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Fulvalenes, Fulvenes and Related Molecules:

An Ab Initio Study

Anthony P. Scott, Israel Agranat, P. Ulrich Biedermann, Noel V. Riggs, and Leo Radom

Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia, and Department of Organic Chemistry, The Hebrew University of Jerusalem, Jerusalem, 91904, Israel

SUPPORTING INFORMATION

(21 pages)

Table S1. Archive Entries Giving Geometries of Structures 1 – 12 and Selected Reference Molecules

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Cyclopropene (1)

@4438\GINC-LEONARD\FOPT\RHF\6-31G(D)\C3H4\APS501\5-Dec-1994\1\\#N RHF 6-31G(D) OPT SCFCYC=100 SCF=DIRECT\\C3H4 cyclic c2v\\0,1\C\X,1,1.\C,1,r1,2,tha1\C,1,r1,2,tha1,3,180.,0\H,1,r2,2,tha2,3,90.,0\H,1,r2,2,tha2,3,-90.,0\H,3,r3,4,tha3,1,180.,0\H,4,r3,3,tha3,1,180.,0\\r1=1.4949435\r2=1.08304908\r3=1.0677535\tha1=154.74036215\tha2=56.46085226\tha3=150.17473392\\Version=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-A1\HF=-115.8230485\RMSD=4.280e-09\RMSF=5.097e-06\Dipole=-0.,0.,-0.2206171\PG=C02V [C2(C1),SGV(C2H2),SGV'(H2)]\\@
@4442\GINC-LEONARD\FOPT\RBLYP\6-31G(D)\C3H4\APS501\6-Dec-1994\1\\#N BLYP 6-31G(D) OPT=READFC GEOM=CHECK GUESS=CHECK SCFCYC=100 SCF=DIRECT\\C3H4 cyclic c2v\\0,1\C\X,1,1.\C,1,r1,2,tha1\C,1,r1,2,tha1,3,180.,0\H,1,r2,2,tha2,3,90.,0\H,1,r2,2,tha2,3,-90.,0\H,3,r3,4,tha3,1,180.,0\H,4,r3,3,tha3,1,180.,0\\r1=1.52196543\r2=1.10240465\r3=1.08737016\tha1=154.59889229\tha2=56.50000447\tha3=149.77803095\\Version=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-A1\HF=-116.5565731\RMSD=2.119e-09\RMSF=1.095e-05\Dipole=-0.,-0.,-0.2007511\PG=C02V [C2(C1),SGV(C2H2),SGV'(H2)]\\@
@4440\GINC-LEONARD\FOPT\RMP2-FC\6-31G(D)\C3H4\APS501\5-Dec-1994\1\\#N MP2=DIRECT 6-31G(D) OPT=READFC GEOM=CHECK GUESS=CHECK SCFCYC=100 SCF=DIRECT\\C3H4 cyclic c2v\\0,1\C\X,1,1.\C,1,r1,2,tha1\C,1,r1,2,tha1,3,180.,0\H,1,r2,2,tha2,3,90.,0\H,1,r2,2,tha2,3,-90.,0\H,3,r3,4,tha3,1,180.,0\H,4,r3,3,tha3,1,180.,0\\r1=1.50687296\r2=1.09125734\r3=1.07869836\tha1=154.39150548\tha2=56.76896056\tha3=149.9719988\\Version=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-A1\HF=-115.8216142\MP2=-116.205251\RMSD=4.167e-09\RMSF=2.706e-05\Dipole=0.,0.,-0.195116\PG=C02V [C2(C1),SGV(C2H2),SGV'(H2)]\\@

Cyclopentadiene (2)

@4446\GINC-LEONARD\FOPT\RHF\6-31G(D)\C5H6\APS501\5-Dec-1994\1\\#N HF/6

-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=(DIRECT) TEST\\Cyclopentad
iene, C2V symmetry\\0,1\X\C,1,r1\X,1,r2,2,90.\C,1,r1,3,90.,2,180.,0\H,
2,r3,1,a1,3,180.,0\H,4,r3,1,a1,3,180.,0\C,3,r4,1,90.,2,0.,0\C,3,r4,1,9
0.,4,0.,0\H,7,r5,3,a2,1,180.,0\H,8,r5,3,a2,1,180.,0\C,3,r6,7,90.,2,180
.,0\X,11,1.,3,90.,7,90.,0\X,11,1.,12,90.,3,180.,0\H,11,r7,13,hcx,12,0.
,0\H,11,r7,13,hcx,12,180.,0\\hcx=53.36905261\r1=0.7383268\r2=1.2547544
3\r3=1.07409614\a1=124.38446674\r4=1.17464059\r5=1.07342483\a2=162.458
19868\r6=0.94318449\r7=1.08889982\\Version=Sun-SVR4-Unix-G92/DFT-RevF.
3\State=1-A1\HF=-192.7917209\RMSD=7.743e-09\RMSF=8.990e-06\Dipole=0.11
99584,0.,-0.\PG=C02V [C2(C1),SGV(C4H4),SGV'(H2)]\\@
@4450\GINC-LEONARD\FOPT\RBLYP\6-31G(D)\C5H6\APS501\6-Dec-1994\1\\#N BL
YP/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=(DIRECT) TEST\\Cyclope
ntadiene, C2V symmetry\\0,1\X\C,1,r1\X,1,r2,2,90.\C,1,r1,3,90.,2,180.,
0\H,2,r3,1,a1,3,180.,0\H,4,r3,1,a1,3,180.,0\C,3,r4,1,90.,2,0.,0\C,3,r4
,1,90.,4,0.,0\H,7,r5,3,a2,1,180.,0\H,8,r5,3,a2,1,180.,0\C,3,r6,7,90.,2
,180.,0\X,11,1.,3,90.,7,90.,0\X,11,1.,12,90.,3,180.,0\H,11,r7,13,hcx,1
2,0.,0\H,11,r7,13,hcx,12,180.,0\\hcx=52.76801591\r1=0.73833363\r2=1.28
355184\r3=1.09269904\a1=124.27396708\r4=1.19011393\r5=1.09125496\a2=16
2.2715927\r6=0.94078421\r7=1.10899125\\Version=Sun-SVR4-Unix-G92/DFT-R
evF.3\State=1-A1\HF=-193.9970694\RMSD=5.236e-09\RMSF=1.451e-05\Dipole=
0.1816657,0.,0.\PG=C02V [C2(C1),SGV(C4H4),SGV'(H2)]\\@
@4448\GINC-LEONARD\FOPT\RMP2-FC\6-31G(D)\C5H6\APS501\5-Dec-1994\1\\#N
MP2=DIRECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=(DIRECT) TEST\
\Cyclopentadiene, C2V symmetry\\0,1\X\C,1,r1\X,1,r2,2,90.\C,1,r1,3,90.
,2,180.,0\H,2,r3,1,a1,3,180.,0\H,4,r3,1,a1,3,180.,0\C,3,r4,1,90.,2,0.,
0\C,3,r4,1,90.,4,0.,0\H,7,r5,3,a2,1,180.,0\H,8,r5,3,a2,1,180.,0\C,3,r6
,7,90.,2,180.,0\X,11,1.,3,90.,7,90.,0\X,11,1.,12,90.,3,180.,0\H,11,r7,
13,hcx,12,0.,0\H,11,r7,13,hcx,12,180.,0\\hcx=53.16880803\r1=0.73240593
\r2=1.27872562\r3=1.08545813\a1=124.66581744\r4=1.17765745\r5=1.084560
27\a2=162.43434862\r6=0.93012725\r7=1.09936644\\Version=Sun-SVR4-Unix-
G92/DFT-RevF.3\State=1-A1\HF=-192.7896863\MP2=-193.4253766\RMSD=4.066e
-09\RMSF=8.091e-05\Dipole=0.162569,0.,-0.\PG=C02V [C2(C1),SGV(C4H4),SG
V'(H2)]\\@

Cycloheptatriene (3-C_s)

@4468\GINC-LEONARD\FOPT\RHF\6-31G(D)\C7H8\APS501\9-Dec-1994\1\\#N HF/6
-31G* OPT=READFC GEOM=CHECK GUESS=CHECK TEST\\cycloheptatriene, Cs sym
metry\\0,1\X\C,1,1.\X,2,1.,1,hf1\X,2,r2,3,hf1,1,180.,0\C,4,r3,2,90.,3,
90.,0\C,4,r3,2,90.,3,-90.,0\X,4,1.,2,hf2,3,0.,0\X,4,r4,7,hf2,2,180.,0\
C,8,r5,4,90.,7,90.,0\C,8,r5,4,90.,7,-90.,0\X,8,1.,4,hf3,7,0.,0\X,8,r6,
11,hf3,4,180.,0\C,12,r7,8,90.,11,90.,0\C,12,r7,8,90.,11,-90.,0\H,5,r8,
2,a1,3,90.,0\H,6,r8,2,a1,3,-90.,0\H,9,r10,5,a3,15,d1,0\H,10,r10,6,a3,1
6,-d1,0\H,13,r11,9,a4,17,d2,0\H,14,r11,10,a4,18,-d2,0\H,2,ch,4,hcx,7,0
.,0\H,2,ch1,4,hcx1,7,180.,0\\d1=3.40541715\d2=27.33656126\hf1=24.32880
151\hf2=114.8035213\hf3=103.14606617\ch=1.08336006\hcx=127.48576805\ch
1=1.08828884\hcx1=125.36277177\r2=0.86119305\r3=1.24012634\r4=1.295901
21\r5=1.53144829\r6=1.18043068\r7=0.66900121\r8=1.07702112\r10=1.07782
535\r11=1.07767769\a1=118.03742488\a3=118.81454876\a4=116.02915658\\Ve
rsion=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-A'\HF=-269.6823296\RMSD=7.1
46e-09\RMSF=2.857e-05\Dipole=-0.1085846,0.,-0.0408552\PG=CS [SG(C1H2),
X(C6H6)]\\@
@4525\GINC-LEONARD\FOPT\RBLYP\6-31G(D)\C7H8\APS501\12-Dec-1994\1\\#N B
LYP/6-31G* OPT=READFC GUESS=CHECK SCF=DIRECT TEST\\cycloheptatriene, C
s symmetry\\0,1\X\C,1,1.\X,2,1.,1,hf1\X,2,r2,3,hf1,1,180.,0\C,4,r3,2,9
0.,3,90.,0\C,4,r3,2,90.,3,-90.,0\X,4,1.,2,hf2,3,0.,0\X,4,r4,7,hf2,2,18
0.,0\C,8,r5,4,90.,7,90.,0\C,8,r5,4,90.,7,-90.,0\X,8,1.,4,hf3,7,0.,0\X,
8,r6,11,hf3,4,180.,0\C,12,r7,8,90.,11,90.,0\C,12,r7,8,90.,11,-90.,0\H,
5,r8,2,a1,3,90.,0\H,6,r8,2,a1,3,-90.,0\H,9,r10,5,a3,15,d1,0\H,10,r10,6
,a3,16,-d1,0\H,13,r11,9,a4,17,d2,0\H,14,r11,10,a4,18,-d2,0\H,2,ch,4,hc
x,7,0.,0\H,2,ch1,4,hcx1,7,180.,0\\d1=6.69924654\d2=22.52161929\hf1=20.
44903571\hf2=116.35145044\hf3=102.18871451\ch=1.10132895\hcx=127.46896
405\ch1=1.10839587\hcx1=125.00515014\r2=0.89171892\r3=1.23069647\r4=1.
32789319\r5=1.54208239\r6=1.17522115\r7=0.68974921\r8=1.09607087\r10=1

.09762739\r11=1.09698879\a1=118.46943216\a3=118.22012412\a4=116.390727
08\\Version=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-A'\HF=-271.3677342\RM
SD=2.703e-09\RMSF=5.152e-05\Dipole=-0.0944761,-0.,-0.066877\PG=CS [SG(
C1H2),X(C6H6)]\\@
@4527\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C7H8\APS501\27-Jan-1995\1\\#N MP2=
FULLDIRECT/6-31G* OPT=FCCARDS SCF=DIRECT TEST\\cycloheptatriene, Cs sy
mmetry\\0,1\X\C,1,1.\X,2,1.,1,hf1\X,2,r2,3,hf1,1,180.,0\C,4,r3,2,90.,3
,90.,0\C,4,r3,2,90.,3,-90.,0\X,4,1.,2,hf2,3,0.,0\X,4,r4,7,hf2,2,180.,0
\C,8,r5,4,90.,7,90.,0\C,8,r5,4,90.,7,-90.,0\X,8,1.,4,hf3,7,0.,0\X,8,r6
,11,hf3,4,180.,0\C,12,r7,8,90.,11,90.,0\C,12,r7,8,90.,11,-90.,0\H,5,r8
,2,a1,3,90.,0\H,6,r8,2,a1,3,-90.,0\H,9,r10,5,a3,15,d1,0\H,10,r10,6,a3,
16,-d1,0\H,13,r11,9,a4,17,d2,0\H,14,r11,10,a4,18,-d2,0\H,2,ch,4,hcx,7,
0.,0\H,2,ch1,4,hcx1,7,180.,0\\d1=5.70517338\d2=25.66056607\hf1=16.1425
3537\hf2=118.60389312\hf3=103.82301209\ch=1.09286658\hcx=127.57634322\
ch1=1.09885863\hcx1=123.83795162\r2=0.90485812\r3=1.19511037\r4=1.3190
5333\r5=1.51907304\r6=1.17552136\r7=0.68638266\r8=1.08860696\r10=1.089
51884\r11=1.08961326\a1=119.45413503\a3=118.76370004\a4=117.02647977\\
Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-A'\HF=-269.6770816\MP2=
-270.5709129\RMSD=5.485e-09\RMSF=1.498e-05\Dipole=-0.0781219,0.,-0.076
6913\PG=CS [SG(C1H2),X(C6H6)]\\@

Cycloheptatriene ($3\text{-}C_{2v}$)

