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J5461-1 SUPPORTING INFORMATION

Hoz et. al.

Supporting Information

Gaussian archive records for the geometry optimized molecules, their fluoride adducts and transition states for inversion of the carbanions. 4 pages.

Optimized geometry of bicyclobutanecarbonitrile.

1\1\GINC-ELA\POPT\RHF\6-31+G(D)\C5H5N1\SHOZ\13-Jan-1994\1\\# RHF/6-31+ G*
OPT SCF=DIRECT\\BCBCN\\0,1\C\C,1,r2\C,1,r3,2,a3\C,2,r4,1,a4,3,d4,0\
H,4,r5,1,a5,3,d5,0\H,1,r6,3,a6,4,d6,0\H,1,r7,3,a7,4,d7,0\H,2,r8,3,a8,4,
d8,0\H,2,r9,3,a9,4,d9,0\C,3,r10,1,a10,2,d10,0\X,10,1.,3,90.,5,0.,0\N,
10,r12,11,90.,3,180.,0\\r2=2.26343794\r3=1.49477304\r4=1.48371981\r5=1
.06972334\r6=1.0802386\r7=1.07723602\r8=1.08021904\r9=1.07724775\r10=1
.4280646\r12=1.13766917\a3=40.8304084\a4=40.32240524\a5=129.38769361\a
6=118.35265647\a7=116.73721143\a8=118.3397068\a9=116.6664198\a10=130.2
0306479\d5=242.41165016\d6=109.84393723\d7=-106.83336173\d8=-109.88783
61\d9=106.91052961\d10=167.41501849\d4=260.58862876\\Version=IBM-RS600 0-
G92RevC.3\HF=-246.6142257\RMSD=6.761e-09\RMSF=1.835e-04\Dipole=-1.72 17718,-
0.0430914,-0.0013176\PG=C01 [X(C5H5N1)]\\@

Optimized geometry of bicyclobutaneS(H)O2.

1\1\GINC-ESHEL\FOPT\RHF\6-31+G(D)\C4H6O2S1\SHOZ\26-Dec-1995\1\\#N RHF/ 6-
31+G* SCF=DIRECT OPT\\BCB-S(H)O2\\0, 1\C\C,1,r2\C,1,r3,2,a3\C,2,r4,1,
a4,3,d4,0\H,4,r5,1,a5,3,d5,0\H,1,r6,3,a6,4,d6,0\H,1,r7,3,a7,4,d7,0\H,2
,r8,3,a8,4,d8,0\H,2,r9,3,a9,4,d9,0\S,3,r10,1,a10,2,d10,0\O,10,r11,3,a1
1,4,d11,0\O,10,r12,3,a12,4,d12,0\H,10,r13,3,a13,11,d13,0\\r2=2.2712488
5\r3=1.48999131\r4=1.48391348\r5=1.07082513\r6=1.0795273\r7=1.07860932
\r8=1.079272\r9=1.07602261\r10=1.73450163\a3=40.53233862\a4=40.3254407
1\a5=129.59629362\a6=118.53997592\a7=117.35432424\a8=117.78859151\a9=1
16.4748278\a10=130.87458055\d5=241.31010864\d6=110.04430086\d7=-106.13
747919\d8=-110.04671504\d9=106.69031285\d10=166.5440573\d4=260.6592744
4\r11=1.43319331\r12=1.4300634\r13=1.33302124\a11=108.10864956\a12=110
.49552962\a13=100.75433296\d11=-62.09392795\d12=-196.3828653\d13=112.8
0501776\\Version=IBM-RS6000-G92RevC.3\HF=-702.0271214\RMSD=6.722e-09\R
MSF=1.326e-05\Dipole=-1.770826,-0.7605228,-0.8710795\PG=C01 [X(C4H6O2S 1)]\\@

Optimized geometry of bicyclobutanecarboxaldehyde.

