Supporting Information

Controlling the action of chlorine radical: from lab to environment

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Contents

DFT-D/aug-cc-pVTZ σ-complex structures (2f)

BLYP-D

1\1\GINC-ABE0121\FOpt\ULC-BLYP\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\06-Dec-20
10\0\\#P LC-BLYP/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full g
foldprint gfinput punch=archive output=wfn guess=read geom=check\\C6H6
Cl benzene.Cl sigma complex optimisation/freq LC-BLYP bb\\0,2\C,0.0025
798448,0.0135728395,0.0005901787\C,0.0083820973,0.0264626831,1.4731193
117\C,1.1555026015,-0.0018248869,2.1762190902\C,2.3994760313,-0.081808
7522,1.5340003056\C,2.455046287,-0.1600970531,0.1350381301\C,1.3344707
596,-0.135042411,-0.6097555922\H,1.3791401832,-0.1932073808,-1.6875405
643\H,3.4158096844,-0.2479692884,-0.3526263269\H,3.3094900226,-0.09526
57478,2.1144156765\H,1.1182852923,0.031847517,3.2560734782\H,-0.949056
049,0.0903449655,1.9693352096\H,-0.6944984493,-0.7277053631,-0.3857351
907\Cl,-0.7499402204,1.5756540618,-0.5996342511\\Version=EM64L-G09RevA
.02\State=2-A'\HF=-691.5141835\S2=0.842782\S2-1=0.\S2A=0.754977\RMSD=5
.432e-09\RMSF=2.245e-05\Dipole=0.4706048,-0.6932836,0.3533734\Quadrupo
le=1.3672215,-3.231282,1.8640605,1.3300347,-0.8124277,1.2897348\PG=CS
[SG(C2H2Cl1),X(C4H4)]\\@

CAM-B3LYP

1\1\GINC-ABE0470\FOpt\UCAM-B3LYP\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\06-Dec-
2010\0\\#P CAM-B3LYP/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=fu
ll gfoldprint gfinput punch=archive output=wfn guess=read geom=check\\
C6H6Cl benzene.Cl sigma complex optimisation/freq CAM-B3LYP bb\\0,2\C,
0.0076424083,-0.0203439272,0.0064432132\C,0.0007451194,-0.0170832902,1
.4730102326\C,1.1583080887,-0.0011061052,2.1826736447\C,2.4038318591,-
0.0516221839,1.5344328469\C,2.4621139056,-0.1598973588,0.1347981952\C,
1.3280757234,-0.1787396411,-0.6118153773\H,1.3701845015,-0.2668827405,
-1.6874046929\H,3.4238719041,-0.2413921795,-0.3521018902\H,3.315349237
5,-0.0300466583,2.1130889637\H,1.1226498417,0.0388749673,3.2624058105\
H,-0.9578990741,0.0166558853,1.9692941324\H,-0.7495120961,-0.667251165
7,-0.4254479137\Cl,-0.7006733337,1.6737955812,-0.5758777093\\Version=E
M64L-G09RevA.02\State=2-A'\HF=-692.3759992\S2=0.807586\S2-1=0.\S2A=0.7
52063\RMSD=5.068e-09\RMSF=4.003e-05\Dipole=0.5657879,-0.8170744,0.4235
716\Quadrupole=1.4931851,-3.5056842,2.0124991,1.6971225,-0.9070032,1.5
625419\PG=CS [SG(C2H2Cl1),X(C4H4)]\\@

M06-2X

1\1\GINC-ABE0391\FOpt\UM062X\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\06-Dec-2010
\0\\#P M062X/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full gfold
print gfinput punch=archive output=wfn\\C6H6Cl benzene.Cl sigma comple
x optimisation/freq M062X sb\\0,2\C,0.0042863555,-0.0231308656,0.00452
26376\C,-0.0027988442,-0.0260733642,1.4736921517\C,1.1557527779,-0.000
1517388,2.1845160185\C,2.4040632041,-0.0431529535,1.5339234357\C,2.462
7553207,-0.1593323235,0.1316195018\C,1.3265537246,-0.1879759713,-0.614
3093391\H,1.3662345051,-0.2804563163,-1.69037424\H,3.4250474075,-0.239
3409451,-0.355193564\H,3.31578135,-0.0132215395,2.1120594622\H,1.12050
4318,0.0413306714,3.2645304428\H,-0.9632088887,0.0032479225,1.96846043
89\H,-0.7606963235,-0.6583169043,-0.4332612518\Cl,-0.6695868218,1.6815
355117,-0.5566862386\\Version=EM64L-G09RevA.02\State=2-A'\HF=-692.3775
083\S2=0.783021\S2-1=0.\S2A=0.750728\RMSD=6.637e-09\RMSF=8.827e-06\Dip
ole=0.5365289,-0.7922692,0.4030201\Quadrupole=1.6462154,-3.7238948,2.0
776794,1.6287301,-0.8017951,1.5356174\PG=CS [SG(C2H2Cl1),X(C4H4)]\\@

ωB97X-D

1\1\GINC-ABE0410\FOpt\UwB97XD\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\06-Dec-201
0\0\\#P wB97XD/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full gfo
ldprint gfinput punch=archive output=wfn guess=read geom=check\\C6H6Cl
 benzene.Cl sigma complex optimisation/freq wB97XD sb\\0,2\C,0.0034574
972,-0.013238161,0.003227859\C,-0.00152566,-0.0138857803,1.4745235591\
C,1.157584569,-0.0007391482,2.184279437\C,2.4047881536,-0.0518660684,1
.5350605945\C,2.4632803959,-0.1597605873,0.1334353668\C,1.3286982903,-
0.1758945135,-0.6148466024\H,1.3710943177,-0.2644089509,-1.6909953904\
H,3.4254174603,-0.2432066338,-0.3533418313\H,3.3166493356,-0.031827298
2,2.1140547576\H,1.1220620216,0.0373203381,3.2645167435\H,-0.960578334
9,0.0195667906,1.971340764\H,-0.7476824466,-0.6728142128,-0.4238516883
\Cl,-0.6985575143,1.6657154091,-0.5739041136\\Version=EM64L-G09RevA.02
\State=2-A'\HF=-692.4124942\S2=0.799252\S2-1=0.\S2A=0.751504\RMSD=6.13
8e-09\RMSF=5.520e-05\Dipole=0.5418888,-0.7903481,0.4062836\Quadrupole=
1.5382618,-3.560728,2.0224662,1.6036606,-0.8524535,1.5050405\PG=CS [SG
(C2H2Cl1),X(C4H4)]\\@

ωPBE

1\1\GINC-ABE0393\FOpt\ULC-wPBE\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\06-Dec-20
10\0\\#P LC-wPBE/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full g
foldprint gfinput punch=archive output=wfn guess=read geom=check\\C6H6
Cl benzene.Cl sigma complex optimisation/freq LC-wPBE bb\\0,2\C,-0.003
5238038,0.0158740081,-0.0034742179\C,0.0029885391,0.0276886074,1.47577
21375\C,1.1564704823,-0.001467234,2.1828465514\C,2.4054711452,-0.08220
5409,1.5378479273\C,2.4614625517,-0.160402962,0.1331078664\C,1.3346544
023,-0.1344957372,-0.615862823\H,1.379693573,-0.1937162522,-1.69549305
3\H,3.4236983865,-0.2492787058,-0.3558274027\H,3.3171378989,-0.0963940
266,2.1193722799\H,1.1186631124,0.0314528542,3.2646696735\H,-0.9560308
811,0.0907529605,1.9732072277\H,-0.700143175,-0.7296050585,-0.38918167
53\Cl,-0.7558541463,1.5767581385,-0.6034850364\\Version=EM64L-G09RevA.
02\State=2-A'\HF=-692.1980889\S2=0.852998\S2-1=0.\S2A=0.756123\RMSD=5.
459e-09\RMSF=2.685e-05\Dipole=0.4594759,-0.6767051,0.3450026\Quadrupol
e=1.3888954,-3.2667185,1.8778232,1.2765312,-0.7943805,1.2584067\PG=CS
[SG(C2H2Cl1),X(C4H4)]\\@

DFT-D/aug-cc-pVTZ σ-complex structures (2f)

BLYP-D

1\1\GINC-ABE0541\FOpt\ULC-BLYP\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\07-Dec-20
10\0\\#P LC-BLYP/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full g
foldprint gfinput punch=archive output=wfn guess=read geom=check\\C6H6
Cl benzne.Cl pi complex optimisation/freq LC-BLYP bb\\0,2\C,0.01061242
16,-0.0083799,-0.0009773664\C,0.0095119171,0.0028319964,1.3676866096\C
,1.2064768148,0.0100379347,2.0566992427\C,2.4092431611,-0.0022348445,1
.3779374268\C,2.4197879952,-0.0134668736,0.0093137253\C,1.2182379,0.00
85246269,-0.6973436228\H,1.2225213798,-0.1278859146,-1.7675546464\H,3.
3535518111,-0.0192169856,-0.5334524074\H,3.3394034589,-0.0010159282,1.
9272924092\H,1.2018862689,0.0226887716,3.1376038798\H,-0.9252941589,0.
0079885415,1.9090751699\H,-0.9184963068,-0.0101963049,-0.5517011442\Cl
,1.2255194754,2.4036372119,-1.2180040318\\Version=EM64L-G09RevA.02\Sta
te=2-A\HF=-691.5083412\S2=0.796402\S2-1=0.\S2A=0.751475\RMSD=4.450e-09
\RMSF=1.658e-05\Dipole=-0.0047418,-0.9792229,0.6260062\Quadrupole=3.04
73793,-4.8750932,1.8277139,-0.0253466,0.0094704,2.0174612\PG=C01 [X(C6
H6Cl1)]\\@

