARDS\\$(CH)2sii2(1+) c,h,
 si:6-31G*,i(7ve-mwb-ecp'93,dzp)\0,1\Si,0.,0.,0.9293591041\C,0.6808542577,0.,2.
 5951367473\C,-0.6808542577,0.,2.5951367473\I,0.,-2.0134386524,-0.4798855739\I,0
 .,2.0134386524,-0.4798855739\H,1.4556524425,0.,3.3576012034\H,-1.4556524425,0.,
 3.3576012034\Version=Convex-Unix-G94RevB.1\State=1-A1\HF=-388.1648579\MP2=-388
 .6908743\RMSD=0.000e+00\RMSF=4.911e-05\Dipole=0.,0.,0.7218839\PG=C02V [C2(Si1),
 SGV(C2H2),SGV'(I2)]\@

(CH)2SiI2+ MP4 SP
 1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\GEN\C2H2I2SI1\GOELLER\16-Jul-1995\0\#\# RMP4/
 GEN NAME=GOELLER SCF=DIRECT PSEUDO=CARDS GUESS=READ GEOM=CHECKPOINT\\$(CH)2sii2(
 1+) c,h,si:6-31G*,i(7ve-mwb-ecp'93,dzp)\0,1\Si,0.,0.,0.9293591041\C,0.68085425
 77,0.,2.5951367473\C,-0.6808542577,0.,2.5951367473\I,0.,-2.0134386524,-0.479885
 5739\I,0.,2.0134386524,-0.4798855739\H,1.4556524425,0.,3.3576012034\H,-1.455652
 4425,0.,3.3576012034\Version=Convex-Unix-G94RevB.1\State=1-A1\HF=-388.1648579\
 MP2=-388.6908743\MP3=-388.7173296\MP4D=-388.73022\MP4DQ=-388.7173283\MP4SDQ=-38
 8.7226923\MP4SDTQ=-388.7451781\RMSD=6.224e-10\PG=C02V [C2(Si1),SGV(C2H2),SGV'(I
 2)]\@

(CH)2Si(CH3)2+ HF OPT
 1\1\FAU-CCC-HP104\FOPT\RHF\6-31G(D)\C4H8SI1\GOELLER\27-Feb-1995\1\#\# RHF/6-31G*
 FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\\$(CH)2si(ch3)2(1+)\0,1\Si\X,1,PX\C,2,C
 X,1,90.\C,2,CX,1,90.,3,180.,0\C,1,Pn,2,A2,3,90.,0\C,1,Pn,2,A2,5,180.,0\H,3,CH,2
 ,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\H,5,nh,1,hnp,2,hnpX,0\H,5,nh,1,hnp,2,-hnpX,
 0\H,6,nh,1,hnp,2,hnpX,0\H,6,nh,1,hnp,2,-hnpX,0\H,5,nh2,1,hnp2,2,0.,0\H,6,nh2,1,
 hnp2,2,0.,0\PX=1.67671204\Pn=1.88529639\CH=1.07521858\CX=0.66546591\nh=1.08748
 308\nh2=1.08474252\A2=125.15205389\HCC=133.82105429\hnp=111.07196268\hnp2=111.2
 531174\hnpX=120.41304508\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A1\HF=-
 444.9911452\RMSD=5.686e-09\RMSF=3.357e-05\Dipole=0.,0.,-0.2015666\PG=C02V [C2(S
 i1),SGV(C2H2),SGV'(C2H2),X(H4)]\@

(CH)2Si(CH3)2+ HF Freq
 FREQ RHF 6-31G(D) C4H8SI1 PG=C02V DIP=0.000000 NIMAG=0
 STATE=1-A1 HF=-444.9911452 ZPE=70.1381709
 *** (CH)2SI(CH3)2(1+)

(CH)2Si(CH3)2+ MP2 OPT
 1\1\FAU-CCC-DERIOC4\FOPT\RMP2-FC\6-31+G(D)\C4H8SI1\GOELLER\22-Apr-1995\1\#\ RMP
 2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2si(ch3)2(1+)\0,1\Si\X,1
 ,PX\C,2,CX,1,90.,3,180.,0\C,1,Pn,2,A2,3,90.,0\C,1,Pn,2,A2,5,180.,0
 \H,3,CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\H,5,nh,1,hnp,2,hnp,0\H,5,nh,1,hnp
 ,2,-hnp,0\H,6,nh,1,hnp,2,hnp,0\H,6,nh,1,hnp,2,-hnp,0\H,5,nh2,1,hnp2,2,0.,0\H
 ,6,nh2,1,hnp2,2,0.,0\PX=1.69193891\Pn=1.87946322\CH=1.08764911\CX=0.67702546\n
 h=1.09592066\nh2=1.09396124\A2=124.36143021\HCC=134.36510144\hnp=111.18732416\h
 np2=110.44504791\hnp=120.19266093\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State
 =1-A1\HF=-444.9938901\MP2=-445.5959517\RMSD=8.837e-10\RMSF=2.854e-05\Dipole=0.,
 0.,-0.2407751\PG=C02V [C2(Si1),SGV(C2H2),SGV'(C2H2),X(H4)]\@