1\1\GINC-ARMON\FOPT\RHF\6-31+G(D)\C5H6O1\SHOZ\14-Jan-1994\1\\# RHF/6-3
1+G* OPT SCF=DIRECT\\BCB-C(H)O.\\0, 1\C\C,1,r2\C,1,r3,2,a3\C,2,r4,1,a4,
3,d4,0\H,4,r5,1,a5,3,d5,0\H,1,r6,3,a6,4,d6,0\H,1,r7,3,a7,4,d7,0\H,2,r8
,3,a8,4,d8,0\H,2,r9,3,a9,4,d9,0\C,3,r10,1,a10,2,d10,0\O,10,r11,3,a11,5
,d11,0\H,10,r12,3,a12,11,d12,0\\r2=2.26266478\r3=1.49089313\r4=1.47873
054\r5=1.07056244\r6=1.08060975\r7=1.07671818\r8=1.080483\r9=1.0788562
3\r10=1.46325845\r11=1.19290056\r12=1.09429643\a3=40.9441327\a4=40.288
25861\a5=129.03591811\a6=118.47767832\a7=116.47460216\a8=118.15312873\
a9=117.28896264\a10=129.31583111\a11=124.58625516\ a12=114.96892638\d5=
244.36742629\d6=109.20194895\d7=-107.63842256\d8=-109.93492908\d9=107.
09014866\d10=161.03102899\d4=258.78188819\d11=95.84092987\d12=180.6944
0993\\Version=IBM-RS6000-G92RevC.3\HF=-267.6104549\RMSD=5.378e-
09\RMSF=3.781e-05\Dipole=-0.9953233,-0.1478916,0.9039775\PG=C01 [X(C5H6O1)]\\ @

Optimized geometry of 3F-cyclobutane-CN anion (CN axial).

1\1\GINC-DOLEV\POPT\RHF\6-31+G(D)\C5H5F1N1(1-)\SHOZ\18-Mar-1994\1\\# R
HF/6-31+G* OPT SCF=DIRECT\\BCBCN + F- at optimal distance\\-1,1\C\C,1,
r2\C,1,r3,2,a3\C,2,r4,1,a4,3,d4,0\H,4,r5,1,a5,3,d5,0\H,1,r6,3,a6,4,d6,
0\H,1,r7,3,a7,4,d7,0\H,2,r8,3,a8,4,d8,0\H,2,r9,3,a9,4,d9,0\C,3,R10,1,a
10,2,d10,0\X,10,1.,3,90.,5,0.,0\N,10,r12,11,90.,3,180.,0\F,4,r13,5,a13
,3,d13,0\\r2=2.18196499\r3=1.53850898\r4=1.52520013\r5=1.08224858\r6=1
.0908752\r7=1.09013988\r8=1.0909003\r9=1.0901167\R10=1.39178736\r12=1.
16040892\a3=44.83701992\a4=44.33538658\a5=112.19950063\a6=114.04578751
\a7=119.05136609\a8=114.00218982\a9=119.08681529\a10=121.5663273\d5=26
1.67940253\d6=112.52517089\d7=-117.84488575\d8=-112.47865117\d9=117.90
674857\d10=128.17172219\d4=203.61406786\d13=179.98051308\r13=1.4009639
2\a13=105.70989047\\Version=IBM-RS6000-G92RevC.3\HF=
-346.0822812\RMSD=4.135e-09\RMSF=9.335e-04\Dipole=
-2.4478466,0.3452356,0.0000832\PG=C01 [X(C5H5F1N1)]\\@

Optimized geometry of 3F-cyclobutane-CN anion (CN equatorial).

1\1\GINC-ETROG\POPT\RHF\6-31+G(D)\C5H5F1N1(1-)\SHOZ\26-Dec-1995\1\\#N
RHF/6-31+G* OPT\\CYCLOBUTANE 1CN.3F F and CN are equatorial\\-1,1\X\X,
1,1.\C,1,R2,2,90.\C,1,R2,2,90.,3,180.,0\C,1,R3,2,90.,4,90.,0\C,1,R4,2,
A2,3,90.,0\X,5,1.,1,90.,2,0.,0\C,5,R5,7,A3,1,180.,0\X,8,1.,5,90.,7,0.,
0\N,8,R6,9,90.,5,180.,0\H,6,R7,1,A4,2,0.,0\F,6,R8,11,A5,1,180.,0\H,3,R
9,4,A6,5,D3,0\H,3,R10,13,A7,1,D4,0\H,4,R9,3,A6,13,0.,0\H,4,R10,15,A7,1,-
D4,0\\R2=1.08185114\R3=1.08600257\R4=1.07523756\R5=1.40069623\R6=1.1
5710304\R7=1.08075932\R8=1.39550093\R9=1.08934085\R10=1.09655633\A2=57
.78756795\A3=129.83672045\A4=124.11948225\A5=105.95587819\A6=145.58553
48\A7=108.1934507\D3=77.40162246\D4=187.54289726\\Version=IBM-RS6000-G
92RevC.3\State=1-A'\HF=-346.0851563\RMSD=7.532e-09\RMSF=8.644e-04\Dipo le=0.,-
2.3198189,0.9667501\PG=CS [SG(C3H1F1N1),X(C2H4)]\\@