CAM-B3LYP

1\1\GINC-ABE0487\FOpt\UCAM-B3LYP\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\07-Dec-
2010\0\\#P CAM-B3LYP/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=fu
ll gfoldprint gfinput punch=archive output=wfn guess=read geom=check\\
C6H6Cl benzne.Cl pi complex optimisation/freq CAM-B3LYP bb\\0,2\C,0.00
24713411,-0.0074891869,-0.0000974891\C,0.0017023938,-0.0016164519,1.37
63099219\C,1.2064037662,0.0011430276,2.0693987127\C,2.4169599472,-0.00
67162517,1.3866271283\C,2.4279251088,-0.0126105683,0.0102631684\C,1.21
82453824,0.0056626728,-0.7005002328\H,1.2225313937,-0.1290779141,-1.77
05037021\H,3.3612733447,-0.0154617742,-0.5329088129\H,3.3467894578,-0.
0060308486,1.9367034712\H,1.2018022626,0.0089385397,3.1504331005\H,-0.
9327814737,0.0030054407,1.9184224522\H,-0.9262062352,-0.006408505,-0.5
512234266\Cl,1.2258454653,2.4399741513,-1.2763490473\\Version=EM64L-G0
9RevA.02\State=2-A\HF=-692.3776321\S2=0.772141\S2-1=0.\S2A=0.750345\RM
SD=4.396e-09\RMSF=1.390e-06\Dipole=-0.0055125,-1.1107297,0.7414229\Qua
drupole=3.2352989,-5.0224671,1.7871682,-0.0271748,0.0109999,2.2796425\
PG=C01 [X(C6H6Cl1)]\\@

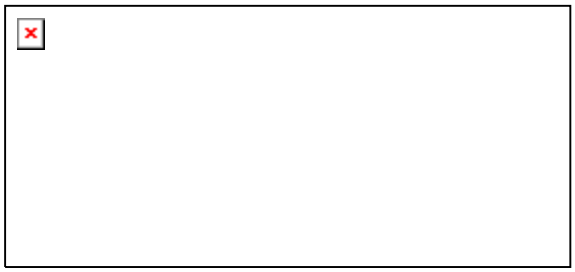
M06-2X

1\1\GINC-ABE0397\FOpt\UM062X\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\07-Dec-2010
\0\\#P M062X/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full gfold
print gfinput punch=archive output=wfn geom=check guess=check\\C6H6Cl
benzne.Cl pi complex optimisation/freq M062X bb\\0,2\C,-0.0013691118,-
0.0116348684,-0.0076456802\C,-0.0016896056,0.0036421265,1.3710119592\C
,1.2064480028,0.012353845,2.0645942104\C,2.4204192791,-0.0014722323,1.
3813582826\C,2.4318122018,-0.0167725236,0.0027479541\C,1.2182856346,0.
0040830497,-0.7107242283\H,1.222562554,-0.1359748805,-1.7811910597\H,3
.3649494409,-0.0187868169,-0.5422396415\H,3.3501330244,0.0033939729,1.
9322875851\H,1.2018644927,0.0293994088,3.1460384205\H,-0.936047193,0.0
124444033,1.9139786556\H,-0.9298166603,-0.0097185616,-0.560585195\Cl,1
.2254100834,2.4023554087,-1.1930560185\\Version=EM64L-G09RevA.02\State
=2-A\HF=-692.3781668\S2=0.763746\S2-1=0.\S2A=0.750127\RMSD=9.552e-09\R
MSF=2.820e-06\Dipole=-0.0054262,-1.1191502,0.7170289\Quadrupole=3.3124
066,-5.2798131,1.9674065,-0.0279442,0.0105908,2.294579\PG=C01 [X(C6H6C
l1)]\\@

ωB97X-D

1\1\GINC-ABE0411\FOpt\UwB97XD\Aug-CC-pVTZ\C6H6Cl1(2)\ACROFT\07-Dec-201
0\0\\#P wB97XD/aug-cc-pVTZ OPT FREQ=noraman int=ultrafine pop=full gfo
ldprint gfinput punch=archive output=wfn guess=read geom=check\\C6H6Cl
 benzne.Cl pi complex optimisation/freq wB97XD bb\\0,2\C,0.0002875739,
-0.0126633827,-0.0043729759\C,-0.0001153334,0.0006718184,1.373756763\C
,1.206428183,0.0079700561,2.0670544983\C,2.4188089924,-0.0044358043,1.
384089565\C,2.4301232943,-0.0177941062,0.0060064383\C,1.2182529078,-0.
0015383742,-0.7058276943\H,1.2225388361,-0.1378341948,-1.7765334713\H,
3.36347898,-0.0229518557,-0.5379699639\H,3.3488208587,-0.0002874306,1.
934546832\H,1.2018390291,0.0223296955,3.1484942096\H,-0.9347700191,0.0
087574401,1.9162488852\H,-0.9284002101,-0.0138892656,-0.5563034318\Cl,
1.2256690848,2.4449777543,-1.2326144329\\Version=EM64L-G09RevA.02\Stat
e=2-A\HF=-692.4121215\S2=0.768964\S2-1=0.\S2A=0.750252\RMSD=6.756e-09\
RMSF=7.489e-07\Dipole=-0.0055707,-1.1407913,0.7401941\Quadrupole=3.299
4285,-5.1836745,1.884246,-0.0278742,0.0109699,2.3320615\PG=C01 [X(C6H6
Cl1)]\\@

MPW1K/6-31+G(d,p) substituted complex structures 1a-1j, 2a-2j and 3a-3j



1a

1\1\GINC-NODE04\SP\RmPWPW91\6-31+G(d,p)\C8H11N1\CHS60A\03-Apr-2008\0\\
#P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C8H1
1N\\0,1\C\N,1,1.437391\C,2,1.3793085,1,118.92309\C,3,1.4031179,2,121.2
8203,1,-12.334199,0\C,4,1.383922,3,120.89691,2,-178.26685,0\C,5,1.3859
065,4,121.22652,3,-0.4734391,0\C,6,1.3859068,5,118.31016,4,-0.2995423,
0\C,3,1.4031223,4,117.43108,5,1.2075457,0\H,8,1.0773842,3,120.40945,4,
178.83778,0\H,7,1.0806147,8,118.77433,3,-179.80718,0\H,6,1.0790909,7,1
20.84415,8,179.85724,0\H,5,1.080615,4,118.77429,3,179.80702,0\H,4,1.07
73863,3,120.40894,8,-178.83804,0\C,2,1.437392,3,118.92554,4,-168.21248
,0\H,14,1.0889882,2,111.03166,3,-61.435693,0\H,14,1.0954523,2,112.8884
7,3,60.254402,0\H,14,1.0850082,2,109.07672,3,-179.37016,0\H,1,1.088989
1,2,111.03127,3,61.433996,0\H,1,1.0850073,2,109.07699,3,179.36884,0\H,
1,1.0954526,2,112.88837,3,-60.255507,0\\Version=x86-Linux-G03RevB.04\S
tate=1-A\HF=-366.1414981\RMSD=3.892e-05\Dipole=-0.6363921,0.1467676,-0
.3874645\PG=C01 [X(C8H11N1)]\\@

1b

1\1\GINC-NODE05\SP\RmPWPW91\6-31+G(d,p)\C6H7N1\CHS60A\03-Apr-2008\0\\#
P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C6H7N
\\0,1\C\C,1,1.3954216\C,1,2.39918,2,30.721419\C,1,2.7652481,2,60.76450
7,3,0.0585549,0\C,1,2.4105381,2,90.87711,3,0.1025695,0\C,1,1.3844364,2
,120.49598,3,0.1184435,0\H,1,1.0813943,2,119.51468,3,-179.50326,0\N,1,
2.416233,2,29.52852,3,-177.42753,0\H,1,3.3807958,2,21.58572,3,-0.37583
81,0\H,1,3.8456991,2,60.578959,3,0.0559034,0\H,1,3.3894327,2,99.99405,
3,0.1180617,0\H,1,2.1311428,2,146.77615,3,0.1603709,0\H,1,3.2694531,2,
21.214445,3,166.53312,0\H,1,2.5871438,2,51.343424,3,172.1618,0\\Versio
n=x86-Linux-G03RevB.04\State=1-A\HF=-287.5456946\RMSD=3.082e-05\Dipole
=-0.425974,-0.3959674,0.2531408\PG=C01 [X(C6H7N1)]\\@

1c

1\1\GINC-NODE07\SP\RmPWPW91\6-31+G(d,p)\C6H6O1\CHS60A\03-Apr-2008\0\\#
P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C6H6O
\\0,1\C\C,1,1.3857141\C,1,2.3931715,2,30.440018\C,1,2.7733828,2,60.374
056,3,0.0000234,0\C,1,2.4010694,2,90.429771,3,-0.0000009,0\C,1,1.38728
62,2,120.57201,3,-0.0000484,0\H,1,1.08016,2,120.1496,3,180.,0\H,1,2.14
42666,2,25.732916,3,179.99999,0\H,1,3.3744203,2,21.323823,3,0.0000106,
0\H,1,3.8523413,2,60.689881,3,0.0000511,0\O,1,3.6557107,2,100.22722,3,
-0.0000809,0\H,1,2.1457642,2,146.41725,3,-0.0002525,0\H,1,3.8214886,2,
114.67034,3,0.0010485,0\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-30
7.3981643\RMSD=2.941e-05\Dipole=-0.3148015,-0.000046,-0.4595045\PG=C01
 [X(C6H6O1)]\\@