@4464\GINC-LEONARD\FOPT\RHF\6-31G(D)\C7H8\APS501\6-Dec-1994\1\\#N HF/6
-31G* OPT=READFC GEOM=CHECK GUESS=CHECK TEST\\cycloheptatriene, C2v sy
mmetry\\0,1\X\C,1,1.\X,2,1.,1,90.\X,2,1.,1,90.,3,180.,0\X,2,r2,3,90.,1
,180.,0\C,5,r3,2,90.,3,90.,0\C,5,r3,2,90.,4,90.,0\X,2,r4,3,90.,1,180.,
0\C,8,r5,2,90.,3,90.,0\C,8,r5,2,90.,4,90.,0\X,2,r6,3,90.,1,180.,0\C,11
,r7,2,90.,3,90.,0\C,11,r7,2,90.,4,90.,0\H,6,r8,2,a1,3,90.,0\H,7,r8,2,a
1,4,90.,0\H,9,r10,6,a3,14,0.,0\H,10,r10,7,a3,15,0.,0\H,12,r11,9,a4,16,
0.,0\H,13,r11,10,a4,17,0.,0\H,2,ch,1,hcx,3,0.,0\H,2,ch,1,hcx,3,180.,0\
\ch=1.09092418\hcx=52.05399287\r2=0.75224267\r3=1.30612795\r4=2.049812
69\r5=1.57479553\r6=3.20205088\r7=0.66395847\r8=1.07878524\r10=1.07747
3\r11=1.07685348\a1=112.34769664\a3=116.05221485\a4=114.52321735\\Vers
ion=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-A1\HF=-269.6755318\RMSD=7.542
e-09\RMSF=6.795e-06\Dipole=0.,0.,-0.1923177\PG=C02V [C2(C1),SGV(C6H6),
SGV'(H2)]\\@
@4528\ ANU-VP\FOPT\RBLYP\6-31G(D)\C7H8\APS501\28-Jan-1995\1\\#N BLYP/6
-31G* OPT=FCCARDS TEST\\cycloheptatriene, C2v symmetry\\0,1\X\C,1,1.\X
,2,1.,1,90.\X,2,1.,1,90.,3,180.,0\X,2,r2,3,90.,1,180.,0\C,5,r3,2,90.,3
,90.,0\C,5,r3,2,90.,4,90.,0\X,2,r4,3,90.,1,180.,0\C,8,r5,2,90.,3,90.,0
\C,8,r5,2,90.,4,90.,0\X,2,r6,3,90.,1,180.,0\C,11,r7,2,90.,3,90.,0\C,11
,r7,2,90.,4,90.,0\H,6,r8,2,a1,3,90.,0\H,7,r8,2,a1,4,90.,0\H,9,r10,6,a3
,14,0.,0\H,10,r10,7,a3,15,0.,0\H,12,r11,9,a4,16,0.,0\H,13,r11,10,a4,17
,0.,0\H,2,ch,1,hcx,3,0.,0\H,2,ch,1,hcx,3,180.,0\\ch=1.1137248\hcx=51.4
3422021\r2=0.76193861\r3=1.31689064\r4=2.09081221\r5=1.58780142\r6=3.2
4076406\r7=0.68149312\r8=1.09850436\r10=1.09725544\r11=1.09612688\a1=1
12.45176591\a3=115.71762286\a4=114.79104241\\Version=Fujitsu-VP-Unix-G
92/DFT-RevG.1\State=1-A1\HF=-271.3597001\RMSD=1.708e-09\RMSF=9.763e-06
\Dipole=0.,0.,-0.1871685\PG=C02V [C2(C1),SGV(C6H6),SGV'(H2)]\\@
@4529\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C7H8\APS501\28-Jan-1995\1\\#N MP2=
FULLDIRECT/6-31G* OPT=FCCARDS TEST\\cycloheptatriene, C2v symmetry\\0,
1\X\C,1,1.\X,2,1.,1,90.\X,2,1.,1,90.,3,180.,0\X,2,r2,3,90.,1,180.,0\C,
5,r3,2,90.,3,90.,0\C,5,r3,2,90.,4,90.,0\X,2,r4,3,90.,1,180.,0\C,8,r5,2
,90.,3,90.,0\C,8,r5,2,90.,4,90.,0\X,2,r6,3,90.,1,180.,0\C,11,r7,2,90.,
3,90.,0\C,11,r7,2,90.,4,90.,0\H,6,r8,2,a1,3,90.,0\H,7,r8,2,a1,4,90.,0\
H,9,r10,6,a3,14,0.,0\H,10,r10,7,a3,15,0.,0\H,12,r11,9,a4,16,0.,0\H,13,
r11,10,a4,17,0.,0\H,2,ch,1,hcx,3,0.,0\H,2,ch,1,hcx,3,180.,0\\ch=1.1022
937\hcx=51.8233967\r2=0.75389536\r3=1.30329679\r4=2.07519455\r5=1.5762
1298\r6=3.22145617\r7=0.67672107\r8=1.09097398\r10=1.08933215\r11=1.08
881983\a1=112.7248907\a3=115.43248962\a4=115.10008959\\Version=Fujitsu
-VP-Unix-G92/DFT-RevG.1\State=1-A1\HF=-269.6725787\MP2=-270.5553654\RM
SD=5.361e-09\RMSF=3.340e-05\Dipole=0.,0.,-0.1709425\PG=C02V [C2(C1),SG
V(C6H6),SGV'(H2)]\\@

Triafulvene (4)

@2264\ ANU-VP\FOPT\RHF\6-31G(D)\C4H4\APS501\2-Jul-1993\1\\#N HF/6-31G*
OPT SCF=DIRECT TEST\\METHYLENECYCLOPROPENE, C2V symmetry\\0,1\C\X,1,C
1X\C,2,X2C,1,90.\H,3,CRH,1,CCRH,2,180.,0\C,2,X2C,1,90.,3,180.,0\H,5,CR
H,1,CCRH,2,180.,0\X,1,1.,2,90.,3,0.,0\C,1,CC,7,90.,2,180.,0\H,8,CHE,1,
CCHE,7,0.,0\H,8,CHE,1,CCHE,7,180.,0\\C1X=1.27083893\X2C=0.6510334\CRH=
1.06865521\CC=1.32015391\CHE=1.07421033\CCRH=148.72679829\CCHE=120.973
97061\\Version=Fujitsu-VP-Unix-G92RevD.3\State=1-A1\HF=-153.6697722\RM
SD=9.735e-09\RMSF=2.973e-05\Dipole=0.,0.,0.9199614\PG=C02V [C2(C1C1),S
GV(C2H4)]\\@
@4345\ ANU-VP\FOPT\RBLYP\6-31G(D)\C4H4\APS501\19-Aug-1994\1\\#N BLYP/6
-31G* OPT=FCCARDS SCF=DIRECT TEST\\METHYLENECYCLOPROPENE, C2V symmetry
\\0,1\C\X,1,C1X\C,2,X2C,1,90.\H,3,CRH,1,CCRH,2,180.,0\C,2,X2C,1,90.,3,
180.,0\H,5,CRH,1,CCRH,2,180.,0\X,1,1.,2,90.,3,0.,0\C,1,CC,7,90.,2,180.
,0\H,8,CHE,1,CCHE,7,0.,0\H,8,CHE,1,CCHE,7,180.,0\\C1X=1.29881796\X2C=0
.6652509\CRH=1.08904169\CC=1.33914275\CHE=1.09258237\CCRH=149.28551515
\CCHE=121.15359402\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-A1\
HF=-154.6280398\RMSD=5.838e-09\RMSF=1.964e-05\Dipole=0.,0.,0.7627592\P
G=C02V [C2(C1C1),SGV(C2H4)]\\@
@2266\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C4H4\APS501\2-Jul-1993\1\\#N MP2=F
ULLDIRECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\ME
THYLENECYCLOPROPENE, C2V symmetry\\0,1\C\X,1,C1X\C,2,X2C,1,90.\H,3,CRH
,1,CCRH,2,180.,0\C,2,X2C,1,90.,3,180.,0\H,5,CRH,1,CCRH,2,180.,0\X,1,1.
,2,90.,3,0.,0\C,1,CC,7,90.,2,180.,0\H,8,CHE,1,CCHE,7,0.,0\H,8,CHE,1,CC
HE,7,180.,0\\C1X=1.2850563\X2C=0.66383317\CRH=1.0807276\CC=1.33156586\
CHE=1.08349396\CCRH=149.25623833\CCHE=120.97552076\\Version=Fujitsu-VP
-Unix-G92RevD.3\State=1-A1\HF=-153.6680011\MP2=-154.1668221\RMSD=5.856
e-09\RMSF=7.187e-05\Dipole=0.,0.,0.7512209\PG=C02V [C2(C1C1),SGV(C2H4)
]\\@

Pentafulvene (5)

@2261\ ANU-VP\FOPT\RHF\6-31G(D)\C6H6\APS501\2-Jul-1993\1\\#N RHF/6-31G
* OPT SCF=DIRECT TEST\\pentafulvene, C2V symmetry\\0,1\C\X,1,CX2\C,2,X
CA,1,90.\C,2,XCA,1,90.,3,180.,0\X,2,XX5,3,90.,1,180.,0\C,5,XCB,2,90.,3
,0.,0\C,5,XCB,2,90.,4,0.,0\H,3,CHA,1,CCA,4,180.,0\H,4,CHA,1,CCA,3,180.
,0\H,6,CHB,3,CCB,1,180.,0\H,7,CHB,4,CCB,1,180.,0\X,1,1.,2,90.,3,90.,0\
C,1,CCE,12,90.,2,180.,0\H,13,CHE,1,CCHE,3,0.,0\H,13,CHE,1,CCHE,4,0.,0\
\CX2=0.89456754\XCA=1.17545337\XX5=1.25924457\XCB=0.73972803\CHA=1.072
63483\CHB=1.07341646\CCE=1.32538336\CHE=1.07553388\CCA=124.3110023\CCB
=126.62663965\CCHE=121.64980915\\Version=Fujitsu-VP-Unix-G92RevD.3\Sta
te=1-A1\HF=-230.6444459\RMSD=7.868e-09\RMSF=1.682e-05\Dipole=0.,0.,-0.
1695015\PG=C02V [C2(C1C1),SGV(C4H6)]\\@
@4344\ ANU-VP\FOPT\RBLYP\6-31G(D)\C6H6\APS501\19-Aug-1994\1\\#N BLYP/6
-31G* OPT=FCCARDS SCF=DIRECT TEST\\pentafulvene, C2V symmetry\\0,1\C\X
,1,CX2\C,2,XCA,1,90.\C,2,XCA,1,90.,3,180.,0\X,2,XX5,3,90.,1,180.,0\C,5
,XCB,2,90.,3,0.,0\C,5,XCB,2,90.,4,0.,0\H,3,CHA,1,CCA,4,180.,0\H,4,CHA,
1,CCA,3,180.,0\H,6,CHB,3,CCB,1,180.,0\H,7,CHB,4,CCB,1,180.,0\X,1,1.,2,
90.,3,90.,0\C,1,CCE,12,90.,2,180.,0\H,13,CHE,1,CCHE,3,0.,0\H,13,CHE,1,
CCHE,4,0.,0\\CX2=0.88902608\XCA=1.18683703\XX5=1.29108815\XCB=0.741944
12\CHA=1.09049143\CHB=1.09177159\CCE=1.35597159\CHE=1.09433686\CCA=124
.27917528\CCB=126.57994976\CCHE=121.70663208\\Version=Fujitsu-VP-Unix-
G92/DFT-RevG.1\State=1-A1\HF=-232.0776519\RMSD=7.953e-09\RMSF=2.762e-0
5\Dipole=0.,0.,-0.2219743\PG=C02V [C2(C1C1),SGV(C4H6)]\\@
@2263\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C6H6\APS501\2-Jul-1993\1\\#N MP2=F
ULLDIRECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\pe
ntafulvene, C2V symmetry\\0,1\C\X,1,CX2\C,2,XCA,1,90.\C,2,XCA,1,90.,3,
180.,0\X,2,XX5,3,90.,1,180.,0\C,5,XCB,2,90.,3,0.,0\C,5,XCB,2,90.,4,0.,
0\H,3,CHA,1,CCA,4,180.,0\H,4,CHA,1,CCA,3,180.,0\H,6,CHB,3,CCB,1,180.,0
\H,7,CHB,4,CCB,1,180.,0\X,1,1.,2,90.,3,90.,0\C,1,CCE,12,90.,2,180.,0\H
,13,CHE,1,CCHE,3,0.,0\H,13,CHE,1,CCHE,4,0.,0\\CX2=0.87632848\XCA=1.177
48537\XX5=1.28527955\XCB=0.73474624\CHA=1.08446911\CHB=1.08526251\CCE=
1.34924609\CHE=1.08665517\CCA=124.6901221\CCB=126.39359971\CCHE=121.52

988074\\Version=Fujitsu-VP-Unix-G92RevD.3\State=1-A1\HF=-230.6415825\M
P2=-231.3982788\RMSD=3.265e-09\RMSF=7.041e-05\Dipole=0.,0.,-0.2540435\
PG=C02V [C2(C1C1),SGV(C4H6)]\\@

Heptafulvene (6)

@570\ ANU-VP\FOPT\RHF\6-31G(D)\C8H8\APS501\25-Jul-1992\1\\#N HF/6-31G*
 OPT SCF=DIRECT TEST\\heptafulvene, c8h8, C2V symmetry\\0,1\C\X,1,1.\C
,1,CC,2,90.\X,1,CXA,2,90.,3,180.,0\C,4,XCA,1,90.,2,90.,0\H,5,CHA,1,CCA
,3,0.,0\C,4,XCA,1,90.,2,-90.,0\H,7,CHA,1,CCA,3,0.,0\X,4,XXB,5,90.,1,18
0.,0\C,9,XCB,4,90.,5,0.,0\H,10,CHB,5,CCB,1,180.,0\C,9,XCB,4,90.,7,0.,0
\H,12,CHB,7,CCB,1,180.,0\X,9,XXG,10,90.,5,180.,0\C,14,XCG,9,90.,10,0.,
0\H,15,CHG,10,CCG,5,180.,0\C,14,XCG,9,90.,12,0.,0\H,17,CHG,12,CCG,7,18
0.,0\H,3,CHE,1,CCE,2,-90.,0\H,3,CHE,1,CCE,2,90.,0\\CC=1.333545\CXA=0.7
10961\XCA=1.290753\CHA=1.076812\XXB=1.302963\XCB=1.565282\CHB=1.076895
\XXG=1.150728\XCG=0.665437\CHG=1.076497\CHE=1.074814\CCA=113.254274\CC
B=115.814111\CCG=114.741125\CCE=121.748705\\Version=Fujitsu-VP-Unix-G9
2RevA\State=1-A1\HF=-307.5367877\RMSD=2.984e-09\RMSF=7.502e-05\Dipole=
-0.1946841,0.,0.\PG=C02V [C2(C1C1),SGV(C6H8)]\\@
@4338\ ANU-VP\FOPT\RBLYP\6-31G(D)\C8H8\APS501\19-Aug-1994\1\\#N BLYP/6
-31G* OPT=FCCARDS SCF=DIRECT TEST\\heptafulvene C2V symmetry\\0,1\C\X,
1,1.\C,1,CC,2,90.\X,1,CXA,2,90.,3,180.,0\C,4,XCA,1,90.,2,90.,0\H,5,CHA
,1,CCA,3,0.,0\C,4,XCA,1,90.,2,-90.,0\H,7,CHA,1,CCA,3,0.,0\X,4,XXB,5,90
.,1,180.,0\C,9,XCB,4,90.,5,0.,0\H,10,CHB,5,CCB,1,180.,0\C,9,XCB,4,90.,
7,0.,0\H,12,CHB,7,CCB,1,180.,0\X,9,XXG,10,90.,5,180.,0\C,14,XCG,9,90.,
10,0.,0\H,15,CHG,10,CCG,5,180.,0\C,14,XCG,9,90.,12,0.,0\H,17,CHG,12,CC
G,7,180.,0\H,3,CHE,1,CCE,2,-90.,0\H,3,CHE,1,CCE,2,90.,0\\CC=1.37002346
\CXA=0.71549788\XCA=1.28772296\CHA=1.09719951\XXB=1.33689497\XCB=1.575
98788\CHB=1.09640324\XXG=1.14805389\XCG=0.68427703\CHG=1.09588907\CHE=
1.09277915\CCA=113.20590116\CCB=115.57371035\CCG=115.12802901\CCE=121.
59289107\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-A1\HF=-309.45
35624\RMSD=9.784e-09\RMSF=4.868e-05\Dipole=-0.3296027,0.,0.\PG=C02V [C
2(C1C1),SGV(C6H8)]\\@
@2258\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C8H8\APS501\1-Jul-1993\1\\#N MP2=F
ULLDIRECT/6-31G* OPT SCF=DIRECT TEST\\heptafulvene, c8h8, C2V symmetry
\\0,1\C\X,1,1.\C,1,CC,2,90.\X,1,CXA,2,90.,3,180.,0\C,4,XCA,1,90.,2,90.
,0\H,5,CHA,1,CCA,3,0.,0\C,4,XCA,1,90.,2,-90.,0\H,7,CHA,1,CCA,3,0.,0\X,
4,XXB,5,90.,1,180.,0\C,9,XCB,4,90.,5,0.,0\H,10,CHB,5,CCB,1,180.,0\C,9,
XCB,4,90.,7,0.,0\H,12,CHB,7,CCB,1,180.,0\X,9,XXG,10,90.,5,180.,0\C,14,
XCG,9,90.,10,0.,0\H,15,CHG,10,CCG,5,180.,0\C,14,XCG,9,90.,12,0.,0\H,17
,CHG,12,CCG,7,180.,0\H,3,CHE,1,CCE,2,-90.,0\H,3,CHE,1,CCE,2,90.,0\\CC=
1.35998351\CXA=0.70268222\XCA=1.28226442\CHA=1.0906867\XXB=1.32898812\
XCB=1.56805763\CHB=1.08915297\XXG=1.14135146\XCG=0.67975969\CHG=1.0887
7477\CHE=1.085675\CCA=113.57224327\CCB=115.32651362\CCG=115.3482362\CC
E=121.52582589\\Version=Fujitsu-VP-Unix-G92RevD.3\State=1-A1\HF=-307.5
324249\MP2=-308.541448\RMSD=9.750e-09\RMSF=5.725e-05\Dipole=-0.2639707
,0.,0.\PG=C02V [C2(C1C1),SGV(C6H8)]\\@