Optimized geometry of 3F-bicyclobutane-S(H)O2- (S(H)O2 axial).

1\1\GINC-ARMON\FOPT\RHF\6-31+G(D)\C4H6F1O2S1(1-)\SHOZ\3-Mar-1994\1\\#
RHF/6-31+G* OPT SCF=DIRECT\\BCB-S(H)O2 + F- at optim. (from bcbf6so2)\ \-
1,1\C\C,1,r2\C,1,r3,2,a3\C,2,r4,1,a4,3,d4,0\H,4,r5,1,a5,3,d5,0\H,1,r
6,3,a6,4,d6,0\H,1,r7,3,a7,4,d7,0\H,2,r8,3,a8,4,d8,0\H,2,r9,3,a9,4,d9,0
\S,3,r10,1,a10,2,d10,0\O,10,r11,3,a11,4,d11,0\O,10,r12,3,a12,4,d12,0\H
,10,r13,3,a13,11,d13,0\F,4,r14,5,a14,3,d14,0\\r2=2.19014009\r3=1.53420
462\r4=1.52869863\r5=1.08339226\r6=1.08884083\r7=1.08903792\r8=1.08884
171\r9=1.08900098\r10=1.65295367\a3=44.457593\a4=44.24832116\a5=112.65
360917\a6=113.36843125\a7=119.40176139\a8=113.36670248\a9=119.39552863
\a10=121.81328567\d5=257.87751288\d6=112.94078242\d7=-118.11705454\d8= -
112.94750132\d9=118.11228577\d10=129.17521708\d4=199.06663293\r11=1.4
5532456\r12=1.45531452\r13=1.35868176\a11=111.17216192\a12=111.2018864
7\a13=111.67573538\d11=-112.39294506\d12=-247.28714123\d13=112.5496259
5\d14=179.99812514\r14=1.39365373\a14=105.79774268\\Version=IBM-RS6000 -
G92RevC.3\HF=-801.5140329\RMSD=6.401e-09\RMSF=1.875e-05\Dipole=-2.140 9099,-
0.6445889,-0.002712\PG=C01 [X(C4H6F1O2S1)]\\@

Optimized geometry of 3F-bicyclobutane-S(H)O2 anion (S(H)O2 equatorial).

1\1\GINC-SHITA\FOPT\RHF\6-31+G(D)\C4H6F1O2S1(1-)\SHOZ\3-Dec-1993\1\\#
RHF/6-31+G* OPT SCF=DIRECT\\CYCLOBUTANE 1-SO2-3F ANION\\-1,1\X\X,1,1.\
C,1,R2,2,90.\C,1,R2,2,90.,3,180.,0\C,1,R3,2,90.,4,90.,0\C,1,R4,2,A2,3,
0.,0\X,5,1.,1,90.,2,0.,0\S,5,R5,7,A3,1,180.,0\O,8,RO,5,AO,7,DO,0\O,8, RO,5,AO,7,-
DO,0\F,6,R7,1,A4,2,0.,0\H,6,R8,11,A5,1,180.,0\H,3,R9,4,A6,5
,D3,0\H,3,R10,13,A7,1,D4,0\H,4,R9,3,A6,13,0.,0\H,4,R10,15,A7,1,-D4,0\H
,8,R11,5,A8,7,180.,0\\R2=1.08693839\R3=1.07952343\R4=1.07117481\R7=1.3
9263799\R8=1.08100727\R9=1.0907947\R10=1.08759207\A2=122.14477496\A4=1
29.77174917\A5=106.02827956\A6=106.38231911\A7=108.52396443\D3=109.676
58303\D4=184.04769442\R5=1.68050078\A3=49.31047699\RO=1.45851226\AO=11
2.61746148\DO=68.08823228\R11=1.33369739\A8=106.75346613\\Version=IBM-
RS6000-G92RevC.3\State=1-A'\HF=-801.5144592\RMSD=3.817e-09\RMSF=6.532e -
05\Dipole=0.,-0.6741679,-1.2485687\PG=CS [SG(C2H2F1S1), X(C2H4O2)]\\@