1d

1\1\GINC-NODE06\SP\RmPWPW91\6-31+G(d,p)\C7H8O1\CHS60A\03-Apr-2008\0\\#
P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C7H8O
\\0,1\C\C,1,1.3929872\C,1,2.4077658,2,30.024243\C,1,2.7659027,2,60.198
412,3,-0.0003967,0\C,1,2.407227,2,90.191454,3,-0.0004803,0\C,1,1.38053
75,2,120.00361,3,-0.000338,0\H,1,1.0791996,2,118.5006,3,179.99982,0\O,
1,2.3244106,2,31.499061,3,179.99807,0\H,1,3.3923862,2,21.220789,3,0.00
13865,0\H,1,3.8461302,2,60.052589,3,-0.0003143,0\H,1,3.3853016,2,99.35
7722,3,-0.0006034,0\H,1,2.129239,2,146.25129,3,-0.0004992,0\C,1,3.6134
753,2,20.684507,3,-179.97715,0\H,1,3.9865148,2,17.527299,3,132.201,0\H
,1,4.3188228,2,32.648541,3,-179.97754,0\H,1,3.986001,2,17.536266,3,-13
2.14867,0\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-346.6907354\RMSD
=3.333e-05\Dipole=0.0939468,0.0002706,0.5344246\PG=C01 [X(C7H8O1)]\\@

1e

1\1\GINC-NODE09\SP\RmPWPW91\6-31+G(d,p)\C7H8\CHS60A\03-Apr-2008\0\\#P
MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C7H8\\0
,1\C\C,1,1.3921466\C,1,2.4189705,2,29.425892\C,1,2.801549,2,59.09791,3

,0.0561861,0\C,1,2.418978,2,88.767449,3,0.1490223,0\C,1,1.3920399,2,11
8.19521,3,0.2928979,0\C,1,1.4994838,2,120.88452,3,-178.5183,0\H,1,2.14
12005,2,26.116277,3,179.89735,0\H,1,3.3931062,2,20.070063,3,0.0873807,
0\H,1,3.8815578,2,59.097537,3,0.0884593,0\H,1,3.3930807,2,98.124387,3,
0.2216721,0\H,1,2.1410943,2,144.31159,3,0.5913176,0\H,1,2.1455844,2,11
6.28155,3,-146.5603,0\H,1,2.1499094,2,96.078231,3,167.40763,0\H,1,2.14
98795,2,143.94704,3,159.12876,0\\Version=x86-Linux-G03RevB.04\State=1-
A\HF=-271.5130288\RMSD=4.347e-05\Dipole=-0.1400092,0.0178855,-0.083017
2\PG=C01 [X(C7H8)]\\@

1f

1\1\GINC-NODE02\FOpt\RmPWPW91\6-31+G(d,p)\C6H6\CHS60A\23-Dec-2006\0\\#
P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H6\\0,1\C,-1.201591
9921,0.0000349432,-0.6935267878\C,-1.2014485074,-0.0000051292,0.693879
1793\C,0.0001357234,-0.0000546434,1.3873697721\C,1.2015920529,0.000160
7569,0.6935267797\C,1.2014485612,-0.0000522669,-0.6938790778\C,-0.0001
359199,-0.00007537,-1.3873698549\H,-0.0005610446,-0.0001626104,-2.4674
749135\H,2.1366611941,-0.0001094935,-1.2342597637\H,2.1371672309,0.000
3029647,1.2332718359\H,0.0005614447,-0.0001365465,2.4674748838\H,-2.13
6661166,-0.0000183971,1.2342597718\H,-2.1371671676,0.0000743391,-1.233
2718775\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-232.2001933\RMSD=6
.527e-09\RMSF=3.533e-05\Dipole=0.0000002,-0.0000164,0.\PG=C01 [X(C6H6)
]\\@

1g

1\1\GINC-NODE10\SP\RmPWPW91\6-31+G(d,p)\C6H5F1\CHS60A\03-Apr-2008\0\\#
P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C6H5F
\\0,1\C\C,1,1.3876353\C,2,1.387194,1,120.48328\C,3,1.3798236,2,118.337
71,1,0.0000494,0\C,4,1.3798236,3,122.54676,2,0.0001963,0\C,1,1.3876353
,2,119.81126,3,-0.0002867,0\H,6,1.079823,1,120.10263,2,-179.99986,0\H,
5,1.0786704,4,119.70344,3,179.99983,0\F,4,1.339,3,118.72662,2,179.9997
1,0\H,3,1.0786704,2,121.95886,1,-179.99992,0\H,2,1.079823,1,120.10263,
6,179.99986,0\H,1,1.079377,2,120.09437,3,180.,0\\Version=x86-Linux-G03
RevB.04\State=1-A'\HF=-331.4064307\RMSD=3.853e-05\Dipole=-0.5774534,-0
.0000016,-0.3346622\PG=CS [SG(C2H1F1),X(C4H4)]\\@

1h

1\1\GINC-NODE09\SP\RmPWPW91\6-31+G(d,p)\C6H5Cl1\CHS60A\03-Apr-2008\0\\
#P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C6H5
Cl\\0,1\C\C,1,1.3868596\C,2,1.386648,1,120.44998\C,3,1.3854764,2,119.0
8391,1,-0.0000934,0\C,4,1.3854764,3,121.20148,2,0.0003856,0\C,1,1.3868
596,2,119.73075,3,-0.0001909,0\H,6,1.0798905,1,120.18059,2,-179.99966,
0\H,5,1.0787582,4,119.94189,3,179.99968,0\Cl,4,1.731909,3,119.39926,2,
179.99992,0\H,3,1.0787582,2,120.9742,1,179.99997,0\H,2,1.0798905,1,120
.18059,6,179.99966,0\H,1,1.07955,2,120.13463,3,179.99975,0\\Version=x8
6-Linux-G03RevB.04\State=1-A'\HF=-691.8033617\RMSD=6.449e-05\Dipole=-0
.6383379,0.0000023,-0.3705472\PG=CS [SG(C2H1Cl1),X(C4H4)]\\@

1i

1\1\GINC-NODE11\SP\RmPWPW91\6-31+G(d,p)\C6H5Br1\CHS60A\03-Apr-2008\0\\
#P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C6H5
Br\\0,1\C\C,1,1.3862412\C,1,2.4076564,2,29.71995\C,1,2.764624,2,59.769
914,3,-0.000024,0\C,1,2.4076564,2,89.819878,3,0.0002666,0\C,1,1.386241
2,2,119.53983,3,0.0005287,0\H,1,1.079384,2,120.23009,3,179.99995,0\H,1
,2.1429523,2,25.830253,3,-179.99998,0\H,1,3.3880629,2,20.690859,3,0.00
02304,0\Br,1,4.637557,2,59.769914,3,0.0006094,0\H,1,3.3880629,2,98.848
968,3,0.000422,0\H,1,2.1429523,2,145.37008,3,0.0009162,0\\Version=x86-
Linux-G03RevB.04\State=1-A'\HF=-2803.4547811\RMSD=4.414e-05\Dipole=-0.
6397615,-0.0000047,-0.3728\PG=CS [SG(C2H1Br1),X(C4H4)]\\@

1j

1\1\GINC-NODE10\SP\RmPWPW91\6-31+G(d,p)\C6H5N1O2\CHS60A\03-Apr-2008\0\
\#P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C6H
5O2N\\0,1\C\C,1,1.3835451\C,2,1.3835451,1,122.51688\C,3,1.3842094,2,11
8.38778,1,-0.0001958,0\C,4,1.3880507,3,120.1505,2,0.0000941,0\C,1,1.38
42094,2,118.38778,3,0.0001958,0\H,6,1.0791773,1,119.64918,2,179.99991,
0\H,5,1.079764,4,119.79672,3,180.,0\H,4,1.0791773,3,119.64918,2,-179.9
9991,0\H,3,1.0774719,2,119.63472,1,179.99996,0\N,2,1.457033,1,118.7415
6,6,-179.99987,0\O,11,1.2093342,2,117.57772,1,-179.98917,0\O,11,1.2093
342,2,117.57772,1,-0.0107755,0\H,1,1.0774719,2,119.63472,3,-179.99996,
0\\Version=x86-Linux-G03RevB.04\State=1-A'\HF=-436.6216759\RMSD=9.218e
-05\Dipole=1.6867076,-0.0002026,-0.9250362\PG=CS [SG(C2H1N1),X(C4H4O2)
]\\@