Triafulvalene (7)

@4296\ ANU-VP\FOPT\RHF\6-31G(D)\C6H4\APS501\3-Aug-1994\1\\#N HF/6-31G*
 OPT=FCCARDS SCF=DIRECT TEST\\triafulvalene, D2H symmetry\\0,1\C\C,1,R
1\X,2,1.,1,90.\X,2,R2,3,90.,1,180.,0\C,4,R3,2,90.,3,90.,0\C,4,R3,2,90.
,5,180.,0\X,1,1.,2,90.,3,0.,0\X,1,R2,7,90.,2,180.,0\C,8,R3,1,90.,7,90.
,0\C,8,R3,1,90.,9,180.,0\H,5,R4,2,A1,4,180.,0\H,6,R4,2,A1,4,180.,0\H,9
,R4,1,A1,8,180.,0\H,10,R4,1,A1,8,180.,0\\R1=1.29865988\R2=1.2965371\R3
=0.647676\R4=1.06877562\A1=148.26065281\\Version=Fujitsu-VP-Unix-G92/D
FT-RevG.1\State=1-AG\HF=-229.2822182\RMSD=4.331e-09\RMSF=2.955e-05\Dip
ole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C4H4)]\\@
@4340\ ANU-VP\FOPT\RBLYP\6-31G(D)\C6H4\APS501\19-Aug-1994\1\\#N BLYP/6
-31G* OPT=FCCARDS SCF=DIRECT TEST\\triafulvalene, D2H symmetry\\0,1\C\
C,1,R1\X,2,1.,1,90.\X,2,R2,3,90.,1,180.,0\C,4,R3,2,90.,3,90.,0\C,4,R3,
2,90.,5,180.,0\X,1,1.,2,90.,3,0.,0\X,1,R2,7,90.,2,180.,0\C,8,R3,1,90.,
7,90.,0\C,8,R3,1,90.,9,180.,0\H,5,R4,2,A1,4,180.,0\H,6,R4,2,A1,4,180.,
0\H,9,R4,1,A1,8,180.,0\H,10,R4,1,A1,8,180.,0\\R1=1.31960285\R2=1.32181

927\R3=0.66217274\R4=1.08905152\A1=148.72040394\\Version=Fujitsu-VP-Un
ix-G92/DFT-RevG.1\State=1-AG\HF=-230.6993364\RMSD=4.958e-09\RMSF=3.176
e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C4H4)]\\@
@4298\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C6H4\APS501\3-Aug-1994\1\\#N MP2=F
ULLDIRECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\tr
iafulvalene, D2H symmetry\\0,1\C\C,1,R1\X,2,1.,1,90.\X,2,R2,3,90.,1,18
0.,0\C,4,R3,2,90.,3,90.,0\C,4,R3,2,90.,5,180.,0\X,1,1.,2,90.,3,0.,0\X,
1,R2,7,90.,2,180.,0\C,8,R3,1,90.,7,90.,0\C,8,R3,1,90.,9,180.,0\H,5,R4,
2,A1,4,180.,0\H,6,R4,2,A1,4,180.,0\H,9,R4,1,A1,8,180.,0\H,10,R4,1,A1,8
,180.,0\\R1=1.31223024\R2=1.30492586\R3=0.6616255\R4=1.08092307\A1=148
.69257626\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-AG\HF=-229.2
790695\MP2=-230.0304188\RMSD=4.728e-09\RMSF=2.781e-05\Dipole=0.,0.,0.\
PG=D02H [C2"(C1.C1),SG(C4H4)]\\@
@4364\GINC-LEONARD\FOPT\RMP2-FC\6-31G(D)\C6H4\APS501\6-Sep-1994\1\\#N
MP2=DIRECT/6-31G* OPT=CALCHFFC SCF=DIRECT TEST\\triafulvalene, C2H sym
metry\\0,1\C\C,1,R1\X,2,1.,1,90.\X,2,R2,3,a2,1,180.,0\C,4,R3,2,90.,3,9
0.,0\C,4,R3,2,90.,5,180.,0\X,1,1.,2,90.,3,180.,0\X,1,R2,7,a2,2,180.,0\
C,8,R3,1,90.,7,90.,0\C,8,R3,1,90.,9,180.,0\H,5,R4,2,A1,4,d1,0\H,6,R4,2
,A1,4,-d1,0\H,9,R4,1,A1,8,d1,0\H,10,R4,1,A1,8,-d1,0\\d1=178.317704\R1=
1.3141345\R2=1.30521976\R3=0.66158348\R4=1.08087774\A1=148.71529877\a2
=96.14977593\\Version=Sun-SVR4-Unix-G92/DFT-RevF.3\State=1-AG\HF=-229.
2784425\MP2=-230.0304916\RMSD=4.256e-09\RMSF=1.543e-05\Dipole=0.,-0.,0
.\PG=C02H [SGH(C2),X(C4H4)]\\@
1\1\ ANU-PC\FOpt\RMP2-FC\6-311+G(2df,p)\C6H4\APS501\12-Sep-1996\0\\#N
MP2=FULLDIRECT/6-311+G(2DF,P) OPT SCF=DIRECT TEST MAXDISK=250000000 MA
XDISK=250000000\\triafulvalene, D2H symmetry\\0,1\C,0.,0.,0.65452977\C
,0.,0.,-0.65452977\C,0.,0.65947566,-1.95512249\C,0.,-0.65947566,-1.955
12249\C,0.,-0.65947566,1.95512249\C,0.,0.65947566,1.95512249\H,0.,1.57
27125573,-2.5285147547\H,0.,-1.5727125573,-2.5285147547\H,0.,-1.572712
5573,2.5285147547\H,0.,1.5727125573,2.5285147547\\Version=SGI-G94RevD.
3\State=1-AG\HF=-229.3528132\MP2=-230.2615681\RMSD=2.288e-09\RMSF=2.43
2e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C4H4)]\\@

Triapentafulvalene (8)

@578\ ANU-VP\FOPT\RHF\6-31G(D)\C8H6\APS501\26-Jul-1992\1\\#N RHF/6-31G
* OPT SCF=DIRECT TEST\\triapentafulvalene C2V symmetry\\0,1\X\X,1,1.\C
,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,90.,1,180.,0\C,5,R3,3,90.,4,9
0.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,6,90.,8,90.,0\C,
9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\H,6,R6,10,A2,9,180.,0\H,7,R6,11,
A2,9,180.,0\H,10,R7,6,A3,5,180.,0\H,11,R7,7,A3,5,180.,0\C,1,R1,2,90.,3
,180.,0\X,16,1.,1,90.,2,0.,0\X,16,R8,17,90.,1,180.,0\C,18,R9,16,90.,17
,90.,0\C,18,R9,16,90.,17,-90.,0\H,19,R10,16,A4,20,180.,0\H,20,R10,16,A
4,19,180.,0\\R1=0.670867\R2=0.872484\R3=1.165222\R4=1.272683\R5=0.7291
07\R6=1.073675\R7=1.073865\R8=1.251627\R9=0.653828\R10=1.068255\A2=127
.12135\A3=126.292789\A4=148.76879\\Version=Fujitsu-VP-Unix-G92RevA\Sta
te=1-A1\HF=-306.291533\RMSD=2.853e-09\RMSF=5.760e-05\Dipole=-1.9175297
,0.,0.\PG=C02V [C2(C1C1),SGV(C6H6)]\\@
@4343\ ANU-VP\FOPT\RBLYP\6-31G(D)\C8H6\APS501\19-Aug-1994\1\\#N BLYP/6
-31G* OPT=FCCARDS SCF=DIRECT TEST\\triapentafulvalene C2V symmetry\\0,
1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,90.,1,180.,0\C,5,
R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,6,90
.,8,90.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\H,6,R6,10,A2,9,180.,
0\H,7,R6,11,A2,9,180.,0\H,10,R7,6,A3,5,180.,0\H,11,R7,7,A3,5,180.,0\C,
1,R1,2,90.,3,180.,0\X,16,1.,1,90.,2,0.,0\X,16,R8,17,90.,1,180.,0\C,18,
R9,16,90.,17,90.,0\C,18,R9,16,90.,17,-90.,0\H,19,R10,16,A4,20,180.,0\H
,20,R10,16,A4,19,180.,0\\R1=0.6810672\R2=0.87323786\R3=1.18078244\R4=1
.30168759\R5=0.73261626\R6=1.09091368\R7=1.09211152\R8=1.28045972\R9=0
.66814506\R10=1.08861317\A2=127.74839263\A3=126.15580465\A4=149.351680
3\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-A1\HF=-308.1770331\R
MSD=5.991e-09\RMSF=1.106e-04\Dipole=-1.6936728,0.,0.\PG=C02V [C2(C1C1)
,SGV(C6H6)]\\@
@4295\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C8H6\APS501\3-Aug-1994\1\\#N MP2=F
ULLDIRECT/6-31G* OPT=FCCARDS SCF=DIRECT TEST\\triapentafulvalene C2V s

ymmetry\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,90.,1,
180.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\
X,5,R4,6,90.,8,90.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\H,6,R6,10
,A2,9,180.,0\H,7,R6,11,A2,9,180.,0\H,10,R7,6,A3,5,180.,0\H,11,R7,7,A3,
5,180.,0\C,1,R1,2,90.,3,180.,0\X,16,1.,1,90.,2,0.,0\X,16,R8,17,90.,1,1
80.,0\C,18,R9,16,90.,17,90.,0\C,18,R9,16,90.,17,-90.,0\H,19,R10,16,A4,
20,180.,0\H,20,R10,16,A4,19,180.,0\\R1=0.67580415\R2=0.85915604\R3=1.1
7157267\R4=1.2955043\R5=0.72562447\R6=1.08489749\R7=1.08545814\R8=1.26
643217\R9=0.6671923\R10=1.08082434\A2=127.65750105\A3=126.04226291\A4=
149.36436834\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-A1\HF=-30
6.2882067\MP2=-307.2929693\RMSD=8.014e-09\RMSF=1.119e-05\Dipole=-1.748
6625,0.,0.\PG=C02V [C2(C1C1),SGV(C6H6)]\\@

Triaheptafulvalene (9)

@574\ ANU-VP\FOPT\RHF\6-31G(D)\C10H8\APS501\25-Jul-1992\1\\#N RHF/6-31
G* OPT=READFC SCF=DIRECT TEST\\triaheptafulvalene C2V symmetry\\0,1\C\
X,1,1.\C,1,CC,2,90.\X,1,CXA,2,90.,3,180.,0\C,4,XCA,1,90.,2,90.,0\H,5,C
HA,1,CCA,3,0.,0\C,4,XCA,1,90.,2,-90.,0\H,7,CHA,1,CCA,3,0.,0\X,4,XXB,5,
90.,1,180.,0\C,9,XCB,4,90.,5,0.,0\H,10,CHB,5,CCB,1,180.,0\C,9,XCB,4,90
.,7,0.,0\H,12,CHB,7,CCB,1,180.,0\X,9,XXG,10,90.,5,180.,0\C,14,XCG,9,90
.,10,0.,0\H,15,CHG,10,CCG,5,180.,0\C,14,XCG,9,90.,12,0.,0\H,17,CHG,12,
CCG,7,180.,0\X,3,1.,1,90.,2,0.,0\X,3,CXT,19,90.,1,180.,0\C,20,XCT,3,90
.,19,90.,0\H,21,CHT,3,CCT,20,180.,0\C,20,XCT,3,90.,21,180.,0\H,23,CHT,
3,CCT,20,180.,0\\CC=1.33508052\CXA=0.69726402\XCA=1.29577379\CHA=1.078
20755\XXB=1.29979923\XCB=1.57758372\CHB=1.07698611\XXG=1.15192421\XCG=
0.66429321\CHG=1.07718147\CXT=1.26700429\XCT=0.65162196\CHT=1.0683246\
CCA=113.5287908\CCB=116.29740946\CCG=114.52591805\CCT=148.79548955\\Ve
rsion=Fujitsu-VP-Unix-G92RevA\State=1-A1\HF=-383.171709\RMSD=4.068e-09
\RMSF=2.739e-05\Dipole=1.4243938,0.,0.\PG=C02V [C2(C1C1),SGV(C8H8)]\\@
@4341\ ANU-VP\FOPT\RBLYP\6-31G(D)\C10H8\APS501\19-Aug-1994\1\\#N BLYP/
6-31G* OPT=FCCARDS SCF=DIRECT TEST\\triaheptafulvalene C2V symmetry\\0
,1\C\X,1,1.\C,1,CC,2,90.\X,1,CXA,2,90.,3,180.,0\C,4,XCA,1,90.,2,90.,0\
H,5,CHA,1,CCA,3,0.,0\C,4,XCA,1,90.,2,-90.,0\H,7,CHA,1,CCA,3,0.,0\X,4,X
XB,5,90.,1,180.,0\C,9,XCB,4,90.,5,0.,0\H,10,CHB,5,CCB,1,180.,0\C,9,XCB
,4,90.,7,0.,0\H,12,CHB,7,CCB,1,180.,0\X,9,XXG,10,90.,5,180.,0\C,14,XCG
,9,90.,10,0.,0\H,15,CHG,10,CCG,5,180.,0\C,14,XCG,9,90.,12,0.,0\H,17,CH
G,12,CCG,7,180.,0\X,3,1.,1,90.,2,0.,0\X,3,CXT,19,90.,1,180.,0\C,20,XCT
,3,90.,19,90.,0\H,21,CHT,3,CCT,20,180.,0\C,20,XCT,3,90.,21,180.,0\H,23
,CHT,3,CCT,20,180.,0\\CC=1.36366908\CXA=0.70132057\XCA=1.29779593\CHA=
1.09755659\XXB=1.33306069\XCB=1.58764957\CHB=1.09626469\XXG=1.1514916\
XCG=0.68193793\CHG=1.09640338\CXT=1.29628837\XCT=0.66584888\CHT=1.0884
205\CCA=113.43100041\CCB=115.8867154\CCG=114.83558064\CCT=149.45993314
\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-A1\HF=-385.5384981\RM
SD=9.651e-09\RMSF=4.944e-05\Dipole=1.1011019,0.,0.\PG=C02V [C2(C1C1),S
GV(C8H8)]\\@
@784\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C10H8\LXR501\20-Sep-1992\1\\#N MP2=
FULLDIRECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\t
riaheptafulvalene C2V symmetry\\0,1\C\X,1,1.\C,1,CC,2,90.\X,1,CXA,2,90
.,3,180.,0\C,4,XCA,1,90.,2,90.,0\H,5,CHA,1,CCA,3,0.,0\C,4,XCA,1,90.,2,
-90.,0\H,7,CHA,1,CCA,3,0.,0\X,4,XXB,5,90.,1,180.,0\C,9,XCB,4,90.,5,0.,
0\H,10,CHB,5,CCB,1,180.,0\C,9,XCB,4,90.,7,0.,0\H,12,CHB,7,CCB,1,180.,0
\X,9,XXG,10,90.,5,180.,0\C,14,XCG,9,90.,10,0.,0\H,15,CHG,10,CCG,5,180.
,0\C,14,XCG,9,90.,12,0.,0\H,17,CHG,12,CCG,7,180.,0\X,3,1.,1,90.,2,0.,0
\X,3,CXT,19,90.,1,180.,0\C,20,XCT,3,90.,19,90.,0\H,21,CHT,3,CCT,20,180
.,0\C,20,XCT,3,90.,21,180.,0\H,23,CHT,3,CCT,20,180.,0\\CC=1.35012212\C
XA=0.68586073\XCA=1.29225365\CHA=1.09142581\XXB=1.32487078\XCB=1.58031
46\CHB=1.08893592\XXG=1.1437696\XCG=0.67775348\CHG=1.08913999\CXT=1.28
329275\XCT=0.66480876\CHT=1.08086503\CCA=113.74911491\CCB=115.69401572
\CCG=115.07697936\CCT=149.48373789\\Version=Fujitsu-VP-Unix-G92RevC\St
ate=1-A1\HF=-383.166643\MP2=-384.421941\RMSD=3.836e-09\RMSF=1.099e-05\
Dipole=1.0620275,0.,0.\PG=C02V [C2(C1C1),SGV(C8H8)]\\@