(CH)2Si(CH3)2+ MP4 SP
 1\1\FAU-CCC-DERIOC3\SP\RMP4SDTQ-FC\6-31+G(D)\C4H8SI1\GOELLER\12-May-1995\0\#\ R
 MP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2si(ch3)2(1
 +)\0,1\Si\X,1,1.6919389059\C,2,0.6770254612,1,90.,3,180.
 .,0\C,1,1.8794632162,2,124.36143021,3,90.,0\C,1,1.8794632162,2,124.36143021,5,1
 80.,0\H,3,1.0876491136,2,134.36510144,1,180.,0\H,4,1.0876491136,2,134.36510144,
 1,180.,0\H,5,1.0959206616,1,111.18732416,2,120.19266093,0\H,5,1.0959206616,1,11
 1.18732416,2,-120.19266093,0\H,6,1.0959206616,1,111.18732416,2,120.19266093,0\H
 ,6,1.0959206616,1,111.18732416,2,-120.19266093,0\H,5,1.0939612426,1,110.4450479
 1,2,0.,0\H,6,1.0939612426,1,110.44504791,2,0.,0\Version=HP-PARisc-HPUX-G92/DFT
 -RevG.2\State=1-A1\HF=-444.9938901\MP2=-445.5959517\MP3=-445.638061\MP4D=-445.6
 539248\MP4DQ=-445.6415549\MP4SDQ=-445.6477633\MP4SDTQ=-445.6712035\RMSD=8.260e-
 10\PG=C02V [C2(Si1),SGV(C2H2),SGV'(C2H2),X(H4)]\@

(CH)2SiH2+ HF OPT
 1\0\FAU-ERLG\FOPT\RHF\6-31G(D)\C2H4SI1\SCHLEYER\1-DEC-1985\1\#\ RHF/6-31G* OPT
 NAME=SCHLEYER\ (CH)2SiH2, C2V\0,1\SI\X,1,SIX\H,1,SIH,2,A1\H,1,SIH,2,A1,3,180.,
 0\C,2,CX,1,90.,3,90.,0\C,2,CX,1,90.,3,-90.,0\H,5,CH,2,A2,1,180.,0\H,6,CH,2,A2,1
 ,180.,0\SIH=1.67546\SIH=1.47258\CX=0.66303\CH=1.07406\A1=125.17316\A2=135.1139
 6\Version=CYBER-NOS-G82RevH\HF=-366.8945529\RMSD=0.405D-10\RMSF=0.419D-05\DIP=
 0.31191\PG=C02V\

(CH)2SiH2+	HF	Freq			
FREQ	RHF	6-31G(D)	C2H4SI1	PG=C02V	DIP=0.000000 NIMAG=0
STATE=1-A1		HF=-366.8945529	ZPE=31.6781638		

*** (CH)2SiH2, C2V

(CH)2SiH2+ MP2 OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C2H4SI1\GOELLER\22-Apr-1995\1\#\ RMP
2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (CH)2SiH2(1)\0,1\Si\X,1,PX\C
,2,CX,1,90.\C,2,CX,1,90.,3,180.,0\H,1,PH,2,A2,3,90.,0\H,1,PH,2,A2,5,180.,0\H,3,
CH,2,HCC,1,180.,0\H,4,CH,2,HCC,1,180.,0\PX=1.69323268\PH=1.48064237\CH=1.08598
32\CX=0.67330387\A2=124.25716641\HCC=135.98250955\Version=Convex-Unix-G92/DFT-
RevG.2\State=1-A1\HF=-366.8964991\MP2=-367.2305013\RMSD=1.786e-09\RMSF=4.412e-0
5\Dipole=-0.,0.,0.1110618\PG=C02V [C2(Si1),SGV(C2H2),SGV'(H2)]\@