2a

meta

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C8H11Cl1N1(2)\CHS60A\05-Apr-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C8H11N.Cl me
ta sigma 1K\\0,2\C,-2.085292788,0.0587283493,-2.0068288503\N,-2.063983
5922,0.2249291658,-0.5788149394\C,-0.8140990916,0.263040176,0.03881046
89\C,0.3580905242,0.3103855887,-0.6582436357\C,1.6650710701,0.21714752
79,0.0007406875\C,1.6413143401,0.2911166732,1.4679634136\C,0.455627580
7,0.2492395111,2.1440855679\C,-0.7648803129,0.2010573116,1.4655698102\
H,-1.679749979,0.0890805522,2.0245973861\H,0.4556456456,0.2418320856,3
.2241767724\H,2.5850548192,0.3148029959,1.9898240979\H,2.3868289058,0.
9015491144,-0.435070817\H,0.3662218202,0.3682323808,-1.733798686\C,-3.
0577693662,1.1673538234,-0.1174611665\H,-3.0715847795,1.225050039,0.96
49096774\H,-2.8802185331,2.1769045592,-0.5072673515\H,-4.0421639875,0.
8416077157,-0.4457861223\H,-1.4735709697,-0.7925120363,-2.2932479538\H
,-3.1075610407,-0.139003638,-2.3196932228\H,-1.7318007163,0.9445265852
,-2.5503889864\Cl,2.485436013,-1.4291169577,-0.4631981171\\Version=x86
-Linux-G03RevB.04\State=2-A\HF=-826.2991017\S2=0.833907\S2-1=0.\S2A=0.
754204\RMSD=6.200e-09\RMSF=5.832e-06\Dipole=-1.0615994,1.0165262,0.185
8192\PG=C01 [X(C8H11Cl1N1)]\\@

2b

ortho

1\1\GINC-NODE08\FOpt\UmPWPW91\6-31+G(d,p)\C6H7Cl1N1(2)\CHS60A\03-Jul-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H7NCl 1k re
opt sigma ortho\\0,2\N,0.5277424036,-0.4788459295,-2.1372838858\C,0.56
88783653,-0.4197528345,-0.7727094551\C,1.7467996229,-0.386560618,-0.05
31508068\C,1.7335200187,-0.4111759173,1.3366482986\C,0.5146943554,-0.4
999773857,2.0386036903\C,-0.6674725777,-0.5382699759,1.3672960285\C,-0
.7211015703,-0.4058093133,-0.0799120893\H,-1.4666369862,-1.031028274,-
0.5575247319\H,-1.6054527034,-0.6266181336,1.8927280252\H,0.5230269162
,-0.562527242,3.1163035687\H,2.6655974214,-0.3773008711,1.8790625126\H
,2.688330159,-0.3541169971,-0.583052357\H,1.3832142282,-0.2837585794,-
2.6217550843\H,-0.2776503441,-0.0609044773,-2.5682752119\Cl,-1.5680314
589,1.3304383735,-0.5068913833\\Version=x86-Linux-G03RevB.04\State=2-A
\HF=-747.7112945\S2=0.819095\S2-1=0.\S2A=0.752939\RMSD=6.777e-09\RMSF=
5.130e-05\Dipole=0.8325586,-0.6566958,-0.2747456\PG=C01 [X(C6H7Cl1N1)]
\\@

meta

1\1\GINC-NODE12\FOpt\UmPWPW91\6-31+G(d,p)\C6H7Cl1N1(2)\CHS60A\03-Apr-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H7N.Cl meta
 1K sigma\\0,2\C,-1.4475068116,-0.3364853023,-1.1484766955\C,-1.440926
9701,-0.3910986914,0.2723356741\C,-0.2520675848,-0.4645041891,0.936908
8587\C,1.0334465281,-0.391910109,0.2372496856\C,0.9562063325,-0.449043
0807,-1.2309656577\C,-0.2485100467,-0.3935556211,-1.8684980628\H,-0.28
36736533,-0.3927519912,-2.9478716248\H,1.8819362094,-0.4803489892,-1.7
836048727\H,1.7584620062,-1.0951949384,0.6364566851\H,-0.2290351763,-0
.514522797,2.0156624884\N,-2.65603767,-0.3308329939,0.934474377\H,-2.6
311490866,-0.5692091187,1.9076451186\H,-3.4319527308,-0.7513675032,0.4
593472985\H,-2.3898778252,-0.2547327548,-1.6696723489\Cl,1.9008061919,
1.2313847653,0.685258459\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-7
47.7026882\S2=0.839286\S2-1=0.\S2A=0.754748\RMSD=5.744e-09\RMSF=1.272e
-05\Dipole=-1.0592592,-1.1910387,-0.2312053\PG=C01 [X(C6H7Cl1N1)]\\@

2c

ortho

1\1\GINC-NODE07\FOpt\UmPWPW91\6-31+G(d,p)\C6H6Cl1O1(2)\CHS60A\09-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H6O---Cl or
tho int sigma 1K\\0,2\C,-0.9388122569,-0.4039427521,0.1125591443\C,-0.

9425335974,-0.4681034203,1.4784555653\C,0.2625303673,-0.5037068623,2.1
853527157\C,1.4922205301,-0.4866534618,1.4965693302\C,1.5331580871,-0.
4366077117,0.1382641223\C,0.3089288168,-0.3495688562,-0.6597193138\H,0
.2983402556,-1.036276396,-1.5025719265\H,2.4711987398,-0.4441663573,-0
.3944600394\H,2.4147805201,-0.5345586256,2.055381787\H,0.2485535761,-0
.5440201193,3.2630831513\H,-1.892041464,-0.4887681518,1.9903988454\O,-
2.0974398859,-0.3984878798,-0.5632425413\H,-1.9729822193,0.0280342277,
-1.4131287232\Cl,0.2893363527,1.2999504027,-1.6471560087\\Version=x86-
Linux-G03RevB.04\State=2-A\HF=-767.5600623\S2=0.83218\S2-1=0.\S2A=0.75
3998\RMSD=6.836e-09\RMSF=2.441e-05\Dipole=0.3051287,-0.6068139,0.36499
8\PG=C01 [X(C6H6Cl1O1)]\\@

meta

1\1\GINC-NODE09\FOpt\UmPWPW91\6-31+G(d,p)\C6H6Cl1O1(2)\CHS60A\02-Apr-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H6O.Cl meta
 sigma a 1K\\0,2\C,-1.5093766089,0.422299425,-1.1084433486\C,-1.508839
3389,0.4883445048,0.2506379589\C,-0.2515112507,0.4069595819,1.01475267
94\C,0.9747695365,0.4205730564,0.2076392725\C,0.9268023515,0.346061358
5,-1.1511895663\C,-0.3082365503,0.3306725832,-1.8326773578\H,-0.329919
3751,0.2645124549,-2.9112515461\O,2.0969608177,0.3062810591,-1.8292808
597\H,1.9389675488,0.3070930009,-2.7699745048\H,1.9283717122,0.4386579
236,0.7103872516\H,-0.2162300086,1.1368514368,1.8190547846\H,-2.430497
3137,0.5527942054,0.8071758089\H,-2.4450454756,0.4471626342,-1.6467454
157\Cl,-0.3037048509,-1.1815754816,2.0200754512\\Version=x86-Linux-G03
RevB.04\State=2-A\HF=-767.5536669\S2=0.845171\S2-1=0.\S2A=0.755256\RMS
D=7.186e-09\RMSF=8.825e-06\Dipole=-0.4164257,0.7642961,-1.186426\PG=C0
1 [X(C6H6Cl1O1)]\\@

para

1\1\GINC-NODE04\FOpt\UmPWPW91\6-31+G(d,p)\C6H6Cl1O1(2)\CHS60A\02-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H6O---Cl\\0
,2\C,-1.2278336055,-0.4731626805,-0.4592869998\C,-1.2376692007,-0.4616
69776,0.9034951237\C,-0.0330626013,-0.4502527325,1.6251424557\C,1.1989
552453,-0.5073174342,0.9469193241\C,1.2370957187,-0.5147936315,-0.4107
285295\C,0.0213576547,-0.3671984442,-1.2140339313\H,0.0284384305,-0.95
80208151,-2.1226449865\H,2.1804637973,-0.5686722348,-0.931149399\H,2.1
039724029,-0.5657480809,1.5319264391\O,0.0071232847,-0.4340434408,2.96
91137811\H,-0.8744473857,-0.3847273854,3.3329585007\H,-2.1795117031,-0
.4866593252,1.4355169892\H,-2.1533930928,-0.4956069073,-1.0127441156\C
l,0.063790118,1.3869500275,-2.0197540196\\Version=x86-Linux-G03RevB.04
\State=2-A\HF=-767.5575667\S2=0.826828\S2-1=0.\S2A=0.753635\RMSD=6.439
e-09\RMSF=2.064e-05\Dipole=-0.5981252,-0.9247739,0.8044818\PG=C01 [X(C
6H6Cl1O1)]\\@