Pentafulvalene (10)

@782\ ANU-VP\FOPT\RHF\6-31G(D)\C10H8\APS501\16-Oct-1992\1\\#N RHF/6-31
G* OPT SCF=DIRECT TEST\\Pentafulvalene, D2H symmetry\\0,1\X\X,1,1.\C,1
,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,90.,1,180.,0\C,5,R3,3,90.,4,90.
,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,8,90.,3,180.,0\C,9
,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\H,6,CH1,3,CC1,7,180.,0\H,7,CH1,3,
CC1,6,180.,0\H,10,CH2,6,CC2,3,180.,0\H,11,CH2,7,CC2,3,180.,0\C,1,R1,2,
90.,3,180.,0\X,16,1.,1,90.,2,0.,0\X,16,R2,17,90.,1,180.,0\C,18,R3,16,9
0.,17,90.,0\C,18,R3,16,90.,17,-90.,0\X,18,1.,16,90.,17,0.,0\X,18,R4,21
,90.,16,180.,0\C,22,R5,18,90.,19,0.,0\C,22,R5,18,90.,20,0.,0\H,19,CH1,
16,CC1,20,180.,0\H,20,CH1,16,CC1,19,180.,0\H,23,CH2,19,CC2,16,180.,0\H
,24,CH2,20,CC2,16,180.,0\\R1=0.66956699\R2=0.89341687\R3=1.17498419\R4
=1.25965736\R5=0.73963617\CH1=1.07121663\CH2=1.07321531\CC1=124.787110
33\CC2=126.55017023\\Version=Fujitsu-VP-Unix-G92RevC\State=1-AG\HF=-38
3.2571167\RMSD=8.343e-09\RMSF=1.742e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C
1.C1),SG(C8H8)]\\@
@4339\ ANU-VP\FOPT\RBLYP\6-31G(D)\C10H8\APS501\19-Aug-1994\1\\#N BLYP/
6-31G* OPT=FCCARDS SCF=DIRECT TEST\\Pentafulvalene, C2V symmetry\\0,1\
X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,90.,1,180.,0\C,5,R3
,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,8,90.,
3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\H,6,CH1,3,CC1,7,180.,
0\H,7,CH1,3,CC1,6,180.,0\H,10,CH2,6,CC2,3,180.,0\H,11,CH2,7,CC2,3,180.
,0\C,1,R1,2,90.,3,180.,0\X,16,1.,1,90.,2,0.,0\X,16,R2,17,90.,1,180.,0\
C,18,R3,16,90.,17,90.,0\C,18,R3,16,90.,17,-90.,0\X,18,1.,16,90.,17,0.,
0\X,18,R4,21,90.,16,180.,0\C,22,R5,18,90.,19,0.,0\C,22,R5,18,90.,20,0.
,0\H,19,CH1,16,CC1,20,180.,0\H,20,CH1,16,CC1,19,180.,0\H,23,CH2,19,CC2
,16,180.,0\H,24,CH2,20,CC2,16,180.,0\\R1=0.68949789\R2=0.88536852\R3=1
.18581941\R4=1.29264886\R5=0.74306114\CH1=1.08890353\CH2=1.09150543\CC
1=124.81903443\CC2=126.56734927\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.
1\State=1-AG\HF=-385.618628\RMSD=1.417e-09\RMSF=3.164e-05\Dipole=0.,0.
,0.\PG=D02H [C2"(C1.C1),SG(C8H8)]\\@
@2260\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C10H8\APS501\2-Jul-1993\1\\#N MP2=
FULLDIRECT/6-31G* OPT SCF=DIRECT TEST\\Pentafulvalene, D2H symmetry\\0
,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,90.,1,180.,0\C,5
,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,8,9
0.,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\H,6,CH1,3,CC1,7,18
0.,0\H,7,CH1,3,CC1,6,180.,0\H,10,CH2,6,CC2,3,180.,0\H,11,CH2,7,CC2,3,1
80.,0\C,1,R1,2,90.,3,180.,0\X,16,1.,1,90.,2,0.,0\X,16,R2,17,90.,1,180.
,0\C,18,R3,16,90.,17,90.,0\C,18,R3,16,90.,17,-90.,0\X,18,1.,16,90.,17,
0.,0\X,18,R4,21,90.,16,180.,0\C,22,R5,18,90.,19,0.,0\C,22,R5,18,90.,20
,0.,0\H,19,CH1,16,CC1,20,180.,0\H,20,CH1,16,CC1,19,180.,0\H,23,CH2,19,
CC2,16,180.,0\H,24,CH2,20,CC2,16,180.,0\\R1=0.68439645\R2=0.87229184\R
3=1.17796186\R4=1.28650735\R5=0.73580626\CH1=1.08327625\CH2=1.0852887\
CC1=125.24298213\CC2=126.39413356\\Version=Fujitsu-VP-Unix-G92RevD.3\S
tate=1-AG\HF=-383.2519325\MP2=-384.5158051\RMSD=2.331e-09\RMSF=3.339e-
05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C8H8)]\\@

Pentaheptafulvalene (11-C_s)

@621\ ANU-VP\FOPT\RHF\6-31G(D)\C12H10\APS501\19-Aug-1992\1\\#N RHF/6-3
1G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\Pentaheptafulva
lene, CS symmetry\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R
2,4,A2,1,180.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90
.,4,0.,0\X,5,R4,8,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\
X,9,1.,5,90.,8,0.,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,
R7,9,90.,12,-90.,0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2
,6,CC2,3,D2,0\H,11,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,1
1,CC3,7,-D3,0\C,1,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,R2a,23
,A2a,1,180.,0\C,24,R3a,22,90.,23,90.,0\C,24,R3a,22,90.,23,-90.,0\X,24,
1.,22,90.,23,0.,0\X,24,R4a,27,A4a,22,180.,0\C,28,R5a,24,90.,25,0.,0\C,
28,R5a,24,90.,26,0.,0\H,25,CH1a,22,CC1a,26,D1a,0\H,26,CH1a,22,CC1a,25,
-D1a,0\H,29,CH2a,25,CC2a,22,D2a,0\H,30,CH2a,26,CC2a,22,-D2a,0\\R1=0.67
807211\R2=0.73332917\R3=1.27250114\R4=1.30734376\R5=1.54586239\R2a=0.8
9737562\R3a=1.16679769\R4a=1.26548813\R5a=0.73303684\R6=1.15754894\R7=
0.66663707\CH1=1.07272759\CH2=1.07682491\CH1a=1.07088852\CH2a=1.073415

05\CH3=1.07624971\A2=93.59260291\A4=73.48636391\A2a=91.12301738\A4a=89
.94068957\A6=80.23316139\CC1=114.41575415\CC2=115.62730449\CC1a=125.77
65172\CC2a=126.2875208\CC3=115.1538797\D1=200.47755251\D2=178.25150704
\D1a=180.80152347\D2a=180.18508018\D3=169.45084518\\Version=Fujitsu-VP
-Unix-G92RevB\State=1-A'\HF=-460.1487906\RMSD=8.574e-09\RMSF=9.848e-06
\Dipole=0.872941,0.,0.0395748\PG=CS [SG(C2),X(C10H10)]\\@
@2397\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C12H10\APS501\3-Aug-1993\1\\#N MP2
=FULLDIRECT/6-31G* OPT=READFC GUESS=CHECK SCF=DIRECT TEST\\Pentaheptaf
ulvalene, CS symmetry\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X
,3,R2,4,A2,1,180.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,
3,90.,4,0.,0\X,5,R4,8,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0
.,0\X,9,1.,5,90.,8,0.,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C
,13,R7,9,90.,12,-90.,0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10
,CH2,6,CC2,3,D2,0\H,11,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,C
H3,11,CC3,7,-D3,0\C,1,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,R2
a,23,A2a,1,180.,0\C,24,R3a,22,90.,23,90.,0\C,24,R3a,22,90.,23,-90.,0\X
,24,1.,22,90.,23,0.,0\X,24,R4a,27,A4a,22,180.,0\C,28,R5a,24,90.,25,0.,
0\C,28,R5a,24,90.,26,0.,0\H,25,CH1a,22,CC1a,26,D1a,0\H,26,CH1a,22,CC1a
,25,-D1a,0\H,29,CH2a,25,CC2a,22,D2a,0\H,30,CH2a,26,CC2a,22,-D2a,0\\R1=
0.69668977\R2=0.71436733\R3=1.26089375\R4=1.33760048\R5=1.55038599\R2a
=0.87336937\R3a=1.16670174\R4a=1.29639847\R5a=0.72619266\R6=1.14149616
\R7=0.68314714\CH1=1.08701264\CH2=1.08943736\CH1a=1.08368449\CH2a=1.08
558296\CH3=1.08872941\A2=94.36365691\A4=75.50009258\A2a=91.23508881\A4
a=89.8702269\A6=82.35659188\CC1=114.5872744\CC2=115.07170234\CC1a=126.
50603748\CC2a=126.02856852\CC3=115.76885809\D1=197.38724247\D2=177.681
26098\D1a=181.41185\D2a=180.14361856\D3=172.69222744\\Version=Fujitsu-
VP-Unix-G92RevD.3\State=1-A'\HF=-460.1411243\MP2=-461.6652553\RMSD=6.9
29e-09\RMSF=2.356e-05\Dipole=1.3268437,0.,0.0401707\PG=CS [SG(C2),X(C1
0H10)]\\@

Pentaheptafulvalene ($11\text{-}C_{2v}$)

@594\ ANU-VP\FOPT\RHF\6-31G(D)\C12H10\APS501\11-Aug-1992\1\\#N RHF/6-3
1G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\pentaheptafulva
lene, c12h10, C2V symmetry\\0,1\C\X,1,1.\C,1,CC,2,90.\X,1,CXA,2,90.,3,
180.,0\C,4,XCA,1,90.,2,90.,0\H,5,CHA,1,CCA,3,0.,0\C,4,XCA,1,90.,2,-90.
,0\H,7,CHA,1,CCA,3,0.,0\X,4,XXB,5,90.,1,180.,0\C,9,XCB,4,90.,5,0.,0\H,
10,CHB,5,CCB,1,180.,0\C,9,XCB,4,90.,7,0.,0\H,12,CHB,7,CCB,1,180.,0\X,9
,XXG,10,90.,5,180.,0\C,14,XCG,9,90.,10,0.,0\H,15,CHG,10,CCG,5,180.,0\C
,14,XCG,9,90.,12,0.,0\H,17,CHG,12,CCG,7,180.,0\X,3,1.,1,90.,2,0.,0\X,3
,CXT,19,90.,1,180.,0\C,20,XCT,3,90.,19,90.,0\H,21,CHT,3,CCT,20,180.,0\
C,20,XCT,3,90.,21,180.,0\H,23,CHT,3,CCT,20,180.,0\X,20,xx,21,90.,3,180
.,0\C,25,cx,20,90.,21,0.,0\H,26,ch,21,cch9,3,180.,0\C,25,cx,20,90.,23,
0.,0\H,28,ch,23,cch9,3,180.,0\\xx=1.26601782\cx=0.73216776\ch=1.073404
77\cch9=126.23933482\CC=1.36029198\CXA=0.72130551\XCA=1.27663174\CHA=1
.07146911\XXB=1.30869743\XCB=1.54913811\CHB=1.07668645\XXG=1.15357176\
XCG=0.66652337\CHG=1.07610918\CXT=0.89935038\XCT=1.16551868\CHT=1.0706
0056\CCA=114.16177663\CCB=115.21931251\CCG=115.04763891\CCT=126.044359
38\\Version=Fujitsu-VP-Unix-G92RevB\State=1-A1\HF=-460.1486107\RMSD=5.
330e-09\RMSF=9.044e-06\Dipole=-0.9443084,0.,0.\PG=C02V [C2(C1C1),SGV(C
10H10)]\\@
@4342\ ANU-VP\FOPT\RBLYP\6-31G(D)\C12H10\APS501\19-Aug-1994\1\\#N BLYP
/6-31G* OPT=FCCARDS SCF=DIRECT TEST\\pentaheptafulvalene, c12h10, C2V
symmetry\\0,1\C\X,1,1.\C,1,CC,2,90.\X,1,CXA,2,90.,3,180.,0\C,4,XCA,1,9
0.,2,90.,0\H,5,CHA,1,CCA,3,0.,0\C,4,XCA,1,90.,2,-90.,0\H,7,CHA,1,CCA,3
,0.,0\X,4,XXB,5,90.,1,180.,0\C,9,XCB,4,90.,5,0.,0\H,10,CHB,5,CCB,1,180
.,0\C,9,XCB,4,90.,7,0.,0\H,12,CHB,7,CCB,1,180.,0\X,9,XXG,10,90.,5,180.
,0\C,14,XCG,9,90.,10,0.,0\H,15,CHG,10,CCG,5,180.,0\C,14,XCG,9,90.,12,0
.,0\H,17,CHG,12,CCG,7,180.,0\X,3,1.,1,90.,2,0.,0\X,3,CXT,19,90.,1,180.
,0\C,20,XCT,3,90.,19,90.,0\H,21,CHT,3,CCT,20,180.,0\C,20,XCT,3,90.,21,
180.,0\H,23,CHT,3,CCT,20,180.,0\X,20,xx,21,90.,3,180.,0\C,25,cx,20,90.
,21,0.,0\H,26,ch,21,cch9,3,180.,0\C,25,cx,20,90.,23,0.,0\H,28,ch,23,cc
h9,3,180.,0\\xx=1.30444135\cx=0.732194\ch=1.09170873\cch9=126.15940795
\CC=1.40853107\CXA=0.71478507\XCA=1.27275042\CHA=1.092435\XXB=1.345124