(CH)2SiH2+ MP4 SP
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4SI1\GOELLER\13-May-1995\0\#\ R
MP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2SiH2(1)\0
,1\Si\X,1,1.6932326759\C,2,0.6733038697,1,90.\C,2,0.6733038697,1,90.,3,180.,0\H
,1,1.4806423675,2,124.25716641,3,90.,0\H,1,1.4806423675,2,124.25716641,5,180.,0
\H,3,1.0859831958,2,135.98250955,1,180.,0\H,4,1.0859831958,2,135.98250955,1,180
,0\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-366.8964991\MP2=-367.230
5013\MP3=-367.2535771\MP4D=-367.2638398\MP4DQ=-367.2561909\MP4SDQ=-367.2600555\
MP4SDTQ=-367.2748046\RMSD=4.941e-11\PG=C02V [C2(Si1),SGV(C2H2),SGV'(H2)]\@
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4SI1\GOELLER\13-May-1995\0\#\ R
MP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2SiH2(1)\0
,1\Si\X,1,1.6932326759\C,2,0.6733038697,1,90.\C,2,0.6733038697,1,90.,3,180.,0\H
,1,1.4806423675,2,124.25716641,3,90.,0\H,1,1.4806423675,2,124.25716641,5,180.,0
\H,3,1.0859831958,2,135.98250955,1,180.,0\H,4,1.0859831958,2,135.98250955,1,180
,0\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-366.8964991\MP2=-367.230
5013\MP3=-367.2535771\MP4D=-367.2638398\MP4DQ=-367.2561909\MP4SDQ=-367.2600555\
MP4SDTQ=-367.2748046\RMSD=4.941e-11\PG=C02V [C2(Si1),SGV(C2H2),SGV'(H2)]\@
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4SI1\GOELLER\13-May-1995\0\#\ R
MP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ (CH)2SiH2(1)\0
,1\Si\X,1,1.6932326759\C,2,0.6733038697,1,90.\C,2,0.6733038697,1,90.,3,180.,0\H
,1,1.4806423675,2,124.25716641,3,90.,0\H,1,1.4806423675,2,124.25716641,5,180.,0
\H,3,1.0859831958,2,135.98250955,1,180.,0\H,4,1.0859831958,2,135.98250955,1,180
,0\Version=Convex-Unix-G92/DFT-RevG.2\State=1-A1\HF=-366.8964991\MP2=-367.230
5013\MP3=-367.2535771\MP4D=-367.2638398\MP4DQ=-367.2561909\MP4SDQ=-367.2600555\
MP4SDTQ=-367.2748046\RMSD=4.941e-11\PG=C02V [C2(Si1),SGV(C2H2),SGV'(H2)]\@

```
(CH2)2SiF2+      HF      OPT
1\1\FAU-CCC-HP110\FOPT\RHF\6-31G(D)\C2H4F2SI1\GOELLER\30-Sep-1994\1\1\#RHF/6-31G
* OPTCYC=99 OPT NAME=GOELLER SCF=DIRECT\\(Ch2)2sif+\\0,1\Si\X,1,PX\C,2,PC,1,90.
\C,2,PC,1,90.,3,180.,0\F,1,PCL,2,HPCL,3,90.,0\F,1,PCL,2,HPCL,3,-90.,0\H,3,HC,2,
HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\PX=1.
6085858\PC=0.81038022\PCL=1.57766379\HPCL=126.56285639\HC=1.07905333\HCP=114.34
540902\D2=114.57196281\\Version=HP-PARisc-HPUX-G92/DFT-RevF.2\State=1-A1\HF=-56
5.9390971\RMSD=2.260e-09\RMSF=4.377e-05\Dipole=0.,0.,0.6528753\PG=C02V [C2(Si1)
,SGV(C2),SGV'(F2),X(H4)]\\@
```

```
(CH2)2SiF2+      HF      Freq
FREQ      RHF      6-31G(D)      C2H4F2SI1      PG=C02V DIP=0.000000      NIMAG=0
STATE=1-A1      HF=-565.9390971      ZPE=40.0269039
*** (CH2)2SIF+
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```
(CH2)2SiF2+      MP2      OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C2H4F2SI1\GOELLER\2-Jul-1995\1\1\#RMP
2/6-31+G* OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\\(Ch2)2sif+ //HF/6-31G*\\0,1\Si
i\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\F,1,PCL,2,HPCL,3,90.,0\F,1,PCL,2,HP
CL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,H
C,2,HCP,1,D2,0\PX=1.61797885\PC=0.81220637\PCL=1.61567218\HPCL=126.26089697\HC
=1.08928208\HCP=114.51582858\D2=114.19702145\\Version=Convex-Unix-G92/DFT-RevG.
2\State=1-A1\HF=-565.9475962\MP2=-566.647862\RMSD=7.204e-09\RMSF=7.459e-05\Dipo
le=0.,-0.,0.8145215\PG=C02V [C2(Si1),SGV(C2),SGV'(F2),X(H4)]\\@
```

```
(CH2)2SiF2+      MP4      SP
1\1\FAU-CCC-DERIOC1\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4F2SI1\GOELLER\06-Jul-1995\0\1\#
RMP4/6-31+G* SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\(Ch2)2sif+ //MP2/6-31+G*\\0
,1\Si\X,1,1.6179788469\C,2,0.8122063745,1,90.\C,2,0.8122063745,1,90.,3,180.,0\F
,1,1.6156721824,2,126.26089697,3,90.,0\F,1,1.6156721824,2,126.26089697,3,-90.,0
\H,3,1.0892820839,2,114.51582858,1,114.19702145,0\H,3,1.0892820839,2,114.515828
58,1,-114.19702145,0\H,4,1.0892820839,2,114.51582858,1,-114.19702145,0\H,4,1.08
92820839,2,114.51582858,1,114.19702145,0\\Version=Convex-Unix-G94RevB.1\State=1
-A1\HF=-565.9475962\MP2=-566.647862\MP3=-566.6611911\MP4D=-566.6753822\MP4DQ=-5
66.6676832\MP4SDQ=-566.6775352\MP4SDTQ=-566.6991377\RMSD=2.273e-09\PG=C02V [C2(
Si1),SGV(C2),SGV'(F2),X(H4)]\\@
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(CH2)2Si(OH)2+ HF OPT
1\1\FAU-CCC-HP104\FOPT\RHF\6-31G(D)\C2H6O2SI1\GOELLER\04-May-1996\1\#\RHF/6-31G
* NAME=GOELLER SCF=DIRECT FOPT=Z-MATRIX OPTCYC=99\ (Ch2)2Si(OH)2 2 H away from
ring, C2\0,1\Si\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\O,1,PCL,2,HPCL,3,D4,
0\O,1,PCL,2,HPCL,4,D4,0\H,3,HC1,2,HCP1,1,D21,0\H,3,HC2,2,HCP2,1,-D22,0\H,4,HC2,
2,HCP2,1,-D22,0\H,4,HC1,2,HCP1,1,D21,0\H,5,HO,1,HON,2,D3,0\H,6,HO,1,HON,2,D3,0\
\PX=1.62501766\PC=0.80435818\PCL=1.63762367\HPCL=124.13227573\HC1=1.07923888\HC
2=1.07913415\HO=0.94752098\HCP1=114.2030613\HCP2=114.41052121\HON=117.9217109\D
21=114.83620265\D22=114.2661816\D3=120.26204041\D4=85.0743511\Version=HP-PARisc
c-HPUX-G94RevC.3\State=1-A\HF=-517.9064785\RMSE=3.463e-09\RMSF=2.561e-05\Dipole
=0.,0.,-0.5861217\PG=C02 [C2(Si1),X(C2H6O2)]\@

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(CH2)2Si(OH)2+ HF Freq
FREQ RHF 6-31G(D) C2H6O2SI1 PG=C02 DIP=0.000000 NIMAG=0
STATE=1-A HF=-517.9064785
*** (CH2)2Si(OH)2 2 H AWAY FROM RING, C2

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(CH2)2Si(OH)2+ MP2 OPT
1\1\FAU-CCC-DERIOC11\FOPT\RMP2-FC\6-31+G(D)\C2H6O2SI1\GOELLER\15-May-1996\0\#\
RMP2/6-31+G* FOPT NAME=GOELLER SCF=DIRECT OPTCYC=99\ (Ch2)2Si(OH)2 2 H away fro
m ring, C2 //HF/6-31G*\0,1\Si,0.,0.,0.205813584\C,0.8006803274,0.0878208664,-1
.427835649\C,-0.8006803274,-0.0878208664,-1.427835649\O,0.,1.3920469069,1.12687
03556\O,0.,-1.3920469069,1.1268703556\H,1.346135473,-0.7640843755,-1.8322337019
\H,1.1559672652,1.0355029291,-1.8306995806\H,-1.1559672652,-1.0355029291,-1.830
6995806\H,-1.346135473,0.7640843755,-1.8322337019\H,-0.719303725,1.4903164739,1
.7742892437\H,0.719303725,-1.4903164739,1.7742892437\Version=HP-PARisc-HPUX-G9
4RevC.3\State=1-A\HF=-517.9126289\MP2=-518.6291215\RMSE=1.929e-09\RMSF=2.447e-0
5\Dipole=0.,0.,-0.4939064\PG=C02 [C2(Si1),X(C2H6O2)]\@

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(CH2)2Si(OH)2+ MP4 SP
1\1\FAU-CCC-DERIOC3\SP\RMP4SDTQ-FC\6-31+G(D)\C2H6O2SI1\GOELLER\17-May-1996\0\#\
RMP4/6-31+G* NAME=GOELLER SCF=DIRECT GUESS=READ GEOM=CHECK\ (Ch2)2Si(OH)2 2 H
away from ring, C2 //MP2/6-31+G*\0,1\Si,0.,0.,0.205813584\C,0.8006803274,0.087
8208664,-1.427835649\C,-0.8006803274,-0.0878208664,-1.427835649\O,0.,1.39204690
69,1.1268703556\O,0.,-1.3920469069,1.1268703556\H,1.346135473,-0.7640843755,-1.
8322337019\H,1.1559672652,1.0355029291,-1.8306995806\H,-1.1559672652,-1.0355029
291,-1.8306995806\H,-1.346135473,0.7640843755,-1.8322337019\H,-0.719303725,1.49