2d

ortho

1\1\GINC-NODE08\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\10-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8O---Cl or
tho exo sigma 1K\\0,2\C,-1.5357906966,0.4088843405,-2.5113059497\O,-1.
4483668915,0.4148216685,-1.1103541858\C,-0.2381633005,0.3747264402,-0.
5474702213\C,0.9575140443,0.3841733684,-1.2120490383\C,2.16256749,0.42
12428312,-0.4917080348\C,2.1534417739,0.5045535152,0.9116351585\C,0.97
96811076,0.4918791895,1.6011196609\C,-0.3049311297,0.280810989,0.92186
53919\H,-1.1141726303,0.8864910368,1.3164420824\H,0.9619168936,0.56393
74163,2.6774046494\H,3.0872051543,0.6000471099,1.4452080583\H,3.098972
8193,0.4227426959,-1.0272282609\H,0.9865504165,0.3937474824,-2.2896663
122\H,-2.5932431332,0.4254963842,-2.7468142021\H,-1.0547104505,1.28874
09272,-2.9388375117\H,-1.0859037601,-0.4929350898,-2.9255212089\Cl,-0.
9262115242,-1.4473214915,1.3729014346\\Version=x86-Linux-G03RevB.04\St
ate=2-A\HF=-806.8518633\S2=0.82993\S2-1=0.\S2A=0.753834\RMSD=8.575e-09
\RMSF=1.170e-05\Dipole=0.4424582,0.8512164,-0.983133\PG=C01 [X(C7H8Cl1
O1)]\\@

meta

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\03-Apr-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8O.Cl meta
 sigma 1K\\0,2\C,-1.8278896416,-0.3495849253,-2.8753493742\O,-1.839058
0981,-0.3533442736,-1.4743194087\C,-0.6617039068,-0.351945735,-0.81202
30938\C,-0.7350589514,-0.4137022475,0.5545881856\C,0.4645530019,-0.346
8037345,1.3930942848\C,1.7417853652,-0.4073144063,0.6647290745\C,1.770
7731572,-0.3620885935,-0.6916802558\C,0.5869358979,-0.312041098,-1.457
5344819\H,0.6553453915,-0.2611502276,-2.5311065199\H,2.7199166455,-0.3
714909564,-1.2067871801\H,2.6512420086,-0.4393146231,1.243747514\H,0.4
262429619,-1.0503511159,2.220047237\H,-1.701922391,-0.4528676288,1.030

3846282\H,-1.3622465236,0.5537869225,-3.2708213485\H,-2.867241578,-0.3
731413881,-3.1826267779\H,-1.3186731734,-1.2272688509,-3.275370665\Cl,
0.4396136417,1.2770256764,2.3595377851\\Version=x86-Linux-G03RevB.04\S
tate=2-A\HF=-806.8454148\S2=0.847235\S2-1=0.\S2A=0.75539\RMSD=3.125e-0
9\RMSF=2.825e-05\Dipole=0.2138925,-0.7814707,-1.2714479\PG=C01 [X(C7H8
Cl1O1)]\\@

para

1\1\GINC-NODE05\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\02-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8O---Cl si
gma p\\0,2\C,-2.4127559406,-0.3738941586,-2.4734285553\O,-2.3219504019
,-0.4217956698,-1.0730835608\C,-1.1095084059,-0.4283095707,-0.50180794
49\C,0.103544508,-0.4391317129,-1.2064126432\C,1.29159338,-0.438173256
6,-0.5293950345\C,1.3502813195,-0.3132690493,0.9242092102\C,0.06183586
51,-0.4595339964,1.6022839959\C,-1.103367524,-0.4703040421,0.911288018
1\H,-2.0540136977,-0.5304922486,1.418898503\H,0.0598623835,-0.49982359
68,2.680382107\H,2.1510622298,-0.8843059337,1.3788954443\H,2.223869418
3,-0.4624386749,-1.0716869347\H,0.1126177793,-0.4739998159,-2.28400843
66\H,-1.9304736605,0.5193824897,-2.8695053984\H,-1.9733235571,-1.26093
88085,-2.9293715624\H,-3.471161429,-0.3419434568,-2.7038571289\Cl,2.02
1613208,1.4614482426,1.329676448\\Version=x86-Linux-G03RevB.04\State=2
-A\HF=-806.8503999\S2=0.823032\S2-1=0.\S2A=0.753296\RMSD=5.583e-09\RMS
F=1.495e-05\Dipole=-0.6911924,-0.9624422,-1.0387477\PG=C01 [X(C7H8Cl1O
1)]\\@

2e

ortho

1\1\GINC-NODE06\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1(2)\CHS60A\10-Apr-200
7\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8---Cl ortho
 sigma 1K\\0,2\C,0.5214941523,0.4656401096,-2.271352677\C,0.5425645547
,0.4356107508,-0.7830506811\C,1.7013778606,0.4768378892,-0.0585251044\
C,1.7015928859,0.4961692269,1.3459010418\C,0.483584414,0.5209479786,2.
0498360017\C,-0.7013878551,0.4785518523,1.3830481322\C,-0.7529766385,0
.3222093126,-0.0780709538\H,-1.5201197897,0.9412189808,-0.5359064268\H
,-1.6412171229,0.5027173256,1.9129198316\H,0.4903244572,0.5910678078,3
.1274498115\H,2.6372224116,0.5236225602,1.8825423225\H,2.6448537955,0.
5198626811,-0.5845432913\H,1.523457441,0.5708051583,-2.678146799\H,0.0
80007947,-0.4472194882,-2.670850328\H,-0.0832200448,1.2973718655,-2.63
61842787\Cl,-1.4769885493,-1.3926617418,-0.4319997293\\Version=x86-Lin
ux-G03RevB.04\State=2-A\HF=-731.6733626\S2=0.843437\S2-1=0.\S2A=0.7551
18\RMSD=6.788e-09\RMSF=2.970e-06\Dipole=0.5533323,0.8569033,0.0975246\
PG=C01 [X(C7H8Cl1)]\\@

meta

1\1\GINC-NODE10\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1(2)\CHS60A\02-Apr-200
8\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8.Cl meta si
gma 1K\\0,2\C,0.4987506989,-0.4240069589,-2.8598657524\C,0.4880196106,
-0.4066999985,-1.362194277\C,1.7181397344,-0.3621599332,-0.6596462465\
C,1.7478737066,-0.3932651122,0.744042178\C,0.5964332896,-0.4302261559,
1.4710806944\C,-0.7182021927,-0.3747525997,0.811621711\C,-0.6772867806
,-0.443845662,-0.6587857613\H,-1.6260291314,-0.4824637543,-1.173835543
3\H,-1.4209845245,-1.0871653266,1.2354712056\H,0.6162103157,-0.4563260
429,2.549583423\H,2.700563037,-0.3993302362,1.2531033932\H,2.644190731
3,-0.3249285505,-1.2144955923\H,1.0854338535,-1.2599709428,-3.23805837
72\H,0.9431113602,0.4897453803,-3.2526712654\H,-0.506991463,-0.5069505
423,-3.2625417739\Cl,-1.5504630929,1.2374781492,1.3050546619\\Version=
x86-Linux-G03RevB.04\State=2-A\HF=-731.6712318\S2=0.843596\S2-1=0.\S2A
=0.755168\RMSD=5.046e-09\RMSF=1.213e-05\Dipole=0.6513966,-0.7794091,-0
.5221837\PG=C01 [X(C7H8Cl1)]\\@

para

1\1\GINC-NODE01\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1(2)\CHS60A\05-Apr-200
7\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8---Cl again
 sigma\\0,2\C,-0.0085646043,-0.375025184,-3.1297482922\C,-0.0096125632
,-0.4352809482,-1.6393350005\C,1.2006399591,-0.4864825261,-0.912205275
\C,1.2249574409,-0.4889768079,0.4475810088\C,-0.0078440547,-0.36405875
92,1.2391903237\C,-1.2450603902,-0.4349081403,0.4477693915\C,-1.220871
2904,-0.433505608,-0.9119819513\H,-2.1552729387,-0.447856497,-1.456011
9715\H,-2.1816949524,-0.4423209553,0.9838993418\H,-0.0223313029,-1.028
8434336,2.0978638306\H,2.160456352,-0.5373667694,0.9835599317\H,2.1334
325602,-0.5416656215,-1.4563788868\H,-0.8992290125,-0.8396575074,-3.54
75122025\H,0.0106853503,0.6596597392,-3.4776795599\H,0.8640051365,-0.8
726252295,-3.5476474926\Cl,0.0287106955,1.3035355363,2.1277815164\\Ver
sion=x86-Linux-G03RevB.04\State=2-A\HF=-731.6720505\S2=0.839993\S2-1=0
.\S2A=0.754835\RMSD=6.006e-09\RMSF=1.838e-06\Dipole=-0.0179582,-0.8074
093,-0.9107717\PG=C01 [X(C7H8Cl1)]\\@