44\XCB=1.5640025\CHB=1.09611601\XXG=1.14581664\XCG=0.68700782\CHG=1.09
555241\CXT=0.88537729\XCT=1.17374971\CHT=1.08968641\CCA=114.06268022\C
CB=115.16667328\CCG=115.44657664\CCT=126.07963766\\Version=Fujitsu-VP-
Unix-G92/DFT-RevG.1\State=1-A1\HF=-463.0001347\RMSD=4.951e-09\RMSF=4.7
21e-05\Dipole=-1.3859236,0.,0.\PG=C02V [C2(C1C1),SGV(C10H10)]\\@
@2652\ ANU-VP\FOPT\RMP2-FC\6-31G(D)\C12H10\APS501\23-Oct-1993\1\\#N MP
2=FULLDIRECT/6-31G* OPT=READFC GUESS=CHECK SCF=DIRECT TEST\\pentahepta
fulvalene, c12h10, C2V symmetry\\0,1\C\X,1,1.\C,1,CC,2,90.\X,1,CXA,2,9
0.,3,180.,0\C,4,XCA,1,90.,2,90.,0\H,5,CHA,1,CCA,3,0.,0\C,4,XCA,1,90.,2
,-90.,0\H,7,CHA,1,CCA,3,0.,0\X,4,XXB,5,90.,1,180.,0\C,9,XCB,4,90.,5,0.
,0\H,10,CHB,5,CCB,1,180.,0\C,9,XCB,4,90.,7,0.,0\H,12,CHB,7,CCB,1,180.,
0\X,9,XXG,10,90.,5,180.,0\C,14,XCG,9,90.,10,0.,0\H,15,CHG,10,CCG,5,180
.,0\C,14,XCG,9,90.,12,0.,0\H,17,CHG,12,CCG,7,180.,0\X,3,1.,1,90.,2,0.,
0\X,3,CXT,19,90.,1,180.,0\C,20,XCT,3,90.,19,90.,0\H,21,CHT,3,CCT,20,18
0.,0\C,20,XCT,3,90.,21,180.,0\H,23,CHT,3,CCT,20,180.,0\X,20,xx,21,90.,
3,180.,0\C,25,cx,20,90.,21,0.,0\H,26,ch,21,cch9,3,180.,0\C,25,cx,20,90
.,23,0.,0\H,28,ch,23,cch9,3,180.,0\\xx=1.29690162\cx=0.72565225\ch=1.0
8556013\cch9=126.01606201\CC=1.39744201\CXA=0.70465134\XCA=1.26464074\
CHA=1.08627548\XXB=1.33868444\XCB=1.55314759\CHB=1.08935972\XXG=1.1383
9886\XCG=0.68303111\CHG=1.08868886\CXT=0.8751117\XCT=1.16561761\CHT=1.
08359726\CCA=114.4394468\CCB=114.84487383\CCG=115.69378919\CCT=126.732
1836\\Version=Fujitsu-VP-Unix-G92RevE.2\State=1-A1\HF=-460.14099\MP2=-
461.6651219\RMSD=9.896e-09\RMSF=6.877e-05\Dipole=-1.3844248,0.,0.\PG=C
02V [C2(C1C1),SGV(C10H10)]\\@

Heptafulvalene (12-C_{2h})

@597\GINC-RSCQC3\FREQ\RHF\6-31G(D)\C14H12\ASCOTT\11-Aug-1992\1\\#N RHF
/6-31G* FREQ=NORAMAN SCF=DIRECT TEST\\Heptafulvalene, C2h symmetry, an
ti bend\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,A2,1,1
80.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X
,5,R4,8,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\X,9,1.,5,9
0.,8,0.,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,R7,9,90.,1
2,-90.,0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2,6,CC2,3,D
2,0\H,11,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,11,CC3,7,-D
3,0\C,1,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,R2,23,A2,1,180.,
0\C,24,R3,22,90.,23,90.,0\C,24,R3,22,90.,23,-90.,0\X,24,1.,22,90.,23,0
.,0\X,24,R4,27,A4,22,180.,0\C,28,R5,24,90.,25,0.,0\C,28,R5,24,90.,26,0
.,0\X,28,1.,24,90.,27,0.,0\X,28,R6,31,A6,24,180.,0\C,32,R7,28,90.,31,9
0.,0\C,32,R7,28,90.,31,-90.,0\H,25,CH1,22,CC1,26,D1,0\H,26,CH1,22,CC1,
25,-D1,0\H,29,CH2,25,CC2,22,D2,0\H,30,CH2,26,CC2,22,-D2,0\H,33,CH3,29,
CC3,25,D3,0\H,34,CH3,30,CC3,26,-D3,0\\R1=0.672674\R2=0.769286\R3=1.262
103\R4=1.303117\R5=1.539763\R6=1.168962\R7=0.666669\CH1=1.076334\CH2=1
.0775\CH3=1.077031\A2=95.990099\A4=58.156131\A6=71.150163\CC1=115.5393
07\CC2=116.912482\CC3=115.458735\D1=220.436421\D2=178.0536\D3=159.8517
49\\Version=IBM-RS6000-G92RevB\State=1-AG\HF=-537.0357874\RMSD=5.892e-
09\RMSF=2.576e-05\Dipole=0.,-0.,-0.\PG=C02H [SGH(C2),X(C12H12)]\\@
@3206\ ANU-VP\FOPT\RBLYP\6-31G(D)\C14H12\APS501\19-May-1994\1\\#N BLYP
/6-31G* OPT=FCCARDS SCF=DIRECT TEST\\Heptafulvalene, C2h symmetry, ant
i bend\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,A2,1,18
0.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,
5,R4,8,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\X,9,1.,5,90
.,8,0.,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,R7,9,90.,12
,-90.,0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2,6,CC2,3,D2
,0\H,11,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,11,CC3,7,-D3
,0\C,1,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,R2,23,A2,1,180.,0
\C,24,R3,22,90.,23,90.,0\C,24,R3,22,90.,23,-90.,0\X,24,1.,22,90.,23,0.
,0\X,24,R4,27,A4,22,180.,0\C,28,R5,24,90.,25,0.,0\C,28,R5,24,90.,26,0.
,0\X,28,1.,24,90.,27,0.,0\X,28,R6,31,A6,24,180.,0\C,32,R7,28,90.,31,90
.,0\C,32,R7,28,90.,31,-90.,0\H,25,CH1,22,CC1,26,D1,0\H,26,CH1,22,CC1,2
5,-D1,0\H,29,CH2,25,CC2,22,D2,0\H,30,CH2,26,CC2,22,-D2,0\H,33,CH3,29,C
C3,25,D3,0\H,34,CH3,30,CC3,26,-D3,0\\R1=0.70189196\R2=0.75583055\R3=1.
26202252\R4=1.33954144\R5=1.55507063\R6=1.16194567\R7=0.68516554\CH1=1
.09584134\CH2=1.09666464\CH3=1.09623232\A2=96.85553252\A4=65.84034543\

A6=75.91931247\CC1=115.00690112\CC2=115.95422154\CC3=115.67470842\D1=2
11.98005568\D2=178.03832556\D3=166.66246376\\Version=Fujitsu-VP-Unix-G
92/DFT-RevG.1\State=1-AG\HF=-540.3638642\RMSD=6.183e-09\RMSF=9.212e-05
\Dipole=0.,0.,0.\PG=C02H [SGH(C2),X(C12H12)]\\@
@4610\GINC-RSCQC2\FOpt\RMP2-FC\6-31G(d)\C14H12\ASCOTT\23-Jun-1995\0\\#
N MP2=DIRECT/6-31G* OPT=FCCARDS SCF=DIRECT TEST MAXDISK=500000000\\Hep
tafulvalene, C2h symmetry, anti bend\\0,1\C,0.6885087182,0.,0.02156536
61\C,1.4365680715,-1.2518897221,-0.0693312911\C,1.4365680715,1.2518897
221,-0.0693312911\C,2.6345258882,-1.5445013208,0.5087567943\C,2.634525
8882,1.5445013208,0.5087567943\C,3.4637616932,-0.6818220869,1.31481153
34\C,3.4637616932,0.6818220869,1.3148115334\H,0.9732533153,-2.04099580
64,-0.6635996891\H,0.9732533153,2.0409958064,-0.6635996891\H,3.0128102
087,-2.5556363818,0.3587581583\H,3.0128102087,2.5556363818,0.358758158
3\H,4.2163873255,-1.1779485807,1.9264390859\H,4.2163873255,1.177948580
7,1.9264390859\C,-0.6885087182,0.,-0.0215653661\C,-1.4365680715,-1.251
8897221,0.0693312911\C,-1.4365680715,1.2518897221,0.0693312911\C,-2.63
45258882,-1.5445013208,-0.5087567943\C,-2.6345258882,1.5445013208,-0.5
087567943\C,-3.4637616932,-0.6818220869,-1.3148115334\C,-3.4637616932,
0.6818220869,-1.3148115334\H,-0.9732533153,-2.0409958064,0.6635996891\
H,-0.9732533153,2.0409958064,0.6635996891\H,-3.0128102087,-2.555636381
8,-0.3587581583\H,-3.0128102087,2.5556363818,-0.3587581583\H,-4.216387
3255,-1.1779485807,-1.9264390859\H,-4.2163873255,1.1779485807,-1.92643
90859\\Version=IBM-RS6000-G94RevB.1\State=1-AG\HF=-537.0268956\MP2=-53
8.8045674\RMSD=9.506e-09\RMSF=1.433e-05\Dipole=0.,0.,0.\PG=C02H [SGH(C
2),X(C12H12)]\\@

Heptafulvalene (12-C_{2v})

@566\ ANU-VP\FOPT\RHF\6-31G(D)\C14H12\APS501\23-Jul-1992\1\\#N RHF/6-3
1G* OPT SCF=DIRECT TEST\\Heptafulvalene, C2V symmetry, syn bend\\0,1\X
\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,A2,1,180.,0\C,5,R3,3
,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,8,A4,3,1
80.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\X,9,1.,5,90.,8,0.,0\X,9,
R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,R7,9,90.,12,-90.,0\H,6,C
H1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2,6,CC2,3,D2,0\H,11,CH2,7
,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,11,CC3,7,-D3,0\C,1,R1,2,9
0.,3,180.,0\X,22,1.,1,90.,2,0.,0\X,22,R2,23,A2,1,180.,0\C,24,R3,22,90.
,23,90.,0\C,24,R3,22,90.,23,-90.,0\X,24,1.,22,90.,23,0.,0\X,24,R4,27,A
4,22,180.,0\C,28,R5,24,90.,25,0.,0\C,28,R5,24,90.,26,0.,0\X,28,1.,24,9
0.,27,0.,0\X,28,R6,31,A6,24,180.,0\C,32,R7,28,90.,31,90.,0\C,32,R7,28,
90.,31,-90.,0\H,25,CH1,22,CC1,26,D1,0\H,26,CH1,22,CC1,25,-D1,0\H,29,CH
2,25,CC2,22,D2,0\H,30,CH2,26,CC2,22,-D2,0\H,33,CH3,29,CC3,25,D3,0\H,34
,CH3,30,CC3,26,-D3,0\\R1=0.673089\R2=0.781184\R3=1.257642\R4=1.302305\
R5=1.533639\R6=1.173643\R7=0.666168\CH1=1.075895\CH2=1.077494\CH3=1.07
6972\A2=93.382674\A4=56.816115\A6=70.124\CC1=116.247914\CC2=116.891405
\CC3=115.540919\D1=221.78809\D2=177.846893\D3=158.512904\\Version=Fuji
tsu-VP-Unix-G92RevA\State=1-A1\HF=-537.0307306\RMSD=4.600e-09\RMSF=3.0
64e-05\Dipole=0.,0.,-0.0210752\PG=C02V [SGV(C2),X(C12H12)]\\@
@3207\ ANU-VP\FOPT\RBLYP\6-31G(D)\C14H12\APS501\18-May-1994\1\\#N BLYP
/6-31G* OPT=FCCARDS SCF=DIRECT TEST\\Heptafulvalene, C2V symmetry, syn
 bend\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,A2,1,180
.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5
,R4,8,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\X,9,1.,5,90.
,8,0.,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,R7,9,90.,12,
-90.,0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2,6,CC2,3,D2,
0\H,11,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,11,CC3,7,-D3,
0\C,1,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,0.,0\X,22,R2,23,A2,1,180.,0\C,
24,R3,22,90.,23,90.,0\C,24,R3,22,90.,23,-90.,0\X,24,1.,22,90.,23,0.,0\
X,24,R4,27,A4,22,180.,0\C,28,R5,24,90.,25,0.,0\C,28,R5,24,90.,26,0.,0\
X,28,1.,24,90.,27,0.,0\X,28,R6,31,A6,24,180.,0\C,32,R7,28,90.,31,90.,0
\C,32,R7,28,90.,31,-90.,0\H,25,CH1,22,CC1,26,D1,0\H,26,CH1,22,CC1,25,-
D1,0\H,29,CH2,25,CC2,22,D2,0\H,30,CH2,26,CC2,22,-D2,0\H,33,CH3,29,CC3,
25,D3,0\H,34,CH3,30,CC3,26,-D3,0\\R1=0.70906292\R2=0.76022255\R3=1.259
20022\R4=1.34101925\R5=1.54900946\R6=1.16571715\R7=0.6838624\CH1=1.093

58305\CH2=1.09646271\CH3=1.096054\A2=93.11601653\A4=71.4213645\A6=78.1
7892368\CC1=115.44130801\CC2=115.36276105\CC3=115.69550079\D1=203.9905
4224\D2=178.39623987\D3=168.07931201\\Version=Fujitsu-VP-Unix-G92/DFT-
RevG.1\State=1-A1\HF=-540.3590676\RMSD=5.944e-09\RMSF=3.580e-05\Dipole
=0.,0.,-0.0183326\PG=C02V [SGV(C2),X(C12H12)]\\@