```

03164739,1.7742892437\H,0.719303725,-1.4903164739,1.7742892437\\Version=HP-PARisc-HPUX-G94RevC.3\State=1-A\HF=-517.9126289\MP2=-518.6291215\MP3=-518.6512308\MP4D=-518.6668911\MP4DQ=-518.6570821\MP4SDQ=-518.6645227\MP4SDTQ=-518.6858639\RM
SD=5.437e-10\PG=C02 [C2(Si1),X(C2H6O2)]\\@

(CH2)2SiCl2+ HF OPT
1\1\FAU-CCC-HP109\FOPT\RHF\6-31G(D)\C2H4CL2SI1\GOELLER\30-Sep-1994\1\\#RHF/6-31
G* OPTCYC=99 OPT NAME=GOELLER SCF=DIRECT\\(Ch2)2sicl+\\0,1\Si\X,1,PX\C,2,PC,1,9
0.\C,2,PC,1,90.,3,180.,0\C1,1,PCL,2,HPCL,3,90.,0\C1,1,PCL,2,HPCL,3,-90.,0\H,3,H
C,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\\P
X=1.63319139\PC=0.79643368\PCL=2.04208921\HPCL=124.80781635\HC=1.07858862\HCP=1
15.121683\D2=113.41940597\\Version=HP-PARisc-HPUX-G92/DFT-RevF.2\State=1-A1\HF=
-1286.0014932\RMSD=8.972e-09\RMSF=3.933e-05\Dipole=0.,0.,0.7686949\PG=C02V [C2(
Si1),SGV(C2),SGV'(C12),X(H4)]\\@

(CH2)2SiCl2+ HF Freq
FREQ RHF 6-31G(D) C2H4CL2SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-1286.0014932 ZPE=38.5560406
*** (CH2)2SiCl2+

(CH2)2SiCl2+ MP2 OPT
1\1\FAU-CCC-DERIOCI\FOPT\RMP2-FC\6-31+G(D)\C2H4CL2SI1\GOELLER\8-Jul-1995\1\\#RM
P2/6-31+G* OPTCYC=99 OPT NAME=GOELLER SCF=DIRECT\\(Ch2)2sicl+ //HF/6-31G*\\0,1\
Si\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\C1,1,PCL,2,HPCL,3,90.,0\C1,1,PCL,2
,HPCL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,-D2,0\H,
4,HC,2,HCP,1,D2,0\\PX=1.64194071\PC=0.79769964\PCL=2.03836644\HPCL=124.24762958
\HC=1.0894358\HCP=115.27247345\D2=113.12589461\\Version=Convex-Unix-G92/DFT-Rev
G.2\State=1-A1\HF=-1286.0039476\MP2=-1286.6090174\RMSD=7.826e-09\RMSF=2.408e-05
\Dipole=0.,-0.,0.6662338\PG=C02V [C2(Si1),SGV(C2),SGV'(C12),X(H4)]\\@

(CH2)2SiCl2+ MP4 SP
1\1\FAU-CCC-DERIOCI\SP\RMP4SDTQ-FC\6-31+G(D)\C2H4CL2SI1\GOELLER\18-Jul-1995\0\\
#RMP4/6-31+G* SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\(Ch2)2sicl+ //MP2/6-31+G*\
\0,1\Si\X,1,1.6419407148\C,2,0.797699641,1,90.\C,2,0.797699641,1,90.,3,180.,0\C
1,1,2.0383664402,2,124.24762958,3,90.,0\C1,1,2.0383664402,2,124.24762958,3,-90.
,0\H,3,1.0894357996,2,115.27247345,1,113.12589461,0\H,3,1.0894357996,2,115.2724
7345,1,-113.12589461,0\H,4,1.0894357996,2,115.27247345,1,-113.12589461,0\H,4,1.