2g

ortho

1\1\GINC-NODE03\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1F1(2)\CHS60A\09-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5F--Cl ort
ho sigma 1K\\0,2\C,-0.9385542033,-0.4217987601,0.0853881123\C,-0.96437
26435,-0.4331689033,1.4409139413\C,0.2492758488,-0.4448566356,2.148551
2502\C,1.4719042786,-0.4890954164,1.450275332\C,1.5079560756,-0.479378
959,0.0899577724\C,0.2837715152,-0.3306210527,-0.7175787662\H,0.248510
4504,-0.9977705914,-1.5743773293\H,2.4443084145,-0.5212922206,-0.44400
83428\H,2.3958501193,-0.5497988681,2.005407763\H,0.2391631275,-0.44620
46607,3.2267655606\H,-1.9147416413,-0.456190945,1.9506434397\F,-2.0720
604653,-0.4635180002,-0.6096476639\Cl,0.327974617,1.3374375089,-1.5683
91057\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-791.5625986\S2=0.843
247\S2-1=0.\S2A=0.755087\RMSD=8.973e-09\RMSF=6.897e-05\Dipole=0.488066
1,-0.7606472,0.9004603\PG=C01 [X(C6H5Cl1F1)]\\@

meta

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1F1(2)\CHS60A\02-Apr-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5F.Cl meta
 sigma 1K\\0,2\C,-1.5111127121,0.4452394429,-0.2296320963\C,-1.4915530
09,0.4479420399,1.132503815\C,-0.2787722405,0.4161797645,1.8419446759\
C,0.9209565009,0.4145283559,1.1130027319\C,0.9754440098,0.4160347337,-
0.2378607091\C,-0.26939443,0.3471112164,-1.0220174619\H,-0.2621794418,
1.0500430262,-1.8509397\H,1.9237238432,0.4222249778,-0.7500234463\F,2.
0597081641,0.4349047462,1.8140273681\H,-0.2460535443,0.4106835653,2.91
9056565\H,-2.420464764,0.4855328958,1.6812157878\H,-2.4433502637,0.469
091053,-0.7717952505\Cl,-0.3036740013,-1.2749371502,-1.9494944707\\Ver
sion=x86-Linux-G03RevB.04\State=2-A\HF=-791.5623532\S2=0.84405\S2-1=0.
\S2A=0.755137\RMSD=7.006e-09\RMSF=4.803e-05\Dipole=-0.6093057,0.745697
2,0.3074995\PG=C01 [X(C6H5Cl1F1)]\\@

para

1\1\GINC-NODE01\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1F1(2)\CHS60A\01-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5F---Cl si
gma\\0,2\C,-1.2404293279,-0.4538561561,-0.4238596683\C,-1.2487242373,-
0.4292733566,0.9374063285\C,-0.0330737029,-0.4104159425,1.6282276304\C
,1.2039279549,-0.4643917991,0.978374262\C,1.2403913078,-0.48937793,-0.
3824212225\C,0.0145420252,-0.3712824403,-1.1888661889\H,0.0195451018,-
1.0291144489,-2.0522937352\H,2.1818988107,-0.5408564125,-0.9061276951\
H,2.1066411359,-0.5055692681,1.5677924881\F,-0.0549950484,-0.387543445
,2.9602128627\H,-2.1714237923,-0.4443135476,1.4963337301\H,-2.16501229
78,-0.478614914,-0.978736427\Cl,0.0531471975,1.3057614908,-2.062473586
6\\Version=x86-Linux-G03RevB.04\State=2-A'\HF=-791.5630215\S2=0.841941
\S2-1=0.\S2A=0.754957\RMSD=6.413e-09\RMSF=5.823e-05\Dipole=-0.0126803,
-0.834989,0.0433741\PG=CS [SG(C2H1Cl1F1),X(C4H4)]\\@

2h

ortho

1\1\GINC-NODE04\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl2(2)\CHS60A\09-Apr-200
7\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Cl---Cl ort
ho sigma 1K\\0,2\C,-1.8220289544,-0.3617375679,0.1619143705\C,-1.81886
12694,-0.3516699119,1.5203182079\C,-0.6078745992,-0.3278874296,2.24104
13132\C,0.6174839207,-0.3728058211,1.5610466242\C,0.6446787381,-0.3913
154194,0.1974713786\C,-0.5752652812,-0.2581525677,-0.6213390007\H,-0.5
596813111,-0.9298279958,-1.4746419734\Cl,2.1318495618,-0.5337724536,-0
.6480774811\H,1.5445592965,-0.4213244382,2.1107903298\H,-0.6175554951,
-0.3082216193,3.3193258443\H,-2.7555680875,-0.3781641028,2.0564225913\
H,-2.7458722178,-0.3848745687,-0.3950078162\Cl,-0.5727129449,1.4045856
907,-1.4683699506\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1151.960
3409\S2=0.847279\S2-1=0.\S2A=0.755428\RMSD=4.185e-09\RMSF=2.131e-05\Di
pole=-0.5117823,-0.7009586,0.8805351\PG=C01 [X(C6H5Cl2)]\\@

meta

1\1\GINC-NODE12\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl2(2)\CHS60A\02-Apr-200
8\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Cl.Cl meta
sigma 1K\\0,2\C,-1.8186677049,0.3899920877,-0.4686561745\C,-1.79742239
74,0.3652133612,0.8920674204\C,-0.5854463494,0.3292062753,1.6036340182
\C,0.6278428521,0.3562379214,0.8886736599\C,0.6676319187,0.3841265107,
-0.468074181\C,-0.5756424485,0.3173352497,-1.2586515143\H,-0.568660333
,1.0374462351,-2.0730654409\H,1.6075917379,0.4116308919,-0.9951246612\
Cl,2.1051744303,0.3798695605,1.7903241489\H,-0.5727218174,0.3007086987
,2.6806982784\H,-2.7260956613,0.3840457848,1.4424966779\H,-2.750991501
1,0.4192441763,-1.0106153711\Cl,-0.5815801744,-1.2860898089,-2.2125799
639\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1151.9591714\S2=0.8499

08\S2-1=0.\S2A=0.755767\RMSD=5.831e-09\RMSF=2.934e-05\Dipole=-0.617010
7,0.7221042,0.2696015\PG=C01 [X(C6H5Cl2)]\\@

para

1\1\GINC-NODE08\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl2(2)\CHS60A\02-Apr-200
7\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Cl---Cl sig
ma II\\0,2\C,-1.2383926064,-0.3619382931,-0.8213512017\C,-1.237970913,
-0.3807674384,0.537280987\C,-0.0206974778,-0.3942691928,1.2437394881\C
,1.2105075654,-0.4293670562,0.5626206961\C,1.2397832726,-0.4111273718,
-0.7957041493\C,0.0109243488,-0.283834617,-1.5999507626\H,0.0062788378
,-0.9609406014,-2.4497102513\H,2.1807642845,-0.4450392562,-1.322480969
7\H,2.126375555,-0.4866466453,1.1301909887\Cl,-0.0388333795,-0.4130465
004,2.9601283719\H,-2.1669361178,-0.4014291078,1.0857587955\H,-2.16887
8682,-0.3587036041,-1.3674961448\Cl,0.052802261,1.3671984434,-2.479897
358\\Version=x86-Linux-G03RevB.04\State=2-A'\HF=-1151.961227\S2=0.8410
72\S2-1=0.\S2A=0.754904\RMSD=5.429e-09\RMSF=3.082e-05\Dipole=-0.015477
8,-0.7739462,0.0111885\PG=CS [SG(C2H1Cl2),X(C4H4)]\\@

2i

ortho

1\1\GINC-NODE05\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Br1Cl1(2)\CHS60A\09-Apr-
2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Br---Cl
ortho sigma 1K\\0,2\C,-0.2066704174,-0.2623569933,0.3476007432\C,-0.20
58643832,-0.2481130268,1.7105806607\C,1.0058400099,-0.2458340717,2.416
8372626\C,2.2313931293,-0.3093520825,1.7243233818\C,2.261760237,-0.322
9147933,0.3664922512\C,1.0357367948,-0.17896878,-0.4428412778\H,1.0170
497889,-0.8556118548,-1.2923448059\H,3.1948586009,-0.3800662865,-0.172
354529\H,3.1547399631,-0.3668337911,2.280711203\H,0.9914288371,-0.2277
070666,3.4952000362\H,-1.1430793582,-0.2686306964,2.244661797\Br,-1.79
93591036,-0.3871872481,-0.6044192383\Cl,1.1193763865,1.4738612861,-1.3
023034406\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-3263.6124074\S2=
0.846601\S2-1=0.\S2A=0.755385\RMSD=8.168e-09\RMSF=5.589e-05\Dipole=0.4
420427,-0.7017061,0.8753342\PG=C01 [X(C6H5Br1Cl1)]\\@

meta

1\1\GINC-NODE11\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Br1Cl1(2)\CHS60A\02-Apr-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Br.Cl me
ta sigma 1K\\0,2\C,-2.2740363109,0.2916229309,-0.847317082\C,-2.253178
8484,0.2757696453,0.5128881385\C,-1.0432553904,0.2495927247,1.22878127
5\C,0.1721581029,0.278004898,0.5191508539\C,0.2156896519,0.2978213315,
-0.83695734\C,-1.0264770424,0.231546892,-1.6302349655\H,-1.0196559169,
0.963064251,-2.4351641115\H,1.1539350454,0.3284102534,-1.3666269559\Br
,1.7677797749,0.3196107808,1.4989848904\H,-1.0382922288,0.2272372527,2
.3059326977\H,-3.1827430243,0.2914686421,1.062254331\H,-3.2045537437,0
.3130756285,-1.3924267422\Cl,-1.0191990135,-1.3562225818,-2.6068415096
\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-3263.6110337\S2=0.849576\
S2-1=0.\S2A=0.755724\RMSD=8.905e-09\RMSF=2.201e-05\Dipole=-0.5994385,0
.7129982,0.2788588\PG=C01 [X(C6H5Br1Cl1)]\\@

para

1\1\GINC-NODE09\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Br1Cl1(2)\CHS60A\02-Apr-
2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Cl---Br
sigma\\0,2\C,-1.229331217,-0.2659490083,-1.4436293839\C,-1.2285759863,
-0.2874707826,-0.0854412942\C,-0.0124857643,-0.3043957421,0.6226429661
\C,1.217706717,-0.3360268442,-0.0601242962\C,1.2474132931,-0.315109703
8,-1.4179971314\C,0.0191699473,-0.1936509018,-2.2237247719\H,0.0141949
145,-0.8825765655,-3.0643133899\H,2.1889322296,-0.3463786428,-1.944145
5069\H,2.1357741971,-0.3932726652,0.5036966804\Br,-0.0325361993,-0.346
6340553,2.4790283996\H,-2.1596595793,-0.3080129579,0.4592425017\H,-2.1
60262807,-0.2600518328,-1.98915607\Cl,0.0609650636,1.4434177939,-3.122
4514548\\Version=x86-Linux-G03RevB.04\State=2-A'\HF=-3263.6130521\S2=0
.840447\S2-1=0.\S2A=0.75485\RMSD=7.008e-09\RMSF=1.003e-05\Dipole=-0.01
55517,-0.7601141,0.0448626\PG=CS [SG(C2H1Br1Cl1),X(C4H4)]\\@