Heptafulvalene (12-C_s) TS for C_{2v} --> C_{2h} isomerization

@751\ ANU-VP\FOPT\RHF\6-31G(D)\C14H12\LXR501\11-Sep-1992\1\\#N RHF/6-3
1G* OPT SCF=DIRECT TEST\\Heptafulvalene, C2H --> C2V T.S., CS symmetry
\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,A2,1,180.,0\C
,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,R4,8
,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\X,9,1.,5,90.,8,0.
,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,R7,9,90.,12,-90.,
0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2,6,CC2,3,D2,0\H,1
1,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,11,CC3,7,-D3,0\C,1
,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,R8,23,A8,1,180.,0\C,24,
R9,22,90.,23,90.,0\C,24,R9,22,90.,23,-90.,0\X,24,1.,22,90.,23,0.,0\X,2
4,R10,27,A10,22,180.,0\C,28,R11,24,90.,25,0.,0\C,28,R11,24,90.,26,0.,0
\X,28,1.,24,90.,27,0.,0\X,28,R12,31,A12,24,180.,0\C,32,R13,28,90.,31,9
0.,0\C,32,R13,28,90.,31,-90.,0\H,25,CH4,22,CC4,26,D4,0\H,26,CH4,22,CC4
,25,-D4,0\H,29,CH5,25,CC5,22,D5,0\H,30,CH5,26,CC5,22,-D5,0\H,33,CH6,29
,CC6,25,D6,0\H,34,CH6,30,CC6,26,-D6,0\\R1=0.67525424\R2=0.80746003\R3=
1.24429455\R4=1.30107624\R5=1.52454912\R6=1.1810113\R7=0.66682028\CH1=
1.07707373\CH2=1.07768638\CH3=1.07715817\R8=0.74152468\R9=1.27514633\R
10=1.30522674\R11=1.54733213\R12=1.16129891\R13=0.6653543\CH4=1.073113
03\CH5=1.07707826\CH6=1.07660143\A2=93.04217526\A4=50.66981875\A6=66.8
8264419\A8=87.67017255\A10=105.91054605\A12=100.1023728\CC1=117.014086
61\CC2=117.44867136\CC3=115.86699171\CC4=114.78462158\CC5=115.70609698
\CC6=115.09993315\D1=230.49028555\D2=177.86251348\D3=155.64691161\D4=1
60.69178882\D5=181.33185713\D6=191.44072875\\Version=Fujitsu-VP-Unix-G
92RevC\State=1-A'\HF=-537.0303856\RMSD=3.603e-09\RMSF=2.045e-05\Dipole
=-0.0752157,0.,-0.0198264\PG=CS [SG(C2),X(C12H12)]\\@

@4262\ ANU-VP\FOPT\RBLYP\6-31G(D)\C14H12\APS501\3-Jul-1994\1\\#N BLYP/
6-31G* OPT=FCCARDS SCF=DIRECT TEST\\Heptafulvalene, C2H --> C2V T.S.,
CS symmetry\\0,1\X\X,1,1.\C,1,R1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,R2,4,A2
,1,180.,0\C,5,R3,3,90.,4,90.,0\C,5,R3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.
,0\X,5,R4,8,A4,3,180.,0\C,9,R5,5,90.,6,0.,0\C,9,R5,5,90.,7,0.,0\X,9,1.
,5,90.,8,0.,0\X,9,R6,12,A6,5,180.,0\C,13,R7,9,90.,12,90.,0\C,13,R7,9,9
0.,12,-90.,0\H,6,CH1,3,CC1,7,D1,0\H,7,CH1,3,CC1,6,-D1,0\H,10,CH2,6,CC2
,3,D2,0\H,11,CH2,7,CC2,3,-D2,0\H,14,CH3,10,CC3,6,D3,0\H,15,CH3,11,CC3,
7,-D3,0\C,1,R1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,R8,23,A8,1,1
80.,0\C,24,R9,22,90.,23,90.,0\C,24,R9,22,90.,23,-90.,0\X,24,1.,22,90.,
23,0.,0\X,24,R10,27,A10,22,180.,0\C,28,R11,24,90.,25,0.,0\C,28,R11,24,
90.,26,0.,0\X,28,1.,24,90.,27,0.,0\X,28,R12,31,A12,24,180.,0\C,32,R13,
28,90.,31,90.,0\C,32,R13,28,90.,31,-90.,0\H,25,CH4,22,CC4,26,D4,0\H,26
,CH4,22,CC4,25,-D4,0\H,29,CH5,25,CC5,22,D5,0\H,30,CH5,26,CC5,22,-D5,0\
H,33,CH6,29,CC6,25,D6,0\H,34,CH6,30,CC6,26,-D6,0\\R1=0.70188111\R2=0.7
5598625\R3=1.2618523\R4=1.33957289\R5=1.5551723\R6=1.16192056\R7=0.685
19395\CH1=1.09600074\CH2=1.09672356\CH3=1.09626261\R8=0.75530396\R9=1.
26216793\R10=1.33961459\R11=1.55528349\R12=1.16187156\R13=0.68516143\C
H4=1.09598346\CH5=1.09671535\CH6=1.0962612\A2=96.92961587\A4=65.621181
38\A6=75.8304316\A8=96.88657168\A10=65.83656182\A12=75.94318223\CC1=11
5.01964644\CC2=115.98396253\CC3=115.65291904\CC4=114.99311835\CC5=115.
97324118\CC6=115.64802407\D1=212.17060022\D2=177.89787412\D3=166.56373
306\D4=211.89891464\D5=177.92238746\D6=166.67016704\\Version=Fujitsu-V
P-Unix-G92/DFT-RevG.1\State=1-A'\HF=-540.3635833\RMSD=4.679e-09\RMSF=9
.993e-05\Dipole=-0.0009712,0.,-0.0004756\PG=CS [SG(C2),X(C12H12)]\\@

Heptafulvalene (12-D_2)

@4521\ ANU-VP\FOPT\RHF\6-31G(D)\C14H12\APS501\8-Jan-1995\1\\#N RHF/6-3
1G* OPT=CALCFC SCF=DIRECT TEST\\Heptafulvalene, D2 symmetry\\0,1\X\X,1
,1.\C,1,r1,2,90.\X,3,1.,1,90.,2,d1,0\X,3,r2,4,90.,1,180.,0\C,5,r3,3,90
.,4,90.,0\C,5,r3,3,90.,4,-90.,0\X,5,1.,3,90.,4,d2,0\X,5,r4,8,90.,3,180

.,0\C,9,r5,5,90.,6,0.,0\C,9,r5,5,90.,7,0.,0\X,9,1.,5,90.,8,d3,0\X,9,r6
,12,90.,5,180.,0\C,13,r7,9,90.,12,90.,0\C,13,r7,9,90.,12,-90.,0\H,6,ch
1,3,cc1,7,hd1,0\H,7,ch1,3,cc1,6,hd1,0\H,10,ch2,6,cc2,3,hd2,0\H,11,ch2,
7,cc2,3,hd2,0\H,14,ch3,10,cc3,6,hd3,0\H,15,ch3,11,cc3,7,hd3,0\C,1,r1,2
,90.,3,180.,0\X,22,1.,1,90.,2,d1,0\X,22,r2,23,90.,1,180.,0\C,24,r3,22,
90.,23,90.,0\C,24,r3,22,90.,23,-90.,0\X,24,1.,22,90.,23,d2,0\X,24,r4,2
7,90.,22,180.,0\C,28,r5,24,90.,25,0.,0\C,28,r5,24,90.,26,0.,0\X,28,1.,
24,90.,27,d3,0\X,28,r6,31,90.,24,180.,0\C,32,r7,28,90.,31,90.,0\C,32,r
7,28,90.,31,-90.,0\H,25,ch1,22,cc1,26,hd1,0\H,26,ch1,22,cc1,25,hd1,0\H
,29,ch2,25,cc2,22,hd2,0\H,30,ch2,26,cc2,22,hd2,0\H,33,ch3,29,cc3,25,hd
3,0\H,34,ch3,30,cc3,26,hd3,0\\d1=7.90784557\d2=8.58621758\d3=-9.267938
2\hd1=184.25631301\hd2=182.3498836\hd3=179.71679972\r1=0.68668001\r2=0
.7490226\r3=1.26972574\r4=1.30846334\r5=1.54087138\r6=1.16357263\r7=0.
66475542\ch1=1.06977018\ch2=1.07692833\ch3=1.07639065\cc1=114.91418982
\cc2=114.92905819\cc3=115.15186288\\Version=Fujitsu-VP-Unix-G92/DFT-Re
vG.1\State=1-A\HF=-537.0227075\RMSD=9.103e-09\RMSF=1.647e-04\Dipole=0.
,0.,0.\PG=D02 [C2"(C1.C1),X(C12H12)]\\@

Heptafulvalene (12-D_{2h})

@967\ ANU-VP\FOPT\RHF\6-31G(D)\C14H12\APS501\24-Oct-1992\1\\#N RHF/6-3
1G* OPT SCF=DIRECT TEST\\Heptafulvalene, D2H symmetry\\0,1\X\X,1,1.\C,
1,r1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,r2,4,90.,1,180.,0\C,5,r3,3,90.,4,90
.,0\C,5,r3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,r4,8,90.,3,180.,0\C,
9,r5,5,90.,6,0.,0\C,9,r5,5,90.,7,0.,0\X,9,1.,5,90.,8,0.,0\X,9,r6,12,90
.,5,180.,0\C,13,r7,9,90.,12,90.,0\C,13,r7,9,90.,12,-90.,0\H,6,ch1,3,cc
1,7,180.,0\H,7,ch1,3,cc1,6,180.,0\H,10,ch2,6,cc2,3,180.,0\H,11,ch2,7,c
c2,3,180.,0\H,14,ch3,10,cc3,6,180.,0\H,15,ch3,11,cc3,7,180.,0\C,1,r1,2
,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,r2,23,90.,1,180.,0\C,24,r3,2
2,90.,23,90.,0\C,24,r3,22,90.,23,-90.,0\X,24,1.,22,90.,23,0.,0\X,24,r4
,27,90.,22,180.,0\C,28,r5,24,90.,25,0.,0\C,28,r5,24,90.,26,0.,0\X,28,1
.,24,90.,27,0.,0\X,28,r6,31,90.,24,180.,0\C,32,r7,28,90.,31,90.,0\C,32
,r7,28,90.,31,-90.,0\H,25,ch1,22,cc1,26,180.,0\H,26,ch1,22,cc1,25,180.
,0\H,29,ch2,25,cc2,22,180.,0\H,30,ch2,26,cc2,22,180.,0\H,33,ch3,29,cc3
,25,180.,0\H,34,ch3,30,cc3,26,180.,0\\r1=0.687574\r2=0.762276\r3=1.264
664\r4=1.309298\r5=1.533329\r6=1.16769\r7=0.664378\ch1=1.067151\ch2=1.
076963\ch3=1.076308\cc1=115.481621\cc2=114.668409\cc3=115.25875\\Versi
on=Fujitsu-VP-Unix-G92RevC\State=1-AG\HF=-537.0218705\RMSD=8.711e-09\R
MSF=2.932e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C12H12)]\\@
@4382\ ANU-VP\FOPT\RBLYP\6-31G(D)\C14H12\APS501\1-Oct-1994\1\\#N BLYP/
6-31G* OPT SCF=DIRECT TEST\\Heptafulvalene, D2H symmetry\\0,1\X\X,1,1.
\C,1,r1,2,90.\X,3,1.,1,90.,2,0.,0\X,3,r2,4,90.,1,180.,0\C,5,r3,3,90.,4
,90.,0\C,5,r3,3,90.,4,-90.,0\X,5,1.,3,90.,4,0.,0\X,5,r4,8,90.,3,180.,0
\C,9,r5,5,90.,6,0.,0\C,9,r5,5,90.,7,0.,0\X,9,1.,5,90.,8,0.,0\X,9,r6,12
,90.,5,180.,0\C,13,r7,9,90.,12,90.,0\C,13,r7,9,90.,12,-90.,0\H,6,ch1,3
,cc1,7,180.,0\H,7,ch1,3,cc1,6,180.,0\H,10,ch2,6,cc2,3,180.,0\H,11,ch2,
7,cc2,3,180.,0\H,14,ch3,10,cc3,6,180.,0\H,15,ch3,11,cc3,7,180.,0\C,1,r
1,2,90.,3,180.,0\X,22,1.,1,90.,2,180.,0\X,22,r2,23,90.,1,180.,0\C,24,r
3,22,90.,23,90.,0\C,24,r3,22,90.,23,-90.,0\X,24,1.,22,90.,23,0.,0\X,24
,r4,27,90.,22,180.,0\C,28,r5,24,90.,25,0.,0\C,28,r5,24,90.,26,0.,0\X,2
8,1.,24,90.,27,0.,0\X,28,r6,31,90.,24,180.,0\C,32,r7,28,90.,31,90.,0\C
,32,r7,28,90.,31,-90.,0\H,25,ch1,22,cc1,26,180.,0\H,26,ch1,22,cc1,25,1
80.,0\H,29,ch2,25,cc2,22,180.,0\H,30,ch2,26,cc2,22,180.,0\H,33,ch3,29,
cc3,25,180.,0\H,34,ch3,30,cc3,26,180.,0\\r1=0.71630934\r2=0.75288448\r
3=1.26071035\r4=1.34372175\r5=1.55031576\r6=1.16379295\r7=0.68309619\c
h1=1.0901273\ch2=1.09623276\ch3=1.09571582\cc1=115.31993692\cc2=114.72
267452\cc3=115.542136\\Version=Fujitsu-VP-Unix-G92/DFT-RevG.1\State=1-
AG\HF=-540.3581134\RMSD=3.886e-09\RMSF=4.307e-05\Dipole=0.,0.,0.\PG=D0
2H [C2"(C1.C1),SG(C12H12)]\\@

Reference Molecules

Divinyl methane (DVM)