0894357996,2,115.27247345,1,113.12589461,0\\Version=HP-PARisc-HPUX-G94RevB.1\\State=1-A\\HF=-1286.0039476\\MP2=-1286.6090174\\MP3=-1286.6535052\\MP4D=-1286.6667102\\MP4DQ=-1286.654941\\MP4SDQ=-1286.6594804\\MP4SDTQ=-1286.6793045\\RMSD=2.342e-09\\PG=C02V [C2(Si1),SGV(C2),SGV'(C12),X(H4)]\\@

(CH2)2Si(NH2)2+ HF OPT
1\\1\\FAU-CCC-HP104\\FOPT\\RHF\\6-31G(D)\\C2H8N2SI1\\GOELLER\\24-Apr-1995\\1\\#RHF/6-31G
* FOPT OPTCYC=99 NAME=GOELLER SCF=DIRECT\\(CH2)2si(NH2)2+\\0,1\\Si\\X,1,PX\\C,2,PC
1,90.\\C,2,PC,1,90.,3,180.,0\\N,1,Pn,2,HPCL,3,D3,0\\N,1,Pn,2,HPCL,4,D3,0\\H,3,HC1,
2,HCP1,1,D21,0\\H,3,HC2,2,HCP2,1,-D22,0\\H,4,HC1,2,HCP1,1,-D21,0\\H,4,HC2,2,HCP2,1
D22,0\\H,5,hn1,2,hcn1,1,hcnx1,0\\H,5,hn2,2,hcn2,1,hcnx2,0\\H,6,hn1,2,hcn1,1,hcnx1
0\\H,6,hn2,2,hcn2,1,hcnx2,0\\PX=1.64915268\\PC=0.79745908\\Pn=1.7085617\\hn1=0.996
77229\\hn2=0.99767548\\HPCL=125.78640464\\hcn1=96.48013978\\hcn2=134.22996318\\HC1=1
.08061096\\HC2=1.08061096\\HCP1=114.51834017\\HCP2=114.51834017\\D21=114.94616906\\D
22=114.94616906\\D3=79.75589562\\hcnx1=159.57715714\\hcnx2=-70.46147267\\Version=H
P-PARisc-HPUX-G92/DFT-RevG.2\\State=1-A\\HF=-478.2141017\\RMSD=5.524e-09\\RMSF=1.48
1e-04\\Dipole=0.,0.,-0.4545821\\PG=C02 [C2(Si1),X(C2H8N2)]\\@

(CH2)2Si(NH2)2+ HF Freq
FREQ RHF 6-31G(D) C2H8N2SI1 PG=C02 DIP=0.000000 NIMAG=0
STATE=1-A HF=-478.2141017 ZPE=71.1396542
*** (CH2)2SI(NH2)2+

(CH2)2Si(NH2)2+ MP2 OPT
1\\1\\FAU-CCC-DERIO4\\FOPT\\RMP2-FC\\6-31+G(D)\\C2H8N2SI1\\GOELLER\\6-Jul-1995\\1\\#RMP
2/6-31+G* FOPT OPTCYC=99 NAME=GOELLER SCF=DIRECT\\(CH2)2si(NH2)2+ //HF/6-31G*\\
0,1\\Si\\X,1,PX\\C,2,PC,1,90.\\C,2,PC,1,90.,3,180.,0\\N,1,Pn,2,HPCL,3,D3,0\\N,1,Pn,2,
HPCL,4,D3,0\\H,3,HC1,2,HCP1,1,D21,0\\H,3,HC2,2,HCP2,1,-D22,0\\H,4,HC1,2,HCP1,1,-D2
1,0\\H,4,HC2,2,HCP2,1,D22,0\\H,5,hn1,2,hcn1,1,hcnx1,0\\H,5,hn2,2,hcn2,1,hcnx2,0\\H,
6,hn1,2,hcn1,1,hcnx1,0\\H,6,hn2,2,hcn2,1,hcnx2,0\\PX=1.65778549\\PC=0.79817824\\Pn
=1.72325536\\hn1=1.01351393\\hn2=1.01456194\\HPCL=126.10473845\\hcn1=96.34792549\\h
cn2=133.50196478\\HC1=1.0905163\\HC2=1.0905163\\HCP1=114.80540267\\HCP2=114.80540267
\\D21=114.49975469\\D22=114.49975469\\D3=78.38415607\\hcnx1=159.17842552\\hcnx2=-71.
87567565\\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\\State=1-A\\HF=-478.2228973\\MP2=-
478.9056482\\RMSD=6.620e-09\\RMSF=1.649e-04\\Dipole=0.,0.,-0.3074648\\PG=C02 [C2(Si
1),X(C2H8N2)]\\@

(CH2)2Si(NH2)2+ MP4 SP
 1\1\FAU-CCC-DERIOC3\SP\RMP4SDTQ-FC\6-31+G(D)\C2H8N2SI1\GOELLER\7-Jul-1995\0\#\#R
 MP4/6-31+G* SCF=DIRECT GEOM=CHECKPOINT GUESS=READ\ (Ch2)2si(NH2)2+ //MP2/6-31+G
 *\0,1\Si\X,1,1.6577854897\C,2,0.7981782422,1,90.\C,2,0.7981782422,1,90.,3,180.
 ,0\N,1,1.723255362,2,126.10473845,3,78.38415607,0\N,1,1.723255362,2,126.1047384
 5,4,78.38415607,0\H,3,1.090516298,2,114.80540267,1,114.49975469,0\H,3,1.0905162
 98,2,114.80540267,1,-114.49975469,0\H,4,1.090516298,2,114.80540267,1,-114.49975
 469,0\H,4,1.090516298,2,114.80540267,1,114.49975469,0\H,5,1.0135139296,2,96.347
 92549,1,159.17842552,0\H,5,1.0145619388,2,133.50196478,1,-71.87567565,0\H,6,1.0
 135139296,2,96.34792549,1,159.17842552,0\H,6,1.0145619388,2,133.50196478,1,-71.
 87567565,0\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A\HF=-478.2228973\MP2
 =-478.9056482\MP3=-478.9422623\MP4D=-478.9577208\MP4DQ=-478.9467123\MP4SDQ=-478
 .9525121\MP4SDTQ=-478.9734398\RMSD=1.450e-09\PG=C02 [C2(Si1),X(C2H8N2)]\#@