2j

ortho

1\1\GINC-NODE11\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1N1O2(2)\CHS60A\10-Apr
-2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5O2N---C
l ortho sigma 1K\\0,2\C,-0.4782279385,-0.3188166023,0.2206554384\C,-0.
5231865059,-0.3177545553,1.58142009\C,0.6708685615,-0.3404268416,2.314
5262833\C,1.9110883522,-0.4140866643,1.6479693312\C,1.9768088473,-0.39
59864285,0.2905352533\C,0.7733276916,-0.2177900743,-0.5499361856\H,0.7
590370264,-0.8662766676,-1.4197884842\H,2.9243644238,-0.4437603404,-0.
2229992826\H,2.8191891196,-0.4951248929,2.2256693898\H,0.6329329642,-0
.3382046801,3.3922045349\H,-1.4831852406,-0.3350043479,2.0717838815\N,

-1.7055069807,-0.416529604,-0.5256488692\O,-1.6066147028,-0.5880730548
,-1.7214179183\O,-2.7515046082,-0.3389260991,0.0816964161\Cl,0.8921818
242,1.4611316698,-1.3106221883\\Version=x86-Linux-G03RevB.04\State=2-A
\HF=-896.7773212\S2=0.841059\S2-1=0.\S2A=0.754757\RMSD=5.226e-09\RMSF=
7.633e-05\Dipole=1.6231965,-0.5699959,1.5099689\PG=C01 [X(C6H5Cl1N1O2)
]\\@

meta

1\1\GINC-NODE07\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1N1O2(2)\CHS60A\02-Apr
-2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5O2N---C
l sigma meta\\0,2\C,-0.4829766369,-0.3343195247,-0.642743162\C,-0.4381
436905,-0.3486885229,0.7143193246\C,0.7560047236,-0.364871275,1.450962
1435\C,1.9702663731,-0.4053675769,0.7449579362\C,1.9991011336,-0.38806
27524,-0.616554378\C,0.7680038074,-0.2498055911,-1.4182266173\H,0.7547
987434,-0.9226349202,-2.271490168\H,2.935217857,-0.4272800815,-1.15147
73702\H,2.8949488959,-0.4653309759,1.2983044387\H,0.7191943838,-0.3701
437506,2.5265202265\N,-1.7029412556,-0.3766334086,1.4490118525\O,-2.72
53512882,-0.4010762478,0.807162838\O,-1.6398695299,-0.3744018087,2.655
6385659\H,-1.4280862324,-0.3367611838,-1.1597267126\Cl,0.7960439662,1.
4064176871,-2.2637597703\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-8
96.7752867\S2=0.854649\S2-1=0.\S2A=0.756232\RMSD=4.170e-09\RMSF=2.875e
-05\Dipole=1.5132676,-0.6831748,-0.4278894\PG=C01 [X(C6H5Cl1N1O2)]\\@

para

1\1\GINC-NODE06\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1N1O2(2)\CHS60A\02-Apr
-2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5O2N---C
l sigma para\\0,2\C,-1.2410101385,-0.266410473,-1.0436760535\C,-1.2427
515864,-0.3052017235,0.3107262595\C,-0.0176666629,-0.3426675243,1.0036
535495\C,1.2218793256,-0.3579813071,0.3360679099\C,1.2496348647,-0.319
7883061,-1.0180687738\C,0.0137831959,-0.2336992082,-1.8282247058\H,0.0
054603463,-0.9954765358,-2.6066375373\H,2.1891650845,-0.329412501,-1.5
483609458\H,2.1271360342,-0.4056341368,0.9182628637\N,-0.0333643357,-0
.3862806962,2.4404472052\O,-1.114324857,-0.3810070399,2.9913072465\O,1
.0353113784,-0.4263249548,3.0134002812\H,-2.1609917245,-0.3138320885,0
.8741708306\H,-2.1689921207,-0.2359713213,-1.5931690425\Cl,0.057098033
4,1.3174963922,-2.8075250554\\Version=x86-Linux-G03RevB.04\State=2-A\H
F=-896.7791554\S2=0.836143\S2-1=0.\S2A=0.754426\RMSD=8.763e-09\RMSF=2.
352e-05\Dipole=0.0029798,-0.5829846,-1.5057973\PG=C01 [X(C6H5Cl1N1O2)]
\\@

3a

ortho

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C8H11Cl1N1(2)\CHS60A\28-Jun-
2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C8H11N---Cl
pi ortho 1k sb\\0,2\C,-1.6885919106,0.5734409519,-1.780005197\N,-1.648
5425528,0.2124622548,-0.381341029\C,-0.4944652503,0.2941509165,0.30885
16437\C,-0.399215263,-0.1477101856,1.6483261786\C,0.7667166365,0.01226
14524,2.348324563\C,1.8980366706,0.6143302986,1.7703899637\C,1.8412229
428,1.0212476835,0.4672249658\C,0.6796791147,0.8261198317,-0.299063509
2\H,0.6158439608,1.2943986058,-1.2647945929\H,2.6985633319,1.468923256
4,-0.0104639113\H,2.7985715126,0.7426712311,2.350157175\H,0.8129869722
,-0.3329156286,3.370755126\H,-1.2429517826,-0.612036801,2.1295056855\C
,-2.8093464766,-0.3984749609,0.2174558278\H,-3.6482087173,-0.305212058
6,-0.4614477406\H,-2.6448388127,-1.4583088608,0.4178323257\H,-3.076978
9112,0.097675643,1.1491153114\H,-2.6637022546,0.3255080321,-2.18125535
48\H,-1.5293173662,1.6437453512,-1.9153684729\H,-0.9292494861,0.022862
2817,-2.3347478948\Cl,1.2696976847,-1.243926045,-1.568760416\\Version=
x86-Linux-G03RevB.04\State=2-A\HF=-826.3105563\S2=0.762673\S2-1=0.\S2A
=0.750103\RMSD=4.835e-09\RMSF=3.461e-06\Dipole=-1.7025649,1.1423062,0.
9718856\PG=C01 [X(C8H11Cl1N1)]\\@

para

1\1\GINC-NODE01\FOpt\UmPWPW91\6-31+G(d,p)\C8H11Cl1N1(2)\CHS60A\08-Jun-
2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C8H11N---Cl
opt 1K\\0,2\C,-2.0039485077,-0.4968835021,-2.4728298128\N,-1.982144752
1,-0.3086269943,-1.0434449528\C,-0.8210702218,-0.4257306447,-0.3554690
845\C,-0.7805223494,-0.2258381862,1.0451037207\C,0.3987644846,-0.31913
37673,1.7301807631\C,1.612808644,-0.5836231176,1.0642081571\C,1.560123
28,-0.8475662585,-0.3196034512\C,0.3866584982,-0.7569199683,-1.0149576
868\H,0.3932806669,-0.9362570482,-2.0767484441\H,2.4716956252,-1.09287
75975,-0.8419978479\H,2.49233421,-0.8408374923,1.6288357956\H,0.410237
596,-0.1548881292,2.7964495432\H,-1.6819007286,0.0079742954,1.58590165
5\C,-3.2007985251,0.0477315918,-0.3601167575\H,-3.1144104768,1.0168903
593,0.1321039522\H,-4.0073216725,0.108671175,-1.0808795292\H,-3.474287
125,-0.6980136522,0.387008389\H,-1.3515427203,0.2147141264,-2.97978899
51\H,-1.6977649273,-1.506402056,-2.7489668667\H,-3.0131341686,-0.34373
10231,-2.8358464147\Cl,2.5609255982,1.6489958306,1.0258204908\\Version
=x86-Linux-G03RevB.04\State=2-A\HF=-826.3081025\S2=0.770938\S2-1=0.\S2
A=0.750263\RMSD=3.802e-09\RMSF=4.867e-06\Dipole=-2.4914158,-1.4447192,
-1.0390955\PG=C01 [X(C8H11Cl1N1)]\\@