Optimized geometry of 3F-cyclobutane-CHO anion.

1\1\GINC-SHITA\FOPT\RHF\6-31+G(D)\C5H6F1O1(1-)\SHOZ\2-Mar-1994\1\\# RH F/6-
31+G* OPT SCF=DIRECT\\BCB-C(H)O + F-. Full optim.\\-1,1\C\C,1,r2\C
,1,r3,2,a3\C,2,r4,1,a4,3,d4,0\H,4,r5,1,a5,3,d5,0\H,1,r6,3,a6,4,d6,0\H,
1,r7,3,a7,4,d7,0\H,2,r8,3,a8,4,d8,0\H,2,r9,3,a9,4,d9,0\C,3,r10,1,a10,2
,d10,0\O,10,r11,3,a11,5,d11,0\H,10,r12,3,a12,11,d12,0\F,4,R13,5,A13,3,
d13,0\\r2=2.18532285\r3=1.51703981\r4=1.53076286\r5=1.08207001\r6=1.09
342103\r7=1.08787608\r8=1.09393516\r9=1.09042574\r10=1.36209587\r11=1.
25489519\r12=1.10673541\a3=44.13332492\a4=44.441366\a5=112.90810918\a6
=115.01153001\a7=118.61940588\a8=114.99642322\a9=120.01133349\a10=133.
43689765\a11=129.68584056\a12=113.17625135\d5=262.15496511\d6=111.3957
5827\d7=-118.0903926\d8=-110.6076065\d9=117.87134011\d10=169.21067214\
d4=205.65942917\d11=90.7313716\d12=180.2752416\d13=180.23860221\R13=1.
39698441\A13=105.92367103\\Version=IBM-RS6000-G92RevC.3\HF=-367.086735
7\RMSD=4.864e-09\RMSF=5.527e-05\Dipole=-2.3803828,-0.2262545,0.9890765 \PG=C01
[X(C5H6F1O1)]\\@

Transition state for the inversion of 3F-cyclobutane-CN anion.

1\1\GINC-SHITA\PTS\RHF\6-31+G(D)\C5H5F1N1(1-)\SHOZ\25-Nov-1993\1\\# RH
F/6-31+G* OPT=(TS,CALCFC) SCF=DIRECT\\3F-CB-CN anion.TS for inversion.
6-31+G*. Starting from FCCNAE4.\\-1,1\X\X,1,1.\C,1,R2,2,90.\C,1,R2,2,
90.,3,180.,0\C,1,R3,2,90.,4,90.,0\C,1,R4,2,A2,3,90.,0\X,5,1.,1,90.,2,0
.,0\C,5,R5,7,A3,1,180.,0\X,8,1.,5,90.,7,0.,0\N,8,R6,9,90.,5,180.,0\F,6
,R7,1,A4,2,0.,0\H,6,R8,11,A5,1,180.,0\H,3,R9,4,A6,5,D3,0\H,3,R10,13,A7
,1,D4,0\H,4,R9,3,A6,13,0.,0\H,4,R10,15,A7,1,-D4,0\\R2=1.09889608\R3=1.
04500149\R4=1.06533085\R5=1.36932434\R6=1.16591497\R7=1.39753396\R8=1.
08192866\R9=1.09560552\R10=1.09210554\A2=112.36328607\A3=100.775052\A4
=130.52421503\A5=105.79343359\A6=112.86096825\A7=107.57961918\D3=104.3
6885591\D4=184.78158855\\Version=IBM-RS6000-G92RevC.3\State=1-A'\HF=-3
46.0812973\RMSD=1.418e-09\RMSF=8.861e-05\Dipole=0.,-2.7557523,-0.13942
44\PG=CS [SG(C3H1F1N1),X(C2H4)]\\@

Transition state for the inversion of 3F-bicyclobutane-S(H)O2 anion, conformation 1.