(CH2)2SiBr2+ HF OPT
 1\1\FAU-CCC-DERIOC2\FOPT\RHF\GEN\C2H4BR2SI1\GOELLER\3-Oct-1994\1\#\#RHF/GEN OPTC
 YC=99 OPT NAME=GOELLER SCF=DIRECT\ (Ch2)2sibr+ SHASv+d\0,1\Si\X,1,PX\C,2,PC,1,
 90.\C,2,PC,1,90.,3,180.,0\Br,1,PCL,2,HPCL,3,90.,0\Br,1,PCL,2,HPCL,3,-90.,0\H,3,
 HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\H
 PX=1.65589001\PC=0.79087557\PCL=2.2222977\HPCL=124.44866427\HC=1.09043377\HCP=1
 15.58196276\D2=112.77044995\Version=HP-PARisc-HPUX-G92/DFT-RevF.2\State=1-A1\H
 F=-5511.0798302\RMSD=7.747e-09\RMSF=4.410e-05\Dipole=0.,0.,0.5787379\PG=C02V [C
 2(Si1),SGV(C2),SGV'(Br2),X(H4)]\#@

(CH2)2SiBr2+ HF Freq
 FREQ RHF GEN C2H4BR2SI1 PG=C02V DIP=0.000000 NIMAG=0
 STATE=1-A1 HF=-5511.0798302 ZPE=37.1957308
 *** (CH2)2SIBR+ SHASV+D

(CH2)2SiBr2+ MP2 OPT
 1\1\FAU-CCC-DERIOC3\FOPT\RMP2-FC\GEN\C2H4BR2SI1\GOELLER\31-Jul-1995\0\#\#RMP2/GE
 N OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\ (Ch2)2sibr+ SHASv+d\0,1\Si,0.,0.,0.5
 806618191\C,0.7928670907,0.,2.2337405517\Br,0.,
 -1.8386279302,-0.6483007088\Br,0.,1.8386279302,-0.6483007088\H,1.263760947,0.90
 71231446,2.6117243823\H,1.263760947,-0.9071231446,2.6117243823\H,-1.263760947,0
 .9071231446,2.6117243823\H,-1.263760947,-0.9071231446,2.6117243823\Version=HP-
 PARisc-HPUX-G94RevB.1\State=1-A1\HF=-5511.2397131\MP2=-5512.050312\RMSD=7.675e-

09\RMSF=1.927e-04\Dipole=0.,0.,0.6664501\PG=C02V [C2(Si1),SGV(C2),SGV'(Br2),X(H4)]\@

(CH2)2SiBr2+ MP4 SP
1\1\FAU-CCC-DERIOC2\SP\RMP4SDTQ-FC\GEN\C2H4BR2SI1\GOELLER\05-Aug-1995\0\#\RMP4/
GEN SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\(\Ch2)2sibr+ SHASv+d\0,1\Si,0.,0.,0.
5806618191\C,0.7928670907,0.,2.2337405517\C,-0.7928670907,0.,2.2337405517\Br,0.
, -1.8386279302, -0.6483007088\Br,0.,1.8386279302, -0.6483007088\H,1.263760947,0.9
071231446,2.6117243823\H,1.263760947, -0.9071231446,2.6117243823\H, -1.263760947,
0.9071231446,2.6117243823\H, -1.263760947, -0.9071231446,2.6117243823\Version=HP
-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-5511.2397131\MP2=-5512.050312\MP3=-5512.0
693889\MP4D=-5512.0853868\MP4DQ=-5512.0741882\MP4SDQ=-5512.0806555\MP4SDTQ=-551
2.1052462\RMSD=2.229e-09\PG=C02V [C2(Si1),SGV(C2),SGV'(Br2),X(H4)]\@

(CH2)2SiI2+ HF OPT
1\1\FAU-CCC-HP111\FOPT\RHF\GEN\C2H4I2SI1\GOELLER\30-Sep-1994\1\#\RHF/GEN OPTCYC
=99 OPT NAME=GOELLER SCF=DIRECT PSEUDO=CARDS\(\Ch2)2sii c,h,si:6-31G*,i(7ve-mwb
-ecp'93,dzp)\0,1\Si\X,1,PX\C,2,PC,1,90.\C,2,PC,1,90.,3,180.,0\I,1,PCL,2,HPCL,3
,90.,0\I,1,PCL,2,HPCL,3,-90.,0\H,3,HC,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,
2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\PX=1.65731446\PC=0.78599379\PCL=2.44916065\H
PCL=123.44161756\HC=1.0783164\HCP=115.68999624\D2=112.67093772\Version=HP-PARI
sc-HPUX-G92/DFT-RevF.2\State=1-A1\HF=-389.3546245\RMSD=5.863e-09\RMSF=8.163e-05
\Dipole=0.,0.,0.5957329\PG=C02V [C2(Si1),SGV(C2),SGV'(I2),X(H4)]\@