@71\ ANU-PC\FOpt\RHF\6-31G(d)\C5H8\APS501\18-Apr-1996\0\\#N HF/6-31G*

OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\divinyl methane, op
en form, C2 symmetry\\0,1\C,0.,0.,0.6650702671\C,-0.0525102088,1.24902
66256,-0.1784470975\C,0.0525102088,-1.2490266256,-0.1784470975\C,0.855
676961,2.2048730679,-0.1759411227\C,-0.855676961,-2.2048730679,-0.1759
411227\H,-0.8737817645,-0.0410796622,1.3110046927\H,0.8737817645,0.041
0796622,1.3110046927\H,-0.9074370226,1.3337630038,-0.8312316491\H,0.90
74370226,-1.3337630038,-0.8312316491\H,1.7265226997,2.1600578964,0.456
277983\H,-1.7265226997,-2.1600578964,0.456277983\H,0.763662768,3.07255
07036,-0.804932507\H,-0.763662768,-3.0725507036,-0.804932507\\Version=
SGI-G94RevD.1\State=1-A\HF=-193.9484342\RMSD=3.856e-09\RMSF=1.800e-04\
Dipole=0.,0.,0.0225488\PG=C02 [C2(C1),X(C4H8)]\\@
@75\GINC-VPP10\FOpt\RBLYP\6-31G(d)\C5H8\APS501\12-Aug-1996\0\\#N BLYP/
6-31G* OPT=FCCARDS SCF=DIRECT TEST MAXDISK=25000000\\divinyl methane,
openform, C2 symmetry\\0,1\C,0.,0.,0.6686584448\C,-0.05681839,1.261883
4542,-0.1782998028\C,0.05681839,-1.2618834542,-0.1782998028\C,0.869604
8537,2.2348586661,-0.1784008624\C,-0.8696048537,-2.2348586661,-0.17840
08624\H,-0.8884925426,-0.0499115296,1.3274259267\H,0.8884925426,0.0499
115296,1.3274259267\H,-0.9275408235,1.3440014615,-0.8424232815\H,0.927
5408235,-1.3440014615,-0.8424232815\H,1.7555205562,2.1865589738,0.4647
041137\H,-1.7555205562,-2.1865589738,0.4647041137\H,0.7777571636,3.119
5799982,-0.8154781021\H,-0.7777571636,-3.1195799982,-0.8154781021\\Ver
sion=Fujitsu-VP-Unix-G94RevD.2\State=1-A\HF=-195.1810989\RMSD=8.188e-0
9\RMSF=1.436e-05\Dipole=0.,0.,0.0295763\PG=C02 [C2(C1),X(C4H8)]\\@
@73\ANU-PC\FOpt\RMP2-FC\6-31G(d)\C5H8\APS501\18-Apr-1996\0\\#N MP2=DI
RECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\divinyl
 methane, open form,C2 symmetry\\0,1\C,0.,0.,0.6831000855\C,-0.0736677
596,1.2382313346,-0.1682514643\C,0.0736677596,-1.2382313346,-0.1682514
643\C,0.8601967996,2.1969217283,-0.1929133515\C,-0.8601967996,-2.19692
17283,-0.1929133515\H,-0.8814251075,-0.063721037,1.3345171356\H,0.8814
251075,0.063721037,1.3345171356\H,-0.9469607575,1.3208810693,-0.815072
2349\H,0.9469607575,-1.3208810693,-0.8150722349\H,1.7456185753,2.14299
01882,0.4348622569\H,-1.7456185753,-2.1429901882,0.4348622569\H,0.7694
765089,3.065825433,-0.836618519\H,-0.7694765089,-3.065825433,-0.836618
519\\Version=SGI-G94RevD.1\State=1-A\HF=-193.9466839\MP2=-194.5822059\
RMSD=4.518e-09\RMSF=5.344e-06\Dipole=0.,0.,0.0154465\PG=C02 [C2(C1),X(
C4H8)]\\@

Divinyl ethene (DVE)

@27\GINC-EIGEN\FOpt\RHF\6-31G(d)\C6H8\ASCOTT\22-Apr-1996\0\\#N HF/6-31
G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST MAXDISK=450000000
\\divinyl ethane, cis C2 symmetry\\0,1\C,0.,0.,0.6812253562\C,0.,0.,2.
0103129514\C,1.2904423704,-0.1549335068,-0.0349837812\C,-1.2904423704,
0.1549335068,-0.0349837812\C,1.5922872377,0.2832381712,-1.24507169\C,-
1.5922872377,-0.2832381712,-1.24507169\H,0.9046490729,-0.1321523946,2.
5764845366\H,-0.9046490729,0.1321523946,2.5764845366\H,2.0644169626,-0
.6337439033,0.5419882694\H,-2.0644169626,0.6337439033,0.5419882694\H,0
.8858045578,0.7954204081,-1.8704155701\H,-0.8858045578,-0.7954204081,-
1.8704155701\H,2.5829589664,0.1534184807,-1.6423393314\H,-2.5829589664
,-0.1534184807,-1.6423393314\\Version=IBM-RS6000-G94RevD.1\State=1-A\H
F=-231.7975878\RMSD=3.357e-09\RMSF=3.385e-06\Dipole=0.,0.,-0.0022322\P
G=C02 [C2(C1C1),X(C4H8)]\\@
@77\GINC-VPP10\FOpt\RBLYP\6-31G(d)\C6H8\APS501\12-Aug-1996\0\\#N BLYP/
6-31G* OPT=FCCARDS SCF=DIRECT TEST MAXDISK=25000000\\divinyl ethane, c
is C2 symmetry\\0,1\C,0.,0.,0.6860778991\C,0.,0.,2.0496226614\C,1.2967
73963,-0.1359951381,-0.0196396108\C,-1.296773963,0.1359951381,-0.01963
96108\C,1.600764572,0.234189854,-1.2824549496\C,-1.600764572,-0.234189
854,-1.2824549496\H,0.9221382956,-0.1239595465,2.6242413275\H,-0.92213
82956,0.1239595465,2.6242413275\H,2.1053738108,-0.5374393052,0.6048512
544\H,-2.1053738108,0.5374393052,0.6048512544\H,0.8732083816,0.6877133
079,-1.9582231032\H,-0.8732083816,-0.6877133079,-1.9582231032\H,2.6185
723937,0.1183669927,-1.6654037982\H,-2.6185723937,-0.1183669927,-1.665
4037982\\Version=Fujitsu-VP-Unix-G94RevD.2\State=1-A\HF=-233.2605984\R

MSD=7.216e-09\RMSF=5.107e-05\Dipole=0.,0.,0.024825\PG=C02 [C2(C1C1),X(
C4H8)]\\@
@29\GINC-EIGEN\FOpt\RMP2-FC\6-31G(d)\C6H8\ASCOTT\22-Apr-1996\0\\#N MP2
=DIRECT/6-31G* FOPT=READFC GEOM=CHECK GUESS=CHECK MAXDISK=450000000 SC
F=DIRECT TEST\\divinyl ethene, cis C2 symmetry\\0,1\C,0.,0.,0.68423943
14\C,0.,0.,2.0363954461\C,1.27916218,-0.1666050179,-0.0290029352\C,-1.
27916218,0.1666050179,-0.0290029352\C,1.5628152345,0.2823174826,-1.263
3085526\C,-1.5628152345,-0.2823174826,-1.2633085526\H,0.9141276083,-0.
1417048957,2.6056182554\H,-0.9141276083,0.1417048957,2.6056182554\H,2.
0703312902,-0.6537210444,0.5409625463\H,-2.0703312902,0.6537210444,0.5
409625463\H,0.834584972,0.8087726736,-1.8692594628\H,-0.834584972,-0.8
087726736,-1.8692594628\H,2.5540561966,0.152423828,-1.6853570442\H,-2.
5540561966,-0.152423828,-1.6853570442\\Version=IBM-RS6000-G94RevD.1\St
ate=1-A\HF=-231.7948214\MP2=-232.5544449\RMSD=6.256e-09\RMSF=9.722e-06
\Dipole=0.,0.,-0.0044473\PG=C02 [C2(C1C1),X(C4H8)]\\@

Tetravinyl ethene (TVE)

@22\GINC-EIGEN\FOpt\RHF\6-31G(d)\C10H12\ASCOTT\22-Apr-1996\0\\#N HF/6-
31G* SCF=DIRECT OPT=READFC GEOM=CHECK GUESS=CHECK TEST MAXDISK=4500000
00\\tetravinyl ethane, D2 symmetry\\0,1\C,0.,0.,-0.6737161978\C,0.,0.,
0.6737161978\C,1.2742268121,0.1163707749,-1.4296215174\C,-1.2742268121
,-0.1163707749,-1.4296215174\C,1.2573574095,0.2371676005,1.4296215174\
C,-1.2573574095,-0.2371676005,1.4296215174\C,1.4405175358,0.7207441136
,-2.5947960103\C,-1.4405175358,-0.7207441136,-2.5947960103\C,1.5828597
155,-0.298526329,2.5947960103\C,-1.5828597155,0.298526329,2.5947960103
\H,2.1368418246,-0.3268191329,-0.9640358422\H,-2.1368418246,0.32681913
29,-0.9640358422\H,1.9655539404,0.8997229776,0.9640358422\H,-1.9655539
404,-0.8997229776,0.9640358422\H,2.4104711859,0.7640882678,-3.05713957
54\H,0.632464726,1.1931086522,-3.121937439\H,-2.4104711859,-0.76408826
78,-3.0571395754\H,-0.632464726,-1.1931086522,-3.121937439\H,2.5275787
398,-0.0744844485,3.0571395754\H,0.935130568,-0.9741923355,3.121937439
\H,-2.5275787398,0.0744844485,3.0571395754\H,-0.935130568,0.9741923355
,3.121937439\\Version=IBM-RS6000-G94RevD.1\State=1-A\HF=-385.5567127\R
MSD=3.604e-09\RMSF=8.719e-06\Dipole=0.,0.,0.\PG=D02 [C2"(C1.C1),X(C8H1
2)]\\@
@79\GINC-VPP10\FOpt\RBLYP\6-31G(d)\C10H12\APS501\12-Aug-1996\0\\#N BLY
P/6-31G* SCF=DIRECT OPT=FCCARDS TEST MAXDISK=25000000\\tetravinyl etha
ne, D2 symmetry\\0,1\C,0.,0.,-0.6996668667\C,0.,0.,0.6996668667\C,1.27
7740201,0.0734273871,-1.4413052846\C,-1.277740201,-0.0734273871,-1.441
3052846\C,1.2489716437,0.2794305558,1.4413052846\C,-1.2489716437,-0.27
94305558,1.4413052846\C,1.4788327423,0.585285134,-2.6789137604\C,-1.47
88327423,-0.585285134,-2.6789137604\C,1.5825987962,-0.1577530285,2.678
9137604\C,-1.5825987962,0.1577530285,2.6789137604\H,2.1521339065,-0.32
49254733,-0.915136166\H,-2.1521339065,0.3249254733,-0.915136166\H,1.98
07797528,0.9020911738,0.915136166\H,-1.9807797528,-0.9020911738,0.9151
36166\H,2.4767548473,0.5848712186,-3.1263202531\H,0.6754286313,1.03147
35918,-3.2693628224\H,-2.4767548473,-0.5848712186,-3.1263202531\H,-0.6
754286313,-1.0314735918,-3.2693628224\H,2.5422283123,0.1160350112,3.12
63202531\H,0.9321693157,-0.8069708628,3.2693628224\H,-2.5422283123,-0.
1160350112,3.1263202531\H,-0.9321693157,0.8069708628,3.2693628224\\Ver
sion=Fujitsu-VP-Unix-G94RevD.2\State=1-A\HF=-387.9801158\RMSD=2.610e-0
9\RMSF=1.808e-05\Dipole=0.,0.,0.\PG=D02 [C2"(C1.C1),X(C8H12)]\\@
@24\GINC-EIGEN\FOpt\RMP2-FC\6-31G(d)\C10H12\ASCOTT\22-Apr-1996\0\\#N M
P2=DIRECT/6-31G* SCF=DIRECT OPT=READFC GEOM=CHECK GUESS=CHECK TEST MAX
DISK=450000000\\tetravinyl ethene, D2 symmetry\\0,1\C,0.,0.,-0.6889886
632\C,0.,0.,0.6889886632\C,1.2689016077,0.0901430633,-1.4281391193\C,-
1.2689016077,-0.0901430633,-1.4281391193\C,1.2450506171,0.2609329853,1
.4281391193\C,-1.2450506171,-0.2609329853,1.4281391193\C,1.4288825625,
0.6568524818,-2.6390358769\C,-1.4288825625,-0.6568524818,-2.6390358769
\C,1.5541661796,-0.2402666156,2.6390358769\C,-1.5541661796,0.240266615
6,2.6390358769\H,2.1446118189,-0.3387444638,-0.9439382848\H,-2.1446118
189,0.3387444638,-0.9439382848\H,1.9697596105,0.9133207225,0.943938284

8\H,-1.9697596105,-0.9133207225,0.9439382848\H,2.4043754595,0.6854089982,-3.1144532525\H,0.6049567019,1.1166501321,-3.1739132498\H,-2.4043754595,-0.6854089982,-3.1144532525\H,-0.6049567019,-1.1166501321,-3.1739132498\H,2.5001613167,-0.0004853252,3.1144532525\H,0.8877284485,-0.9081950949,3.1739132498\H,-2.5001613167,0.0004853252,3.1144532525\H,-0.8877284485,0.9081950949,3.1739132498\\Version=IBM-RS6000-G94RevD.1\State=1-A\HF=-385.5511764\MP2=-386.8260732\RMSD=4.824e-09\RMSF=1.595e-05\Dipole=0.,0.,0.\PG=D02 [C2"(C1.C1),X(C8H12)]\\@

Napthalene

@5335\ ANU-PC\FOpt\RHF\6-31G(d)\C10H8\APS501\07-Jun-1996\1\\#N HF/6-31G* OPT=(READFC,Z-MATRIX) GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\napthalene\\0,1\X\C,1,cxc\X,1,xx1,2,90.\X,1,xx1,2,90.,3,180.,0\C,1,cxc,3,90.,2,180.,0\C,3,cxm,1,90.,2,0.,0\C,4,cxm,1,90.,2,0.,0\C,3,cxm,1,90.,5,0.,0\C,4,cxm,1,90.,5,0.,0\X,3,xx2,6,90.,1,180.,0\X,4,xx2,7,90.,1,180.,0\C,10,cxe,3,90.,6,0.,0\C,11,cxe,4,90.,7,0.,0\C,10,cxe,3,90.,8,0.,0\C,11,cxe,4,90.,9,0.,0\H,6,ch1,2,hcc1,1,180.,0\H,8,ch1,5,hcc1,1,180.,0\H,7,ch1,2,hcc1,1,180.,0\H,9,ch1,5,hcc1,1,180.,0\H,12,ch2,10,hcc2,3,180.,0\H,14,ch2,10,hcc2,3,180.,0\H,13,ch2,11,hcc2,4,180.,0\H,15,ch2,11,hcc2,4,180.,0\\xx1=1.2428043\cxc=0.70457364\cxm=1.39269864\xx2=1.17329393\cxe=0.70833277\ch1=1.07612699\hcc1=118.83247535\ch2=1.07540134\hcc2=119.48777655\\Version=SGI-G94RevD.1\State=1-AG\HF=-383.3550459\RMSD=8.880e-09\RMSF=2.058e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C8H8)]\\@
@81\GINC-VPP05\FOpt\RBLYP\6-31G(d)\C10H8\APS501\13-Aug-1996\1\\#N BLYP/6-31G* OPT=(Z-MATRIX,FCCARDS) SCF=DIRECT TEST MAXDISK=20000000\\napthalene\\0,1\X\C,1,cxc\X,1,xx1,2,90.\X,1,xx1,2,90.,3,180.,0\C,1,cxc,3,90.,2,180.,0\C,3,cxm,1,90.,2,0.,0\C,4,cxm,1,90.,2,0.,0\C,3,cxm,1,90.,5,0.,0\C,4,cxm,1,90.,5,0.,0\X,3,xx2,6,90.,1,180.,0\X,4,xx2,7,90.,1,180.,0\C,10,cxe,3,90.,6,0.,0\C,11,cxe,4,90.,7,0.,0\C,10,cxe,3,90.,8,0.,0\C,11,cxe,4,90.,9,0.,0\H,6,ch1,2,hcc1,1,180.,0\H,8,ch1,5,hcc1,1,180.,0\H,7,ch1,2,hcc1,1,180.,0\H,9,ch1,5,hcc1,1,180.,0\H,12,ch2,10,hcc2,3,180.,0\H,14,ch2,10,hcc2,3,180.,0\H,13,ch2,11,hcc2,4,180.,0\H,15,ch2,11,hcc2,4,180.,0\\xx1=1.25263457\cxc=0.72402877\cxm=1.41267034\xx2=1.19859136\cxe=0.71256274\ch1=1.09519595\hcc1=118.67255682\ch2=1.09421901\hcc2=119.63390115\\Version=Fujitsu-VP-Unix-G94RevD.2\State=1-AG\HF=-385.7117438\RMSD=5.208e-09\RMSF=7.221e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C8H8)]\\@
@5337\ ANU-PC\FOpt\RMP2-FC\6-31G(d)\C10H8\APS501\07-Jun-1996\1\\#N MP2=DIRECT/6-31G* OPT=(READFC,Z-MATRIX) GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\napthalene\\0,1\X\C,1,cxc\X,1,xx1,2,90.\X,1,xx1,2,90.,3,180.,0\C,1,cxc,3,90.,2,180.,0\C,3,cxm,1,90.,2,0.,0\C,4,cxm,1,90.,2,0.,0\C,3,cxm,1,90.,5,0.,0\C,4,cxm,1,90.,5,0.,0\X,3,xx2,6,90.,1,180.,0\X,4,xx2,7,90.,1,180.,0\C,10,cxe,3,90.,6,0.,0\C,11,cxe,4,90.,7,0.,0\C,10,cxe,3,90.,8,0.,0\C,11,cxe,4,90.,9,0.,0\H,6,ch1,2,hcc1,1,180.,0\H,8,ch1,5,hcc1,1,180.,0\H,7,ch1,2,hcc1,1,180.,0\H,9,ch1,5,hcc1,1,180.,0\H,12,ch2,10,hcc2,3,180.,0\H,14,ch2,10,hcc2,3,180.,0\H,13,ch2,11,hcc2,4,180.,0\H,15,ch2,11,hcc2,4,180.,0\\xx1=1.24157202\cxc=0.7162571\cxm=1.4035393\xx2=1.19083332\cxe=0.70736746\ch1=1.08918938\hcc1=118.91617188\ch2=1.08763339\hcc2=119.69607307\\Version=SGI-G94RevD.1\State=1-AG\HF=-383.3521439\MP2=-384.6146547\RMSD=8.800e-09\RMSF=4.156e-05\Dipole=0.,0.,0.\PG=D02H [C2"(C1.C1),SG(C8H8)]\\@