1\1\GINC-ESHEL\FTS\RHF\6-31+G(D)\C4H6F1O2S1(1-)\SHOZ\22-Dec-1993\1\\#

RHF/6-31+G* OPT=(TS,CALCFC)\\CYCLOBUTANE 1-SO2-3F ANION. Starting from Planar Geomwith Os opposite to the F.\\-1,1\X\X,1,1.\C,1,R2,2,90.\C,1
,R2,2,90.,3,180.,0\C,1,R3,2,90.,4,90.,0\C,1,R4,2,A2,3,90.,0\X,5,1.,1,9
0.,2,0.,0\S,5,R5,7,A3,1,180.,0\O,8,RO,5,AO,7,DO,0\O,8,RO,5,AO,7,-DO,0\
F,6,R7,1,A4,2,0.,0\H,6,R8,11,A5,1,180.,0\H,3,R9,4,A6,5,D3,0\H,3,R10,13
,A7,1,D4,0\H,4,R9,3,A6,13,0.,0\H,4,R10,15,A7,1,-D4,0\H,8,R11,5,A8,7,0.
,0\\R2=1.10361466\R3=1.03691698\R4=1.06323565\R7=1.39460131\R8=1.08140
687\R9=1.09360885\R10=1.08662624\A2=111.96520089\A4=130.06361996\A5=10
6.1838651\A6=112.65724313\A7=108.40680552\D3=104.03822842\D4=183.87245
915\R5=1.6295214\RO=1.45957248\AO=111.65589124\DO=112.22892231\R11=1.3
46394\A8=111.65284474\A3=104.42999674\\Version=IBM-RS6000-G92RevC.3\St
ate=1-A\HF=-801.5121982\RMSD=5.215e-09\RMSF=2.104e-06\Dipole=0.,-1.34
7947,0.7125921\PG=CS [SG(C2H2F1S1),X(C2H4O2)]\\@

Transition state for the inversion of 3F-bicyclobutane-S(H)O2 anion, conformation 2.

1\1\GINC-ETROG\PTS\RHF\6-31+G(D)\C4H6F1O2S1(1-)\SHOZ\14-Jan-1994\1\\#
RHF/6-31+G* OPT=(TS,CALCFC) SCF=DIRECT\\CYCLOBUTANE 1-SO2-3F ANION.
TS . SO2 asymmetric starting point.\\-1,1\X\X,1,1.\C,1,R2,2,90.\C,1,R2,2
,90.,3,180.,0\C,1,R3,2,90.,4,90.,0\C,1,R4,2,A2,3,90.,0\X,5,1.,1,90.,2,
0.,0\S,5,R5,7,AS,1,D8,0\O,8,RO,5,AO,7,DO,0\O,8,R12,5,A10,7,D10,0\F,6,R
7,1,A4,2,0.,0\H,6,R8,11,A5,1,180.,0\H,3,R9,4,A6,5,D3,0\H,3,R10,13,A7,1
,D4,0\H,4,R9,3,A6,13,0.,0\H,4,R10,15,A7,1,-D4,0\H,8,R11,5,A8,7,D17,0\\
R2=1.10517701\R3=1.0316199\R4=1.06333539\R7=1.39187085\R8=1.08211969\R
9=1.09185424\R10=1.08976357\A2=111.31742815\A4=129.94423276\A5=105.991
62735\A6=113.04663217\A7=107.96133417\D3=103.17718597\D4=184.46872165\
R5=1.62684277\RO=1.4590173\AO=111.5688437\DO=67.98110781\R11=1.3484427
9\A8=111.69148989\D8=180.00489585\R12=1.45902499\A10=111.57409712\D10=
-67.96729381\D17=180.00606798\AS=90.47477687\\Version=IBM-RS6000-G92Re
vC.3\HF=-801.5113061\RMSD=4.699e-09\RMSF=6.896e-05\Dipole=-0.0002327,-
1.6356679,-1.2773053\PG=C01 [X(C4H6F1O2S1)]\\@