(CH2)2SiI2+ HF Freq
FREQ RHF GEN C2H4I2SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-389.3546245 ZPE=37.6474619
*** (CH2)2SII C,H,SI:6-31G*,I(7VE-MWB-ECP'93,DZP)

(CH2)2SiI2+ MP2 OPT
1\1\FAU-CCC-DERIOC3\FOPT\RMP2-FC\GEN\C2H4I2SI1\GOELLER\15-Jul-1995\0\#\RMP2/GEN
OPTCYC=99 OPT NAME=GOELLER SCF=DIRECT PSEUDO=READ\(\Ch2)2sii c,h,si:6-31G*,i(7
ve-mwb-ecp'93,dzp)\0,1\Si,0.,0.,0.8321136709\C,0.7873250927,0.,2.499872934\C,-
0.7873250927,0.,2.499872934\I,0.,-2.0545645129,-0.5011930201\I,0.,2.0545645129,
-0.5011930201\H,1.2633572214,0.907790198,2.8695983836\H,1.2633572214,-0.9077901
98,2.8695983836\H,-1.2633572214,0.907790198,2.8695983836\H,-1.2633572214,-0.907
790198,2.8695983836\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-389.357218

\MP2=-389.8971009\RMSD=4.572e-09\RMSF=7.393e-05\Dipole=0.,0.,0.5512903\PG=C02V
[C2(Si1),SGV(C2),SGV'(I2),X(H4)]\@

(CH2)2SiI2+ MP4 SP
1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\GEN\C2H4I2SI1\GOELLER\16-Jul-1995\0\#\RMP4/G
EN SCF=DIRECT PSEUDO=READ GUESS=READ GEOM=CHECKPOINT\ (Ch2)2sii c,h,si:6-31G*,i
(7ve-mwb-ecp'93,dzp)\0,1\Si,0.,0.,0.8321136709\C,0.7873250927,0.,2.499872934\C
, -0.7873250927,0.,2.499872934\I,0.,-2.0545645129,-0.5011930201\I,0.,2.054564512
9,-0.5011930201\H,1.2633572214,0.907790198,2.8695983836\H,1.2633572214,-0.90779
0198,2.8695983836\H,-1.2633572214,0.907790198,2.8695983836\H,-1.2633572214,-0.9
07790198,2.8695983836\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-389.3572
18\MP2=-389.8971009\MP3=-389.9311651\MP4D=-389.9442654\MP4DQ=-389.9327508\MP4SD
Q=-389.9375145\MP4SDTQ=-389.9569121\RMSD=5.311e-10\PG=C02V [C2(Si1),SGV(C2),SGV
'(I2),X(H4)]\@

(CH2)2Si(CH3)2+ HF OPT
1\1\FAU-CCC-HP112\FOPT\RHF\6-31G(D)\C4H10SI1\GOELLER\19-Apr-1995\1\#\RHF/6-31G*
OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\ (Ch2)2Si(CH3)2+\0,1\Si\X,1,PX\C,2,PC,
1,90.\C,2,PC,1,90.,3,180.,0\C,1,PC2,2,HPC,3,90.,0\C,1,PC2,2,HPC,3,-90.,0\H,3,HC
,2,HCP,1,D2,0\H,3,HC,2,HCP,1,-D2,0\H,4,HC,2,HCP,1,D2,0\H,5
,HC2,1,HCP2,2,0.,0\H,6,HC2,1,HCP2,2,0.,0\H,5,HC3,1,HCP3,2,D3,0\H,5,HC3,1,HCP3,2
, -D3,0\H,6,HC3,1,HCP3,2,D3,0\H,6,HC3,1,HCP3,2,-D3,0\PX=1.67252526\PC=0.7843823
8\PC2=1.88223397\HPC=123.10050043\HC=1.07961876\HC2=1.08558634\HC3=1.08662788\H
CP=115.18552527\HCP2=110.78717568\HCP3=111.32606713\D2=113.91202731\D3=119.9744
28\Version=HP-PARisc-HPUX-G92/DFT-RevG.2\State=1-A1\HF=-446.1841808\RMSD=2.215
e-09\RMSF=4.295e-05\Dipole=0.,0.,-0.3832027\PG=C02V [C2(Si1),SGV(C2H2),SGV'(C2)
,X(H8)]\@

(CH2)2Si(CH3)2+ HF Freq
FREQ RHF 6-31G(D) C4H10SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-446.1841808 ZPE=85.420019
*** (CH2)2Si(CH3)2+

(CH2)2Si(CH3)2+ MP2 OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C4H10SI1\GOELLER\15-Jul-1995\0\#\RMP
2/6-31+G* OPTCYC=99 FOPT NAME=GOELLER SCF=DIRECT\ (Ch2)2Si(CH3)2+ //HF/6-31G*\0,
1\Si,0.,0.,-0.1917670654\C,0.7825803909,0.,1.4920951225\C,-0.7825803909,0.,1.

4920951225\C,0.,-1.5866448194,-1.1953298695\C,0.,1.5866448194,-1.1953298695\H,1.2535370343,0.9030980728,1.8796341044\H,1.2535370343,-0.9030980728,1.8796341044\H,-1.2535370343,0.9030980728,1.8796341044\H,-1.2535370343,-0.9030980728,1.8796341044\H,0.,-2.4519542344,-0.5245439911\H,0.,2.4519542344,-0.5245439911\H,-0.8852134358,-1.6560946004,-1.8364731389\H,0.8852134358,-1.6560946004,-1.8364731389\H,0.8852134358,1.6560946004,-1.8364731389\H,-0.8852134358,1.6560946004,-1.8364731389\\Version=Convex-Unix-G94RevB.1\State=1-A1\HF=-446.1872274\MP2=-446.8027247\RMSD=8.933e-09\RMSF=2.277e-05\Dipole=0.,0.,-0.3656819\PG=C02V [C2(Si1),SGV(C2H2),SGV'(C2),X(H8)]\\@