Azulene

@5340\ ANU-PC\FOpt\RHF\6-31G(d)\C10H8\APS501\08-Jun-1996\1\\#N HF/6-31G* OPT=(READFC,Z-MATRIX) GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST\\azulene\\0,1\X\C,1,cxm\X,1,xx7a,2,90.\X,1,xx5a,2,90.,3,180.,0\C,1,cxm,3,90.,2,180.,0\C,3,cx7a,1,90.,2,0.,0\C,3,cx7a,1,90.,5,0.,0\C,4,cx5a,1,90.,2,0.,0\C,4,cx5a,1,90.,5,0.,0\X,3,xx7b,6,90.,2,180.,0\C,10,cx7b,3,90.,6,0.,0\C,10,cx7b,3,90.,7,0.,0\C,10,cx7c,11,90.,6,180.,0\C,4,cx5b,8,90.,2,180.,0\H,6,ch1,2,hcc1,1,180.,0\H,7,ch1,5,hcc1,1,180.,0\H,11,ch2,10,hcc2,3,180.,0\H,12,ch2,10,hcc2,3,180.,0\X,13,1.,10,90.,11,90.,0\H,13,ch3

,19,90.,10,180.,0\H,8,ch4,2,hcc3,1,180.,0\H,9,ch4,5,hcc3,1,180.,0\X,14
,1.,4,90.,8,90.,0\H,14,ch5,23,90.,4,180.,0\\cxm=0.74254002\xx7a=1.1010
9657\xx7b=1.34823229\xx5a=1.3370016\cx7a=1.5831702\cx5a=1.14157904\cx7
b=1.25863442\cx7c=0.58570891\cx5b=0.79784402\ch1=1.07769914\hcc1=115.2
8767474\ch2=1.07587552\hcc2=140.65216587\ch3=1.07706538\ch4=1.07285211
\hcc3=125.38268695\ch5=1.07414001\\Version=SGI-G94RevD.1\State=1-A1\HF
=-383.2826206\RMSD=8.375e-09\RMSF=2.099e-05\Dipole=0.6043854,0.,0.\PG=
C02V [C2(H1C1C1H1),SGV(C8H6)]\\@
@83\GINC-VPP05\FOpt\RBLYP\6-31G(d)\C10H8\APS501\15-Aug-1996\1\\#N BLYP
/6-31G* OPT=(Z-MATRIX,FCCARDS) SCF=DIRECT TEST MAXDISK=25000000\\azule
ne, C2v symmetry\\0,1\X\C,1,cxm\X,1,xx7a,2,90.\X,1,xx5a,2,90.,3,180.,0
\C,1,cxm,3,90.,2,180.,0\C,3,cx7a,1,90.,2,0.,0\C,3,cx7a,1,90.,5,0.,0\C,
4,cx5a,1,90.,2,0.,0\C,4,cx5a,1,90.,5,0.,0\X,3,xx7b,6,90.,2,180.,0\C,10
,cx7b,3,90.,6,0.,0\C,10,cx7b,3,90.,7,0.,0\C,10,cx7c,11,90.,6,180.,0\C,
4,cx5b,8,90.,2,180.,0\H,6,ch1,2,hcc1,1,180.,0\H,7,ch1,5,hcc1,1,180.,0\
H,11,ch2,10,hcc2,3,180.,0\H,12,ch2,10,hcc2,3,180.,0\X,13,1.,10,90.,11,
90.,0\H,13,ch3,19,90.,10,180.,0\H,8,ch4,2,hcc3,1,180.,0\H,9,ch4,5,hcc3
,1,180.,0\X,14,1.,4,90.,8,90.,0\H,14,ch5,23,90.,4,180.,0\\cxm=0.756407
55\xx7a=1.11413722\xx7b=1.36915662\xx5a=1.35760022\cx7a=1.6060412\cx5a
=1.1579319\cx7b=1.27495857\cx7c=0.59787159\cx5b=0.81297617\ch1=1.09776
712\hcc1=115.30468267\ch2=1.09537681\hcc2=140.80128572\ch3=1.09675708\
ch4=1.09088829\hcc3=125.12655756\ch5=1.09240938\\Version=Fujitsu-VP-Un
ix-G94RevD.2\State=1-A1\HF=-385.6629083\RMSD=4.778e-09\RMSF=5.518e-05\
Dipole=0.3601966,0.,0.\PG=C02V [C2(H1C1C1H1),SGV(C8H6)]\\@
1\1\GINC-VPP06\FOpt\RMP2-FC\6-31G(d)\C10H8\APS501\18-Jul-1996\0\\#N MP
2=DIRECT/6-31G* OPT=READFC GEOM=CHECK GUESS=CHECK SCF=DIRECT TEST MAXD
ISK=225000000\\azulene, Cs symmetry\\0,1\C,-0.000574526,0.9331192651,0
.\C,-0.8912807216,-0.2763103499,0.\C,1.390912315,0.960664709,0.\C,-0.5
049277798,-1.6132214749,0.\C,-0.8474309729,2.0539112801,0.\C,-2.212791
5672,0.2002669211,0.\C,2.287991719,-0.112977791,0.\C,0.7862608073,-2.1
515484015,0.\C,2.016290036,-1.4852002975,0.\C,-2.178237577,1.604577234
8,0.\H,1.8400543055,1.9561846265,0.\H,-1.322428793,-2.3374231496,0.\H,
3.3431653557,0.1565954731,0.\H,0.841532459,-3.2392071657,0.\H,2.894009
8357,-2.1317531706,0.\H,-0.5176620185,3.0880568356,0.\H,-3.1026436664,
-0.4213299422,0.\H,-3.053297875,2.2491899215,0.\\Version=Fujitsu-VP-Un
ix-G94RevD.2\State=1-A'\HF=-383.2802622\MP2=-384.5571245\RMSD=3.711e-0
9\RMSF=1.689e-04\Dipole=0.3190489,-0.2348267,0.\PG=CS [SG(C10H8)]\\@

Table S2. Calculated (HF/6-31G*, B-LYP/6-31G* and MP2/6-31G*) Total Energies (E, hartrees) and Relative Energies (ΔE, kJ mol^{-1}) [a]

molecule	conformation	symmetry	HF		B-LYP		MP2	
			E	ΔE	E	ΔE	E	ΔE
1	planar	C_{2v}	-115.82305		-116.55657		-116.20525	
2	planar	C_{2v}	-192.79172		-193.99707		-193.42538	
3-C_s	folded	C_s	-269.68233	0	-271.36773	0	-270.57091	0
3-C_{2v}	planar	C_{2v}	-269.67553[b]	17.9	-271.35970[b]	21.1	-270.55537[b]	40.8
4	planar	C_{2v}	-153.66978[c]		-154.62804		-154.16682	
5	planar	C_{2v}	-230.64445[c]		-232.07765		-231.39828	
6	planar	C_{2v}	-307.53679		-309.45356		-308.54145	
7	planar	D_{2h}	-229.28222		-230.69934		-230.03042[b,d]	
8	planar	C_{2v}	-306.29153		-308.17703		-307.29297	
9	planar	C_{2v}	-383.17171	224	-385.53850	210	-384.42194	246
10	planar	D_{2h}	-383.25712	0	-385.61863	0	-384.51581	0
11-C_s	folded	C_s	-460.14879	0	-463.00013[e]		-461.66526	0
11-C_{2v}	planar	C_{2v}	-460.14861[b]	0.5	-463.00013		-461.66512[b]	0.4
12-C_{2h}	*anti*-folded	C_{2h}	-537.03579	0	-540.36386	0.0	-538.79664[f,g]	0.0
12-C_{2v}	*syn*-folded	C_{2v}	-537.03073	13.3	-540.35907[h]	12.6	-538.79052[f]	16.1
12-C_s	*syn*-folded	C_s	-537.03037[b]	14.2			-538.79080[f]	15.3
12-D_2	twisted	D_2	-537.02271[h]	34.3				
12-D_{2h}	planar	D_{2h}	-537.02187[i]	36.5	-540.35811[i]	15.1	-538.78147[f]	39.8

[a] HF/6-31G* total energies (hartrees) for reference molecules are: C_2H_4 -78.03172, divinylmethane (DVM) -193.94843, 1,1-divinylethene (DVE) -231.79759, 1,2,2,2-tetravinylethene (TVE) -385.55671. B-LYP/6-31G* energies are: C_2H_4 -78.53712, DVM -195.18110, DVE -233.26060, TVE -387.98012. MP2/6-31G* energies are: C_2H_4 -78.28503, DVM -194.58221, DVE -232.55444, TVE -386.82607.

[b] Number of imaginary frequencies = 1.

[c] See also Reference 36e.

[d] Total energy for C_{2h} conformation is -230.03049 hartrees.

[e] Preferred B-LYP structure is planar C_{2v}.

[f] Calculated at HF/6-31G* optimized geometry.

[g] Total energy for the MP2/6-31G* optimized geometry is -538.80457 hartrees.

[h] Number of imaginary frequencies = 2.

[i] Number of imaginary frequencies = 3.

Table S3. Selected Structural Parameters Associated With the Cycloheptatrienylidene Ring Pertaining to Overcrowding in 6, 9, 11 and 12

molecule	conformation	symmetry	method	$r(C_1=C_{1'})$	$r(H\cdots H)^a$	$<C_2C_1C_7$	$\chi(C_1)^b$	α^c	β^c
6	planar	C_{2v}	HF	1.334	2.303	122.3	-	-	-
	planar	C_{2v}	B-LYP	1.370	2.334	121.9	-	-	-
	planar	C_{2v}	MP2	1.360	2.311	122.6	-	-	-
9	planar	C_{2v}	HF	1.336	3.245	123.4	-	-	-
	planar	C_{2v}	B-LYP	1.364	3.314	123.2	-	-	-
	planar	C_{2v}	MP2	1.350	3.267	124.1	-	-	-
11-C_s	folded	C_s	HF	1.356	2.121	120.1	4.1	16.5	9.8
	planar	C_{2v}	B-LYP	1.409	2.042	121.4	0.0	0.0	0.0
	folded	C_s	MP2	1.393	2.078	120.9	4.9	14.5	7.6
12-C_{2h}	*anti*-folded	C_{2h}	HF	1.345	2.377	117.3	7.3	31.8	18.9
	anti-folded	C_{2h}	B-LYP	1.404	2.129	118.2	8.2	24.2	14.1
	anti-folded	C_{2h}	MP2	1.378	2.356	117.9	9.5	32.7	18.4
	anti-folded	C_i	exp[d]	1.373	2.126	117.5	8.1	24.7	15.7

[a] $r(H\cdots H)$ is the distance between the closest-contact hydrogen pairs.

[b] Pyramidalization angle at C_1, see Scheme 1.

[c] α : angle between $C_1C_2C_7$ plane and $C_2C_3C_6C_7$ plane, β: angle between $C_2C_3C_6C_7$ plane and $C_3C_4C_5C_6$ plane, see Scheme 1.

[d] From Reference 14.

Table S4. Dihedral Angles within the Cycloheptatrienylidene Rings of the Non-planar Conformations of 3, 11 and 12

				central double bond							
				cis	*trans*						
molecule	conformation	symmetry	theory	$<C_2C_1C_{1'}C_{2'}$	$<C_2C_1C_{1'}C_{7'}$	$<C_{1'}C_1C_2C_3$	$<C_{1'}C_1C_2H_2$	$<C_7C_1C_2C_3$	$<C_1C_2C_3C_4$	$<C_2C_3C_4C_5$	$<C_3C_4C_5C_6$
3-C_s	folded	C_s	HF	–	–	–	–	62.1	5.1	31.9	0.0
	folded	C_s	B-LYP	–	–	–	–	66.1	9.1	29.7	0.0
	folded	C_s	MP2	–	–	–	–	71.4	8.8	33.1	0.0
11-C_s	folded	C_s	HF	2.9	178.8[a]	162.8	16.6	21.4	0.5	12.5	0.0
	folded	C_s	MP2	3.4	178.5[a]	166.2	12.4	18.8	1.4	9.8	0.0
12-C_{2h}	*anti*-folded	C_{2h}	HF	7.3	180.0	146.4	33.4	40.7	1.1	23.7	0.0
	anti-folded	C_{2h}	B-LYP	8.2	180.0	156.6	24.0	31.4	1.4	17.8	0.0
	anti-folded	C_{2h}	MP2	10.4	180.0	169.8	31.0	41.6	1.8	23.0	0.0
	anti-folded	C_i	exp[b]	8.1	180.0	155.9	21.1	32.3	0.6	20.0	0.1
						155.8[c]	25.2[d]	32.1[e]	0.3[f]	20.0[g]	

[a] $<C_2C_1C_{1'}C_{5'}$. [b] From Reference 14. [c] $<C_{1'}C_1C_7C_6$. [d] $<C_{1'}C_1C_7H_7$. [e] $<C_2C_1C_7C_6$. [f] $<C_1C_7C_6C_5$. [g] $<C_7C_6C_5C_4$.