(CH2)2Si(CH3)2+ MP4 SP
1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\6-31+G(D)\C4H10SI1\GOELLER\17-Jul-1995\0\\#RMP4/6-31+G* SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\\(Ch2)2Si(CH3)2+ //MP2/6-31+G*\\0,1\Si,0.,0.,-0.1917670654\C,0.7825803909,0.,1.4920951225\C,-0.7825803909,0.,1.4920951225\C,0.,-1.5866448194,-1.1953298695\C,0.,1.5866448194,-1.1953298695\H,1.2535370343,0.9030980728,1.8796341044\H,1.2535370343,-0.9030980728,1.8796341044\H,-1.2535370343,0.9030980728,1.8796341044\H,-1.2535370343,-0.9030980728,1.8796341044\H,0.,-2.4519542344,-0.5245439911\H,0.,2.4519542344,-0.5245439911\H,-0.8852134358,-1.6560946004,-1.8364731389\H,0.8852134358,-1.6560946004,-1.8364731389\H,0.8852134358,1.6560946004,-1.8364731389\H,-0.8852134358,1.6560946004,-1.8364731389\\Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-446.1872274\MP2=-446.8027247\MP3=-446.8522513\MP4D=-446.8682149\MP4DQ=-446.8571921\MP4SDQ=-446.8627773\MP4SDTQ=-446.8832338\RMSD=1.605e-09\PG=C02V [C2(Si1),SGV(C2H2),SGV'(C2),X(H8)]\\@

(CH2)2SiH2+ HF OPT
1\1\FAU-IOC-DERIOC1\FOPT\RHF\6-31G(D)\C2H6SI1\MAERKER\27-Jan-1995\1\\#HF/6-31G* FOPT NAME=MAERKER SCF=INCORE\\SILYLCYCLOPROPANE C2V\\0,1\Si\X,1,six\C,2,cx,1,90.\C,2,cx,1,90.,3,180.,0\H,1,sih,2,hsix,3,90.,0\H,1,sih,2,hsix,3,-90.,0\X,3,1.,1,xcsi,2,180.,0\X,4,1.,1,xcsi,2,180.,0\H,3,ch,7,hcx,1,90.,0\H,3,ch,7,hcx,1,-90.,0\H,4,ch,8,hcx,1,90.,0\H,4,ch,8,hcx,1,-90.,0\\six=1.67978565\cx=0.77725436\sih=1.46842876\hsix=123.21124443\xcsi=153.70494363\ch=1.0785466\hcx=56.10784749\\Version=Convex-Unix-G92RevC.2\State=1-A1\HF=-368.0890352\RMSD=8.811e-09\RMSF=2.062e-05\Dipole=0.,-0.,-0.029084\PG=C02V [C2(Si1),SGV(C2),SGV'(H2),X(H4)]\\@

(CH2)2SiH2+ HF Freq

FREQ RHF 6-31G(D) C2H6SI1 PG=C02V DIP=0.000000 NIMAG=0
STATE=1-A1 HF=-368.0890352 ZPE=46.8545528
*** SILYLCYCLOPROPANE C2V

(CH2)2SiH2+ MP2 OPT
1\1\FAU-CCC-DERIOC1\FOPT\RMP2-FC\6-31+G(D)\C2H6SI1\GOELLER\16-Jul-1995\0\#\RMP2
/6-31+G* FOPT OPTCYC=99 SCF=DIRECT\ \SILYLCYCLOPROPANE C2V //HF/6-31G*\ \0,1\Si,0
. ,0. , -0.8429844531\C,0.774287806,0. ,0.8504691228\C, -0.774287806,0. ,0.8504691228
\H,0. , -1.2461748371, -1.6350349393\H,0. ,1.2461748371, -1.6350349393\H,1.254865216
4, -0.9054801363,1.216555687\H,1.2548652164,0.9054801363,1.216555687\H, -1.254865
2164,0.9054801363,1.216555687\H, -1.2548652164, -0.9054801363,1.216555687\ \Versio
n=Convex-Unix-G94RevB.1\State=1-A1\HF=-368.0911016\MP2=-368.4389132\RMSE=3.937e
-09\RMSE=3.842e-05\Dipole=0. ,0. ,0.0074568\PG=C02V [C2(Si1),SGV(C2),SGV'(H2),X(H
4)]\ \@

(CH2)2SiH2+ MP4 SP
1\1\FAU-CCC-DERIOC4\SP\RMP4SDTQ-FC\6-31+G(D)\C2H6SI1\GOELLER\20-Jul-1995\0\#\RM
P4/6-31+G* SCF=DIRECT GUESS=READ GEOM=CHECKPOINT\ \SILYLCYCLOPROPANE C2V //MP2/6
-31+G*\ \0,1\Si,0. ,0. , -0.8429844531\C,0.774287806,0. ,0.8504691228\C, -0.774287806
,0. ,0.8504691228\H,0. , -1.2461748371, -1.6350349393\H,0. ,1.2461748371, -1.63503493
93\H,1.2548652164, -0.9054801363,1.216555687\H,1.2548652164,0.9054801363,1.21655
5687\H, -1.2548652164,0.9054801363,1.216555687\H, -1.2548652164, -0.9054801363,1.2
16555687\ \Version=HP-PARisc-HPUX-G94RevB.1\State=1-A1\HF=-368.0911016\MP2=-368.
4389132\MP3=-368.4693866\MP4D=-368.4798498\MP4DQ=-368.4734473\MP4SDQ=-368.47664
04\MP4SDTQ=-368.4884957\RMSE=2.512e-10\PG=C02V [C2(Si1),SGV(C2),SGV'(H2),X(H4)]
\ \@