3b

ortho

1\1\GINC-NODE14\FOpt\UmPWPW91\6-31+G(d,p)\C6H7Cl1N1(2)\CHS60A\05-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H7N---Cl or
tho pi B1K\\0,2\C,-1.6530528132,0.6277896745,-0.0637621307\C,-1.624775
5264,0.6926963127,1.3095019715\C,-0.410648049,0.6986358101,2.017911509
8\C,0.7692145108,0.6348236412,1.3304529505\C,0.776214623,0.5193873371,
-0.0761780385\C,-0.457336471,0.556137959,-0.7862032659\N,-0.4406543439
,0.537210539,-2.141664732\H,-1.3020695885,0.3331997235,-2.6103866484\H
,0.3667167177,0.1268773302,-2.5740259672\H,1.685913974,0.7264927973,-0
.6157451712\H,1.7147632611,0.646117661,1.849332571\H,-0.4158244247,0.7
619163017,3.0947149892\H,-2.5568157214,0.7401606359,1.8529728337\H,-2.
5951718019,0.6309465886,-0.5921306084\Cl,1.2817276674,-1.7707652481,-0
.4590245208\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-747.7121421\S2
=0.775017\S2-1=0.\S2A=0.750428\RMSD=3.539e-09\RMSF=3.088e-05\Dipole=-1
.0097023,1.2837906,-0.2405502\PG=C01 [X(C6H7Cl1N1)]\\@

para

1\1\GINC-NODE03\FOpt\UmPWPW91\6-31+G(d,p)\C6H7Cl1N1(2)\CHS60A\02-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H7N---Cl\\0
,2\C,-1.2130992174,-0.5849790083,-0.5413966311\C,-1.2380552444,-0.6045
892959,0.8257426737\C,-0.0358482757,-0.6180326265,1.5572680527\C,1.189
2698164,-0.6456428257,0.8651957191\C,1.2094307927,-0.6259135482,-0.502
0105096\C,0.0109536013,-0.5430238603,-1.2438455427\H,0.0250718413,-0.7
278292545,-2.3042840722\H,2.1515146034,-0.6388852798,-1.0273472059\H,2
.1132432829,-0.6802266616,1.4240512399\N,-0.0582725009,-0.6416944718,2
.9137027033\H,-0.9117989192,-0.4453822776,3.3959704986\H,0.7851572912,
-0.4734573131,3.4235545743\H,-2.1803512411,-0.6075360741,1.3542442265\
H,-2.1375231944,-0.5663963083,-1.0970630206\Cl,0.0603932356,1.78615655
65,-1.8429863375\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-747.71035
43\S2=0.775729\S2-1=0.\S2A=0.750426\RMSD=3.990e-09\RMSF=9.125e-06\Dipo
le=-0.057386,-1.4163851,2.0408958\PG=C01 [X(C6H7Cl1N1)]\\@

3c

ortho

1\1\GINC-NODE01\FOpt\UmPWPW91\6-31+G(d,p)\C6H6Cl1O1(2)\CHS60A\05-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H6O---Cl or
tho internal H pi 1K\\0,2\C,-0.3756655925,0.5529136028,-0.7994713038\C
,-0.3657206601,0.5506846107,0.6210883282\C,0.8795390931,0.5416321103,1
.2928575278\C,2.048201367,0.4913413884,0.5834065962\C,2.0119613176,0.4
915159759,-0.8203958015\C,0.814250724,0.5241890086,-1.5087042352\H,0.7
79123318,0.5101134342,-2.5863292212\H,2.937490049,0.4553940745,-1.3753
397475\H,2.997189217,0.4680146975,1.095878067\H,0.883565455,0.56498111
12,2.3711678646\H,-1.2384393978,0.9120152383,1.1419482456\O,-1.5267743
282,0.5744231126,-1.4705905147\H,-2.2250754695,0.2094596327,-0.9227853
769\Cl,-1.2938268259,-1.5664131335,0.9310292715\\Version=x86-Linux-G03
RevB.04\State=2-A\HF=-767.5596441\S2=0.789834\S2-1=0.\S2A=0.751094\RMS
D=7.265e-09\RMSF=1.890e-05\Dipole=0.8182443,1.1089653,-0.0977052\PG=C0
1 [X(C6H6Cl1O1)]\\@

para

1\1\GINC-NODE09\FOpt\UmPWPW91\6-31+G(d,p)\C6H6Cl1O1(2)\CHS60A\24-Dec-2
006\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H6O---Cl ph
enol para complex 1K\\0,2\C,-1.0248075118,0.6302250169,-0.7855919839\C
,-1.0275306858,0.6146211668,0.623431111\C,0.2088061091,0.62786771,1.30
34204074\C,1.3899104333,0.5751669531,0.6107222027\C,1.36799289,0.53937
43776,-0.7868801147\C,0.1571944251,0.5747078483,-1.482907736\H,-1.9642
95426,0.6556484361,-1.3148241003\H,-1.9345513721,0.8414825211,1.158116
9836\H,0.2153295129,0.6510606504,2.3817959948\H,2.3431001189,0.5581259
962,1.1148494386\O,2.5501371025,0.4789089827,-1.4114708372\H,0.1544120
138,0.5579871205,-2.5638849776\Cl,-1.651665082,-1.7000866194,0.9400768
188\H,2.4338207675,0.4341175086,-2.3587558797\\Version=x86-Linux-G03Re
vB.04\State=2-A\HF=-767.5580128\S2=0.782355\S2-1=0.\S2A=0.750719\RMSD=
7.826e-09\RMSF=2.468e-05\Dipole=0.6820073,1.3474107,-1.0337211\PG=C01
[X(C6H6Cl1O1)]\\@

3d

ortho

1\1\GINC-NODE14\Freq\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\07-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) FREQ=NORAMAN GEOM=CHECKPOINT IOP(3/76=05
72004280)\\C7H8O---Cl ortho pi 1K freq\\0,2\C,-2.9567907167,-0.067968
5007,-0.1005425435\O,-1.7977615175,0.326314924,0.5906087532\C,-0.64878
04923,-0.2858826614,0.3207439637\C,0.4939526183,0.2782555061,0.9433145
255\C,1.733763042,-0.3799973973,0.8247971645\C,1.8613622289,-1.4832232
665,0.0170059409\C,0.7394255972,-1.9751714803,-0.6529912079\C,-0.51017
02737,-1.391239622,-0.5065874754\H,-1.3588531934,-1.8088052061,-1.0221
807281\H,0.8389524088,-2.8373716185,-1.2957193465\H,2.8177870804,-1.96
74794918,-0.1018237038\H,2.5852397701,0.0262488824,1.3476755027\H,0.33
23693055,1.0153391186,1.7125374439\H,-3.2231764555,-1.0985991771,0.132
4371029\H,-2.8250341809,0.0482836685,-1.1752977387\H,-3.7450707041,0.5
923790669,0.2398833154\Cl,0.8637238874,2.0735794057,-0.5668720047\\Ver
sion=x86-Linux-G03RevB.04\State=2-A\HF=-806.8501749\S2=0.787477\S2-1=0
.\S2A=0.75098\RMSD=8.080e-09\RMSF=1.327e-05\Dipole=-0.7762814,-1.68672
31,0.2454831\..\PG=C01 [X(C7H8Cl1O1)]\..\@

para

1\1\GINC-NODE10\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\24-Dec-2
006\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8O---Cl an
isole p complex 1K\\0,2\C,-1.485324324,-0.5005667331,-0.6920751195\C,-
1.4824696691,-0.5133772841,0.7202057245\C,-0.3039286945,-0.5183148284,
1.4125305592\C,0.9171155074,-0.5396500701,0.7202401929\C,0.9373315287,
-0.575898404,-0.676763272\C,-0.2532078273,-0.5759234347,-1.3678654543\
Cl,-1.9455423408,1.8352302309,-1.1099356864\H,-2.4011263823,-0.6848772
504,-1.228058774\H,-2.4219575474,-0.4910449041,1.2497602449\H,-0.27928
57934,-0.5035757566,2.4907493198\O,2.0103931436,-0.530120422,1.4846857
004\H,1.8685161737,-0.6031709024,-1.2176678169\H,-0.2466586,-0.6023502
45,-2.4462935513\C,3.2767394192,-0.5261532831,0.8728795608\H,3.4321757
131,-1.4294259006,0.284097811\H,3.9970805643,-0.4968870336,1.681476535
8\H,3.4047948734,0.3526856681,0.2424441466\\Version=x86-Linux-G03RevB.
04\State=2-A\HF=-806.8511405\S2=0.780803\S2-1=0.\S2A=0.750651\RMSD=5.0
23e-09\RMSF=1.791e-05\Dipole=1.4570686,-1.43062,0.2790474\PG=C01 [X(C7
H8Cl1O1)]\\@

3e

ortho

1\1\GINC-NODE02\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1(2)\CHS60A\07-Apr-200
7\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8---Cl ortho
 pi 1K\\0,2\C,1.3257980047,-1.8397298602,0.8090857999\H,0.9270892663,-

1.7367888747,1.8178200705\H,2.4105522244,-1.8220790037,0.8629416702\H,
1.0170358705,-2.8147344882,0.4344393508\C,0.8051567831,-0.7424225856,-
0.0552280084\C,1.6291693823,0.2316862756,-0.5857004191\C,1.1160515724,
1.2428422553,-1.3935466178\C,-0.243382837,1.2946525038,-1.6991248446\C
,-1.0881895688,0.339859472,-1.184928129\C,-0.5881848721,-0.6593688015,
-0.3203688836\H,-1.2084818274,-1.5141726704,-0.0985646898\H,-2.1440805
092,0.3571282927,-1.405539809\H,-0.6264090842,2.0756952133,-2.33760647
22\H,1.7831528273,1.9920142536,-1.793826643\H,2.688475284,0.2030981916
,-0.3759241284\Cl,-1.3285791082,0.2385131488,1.7338310157\\Version=x86
-Linux-G03RevB.04\State=2-A\HF=-731.671486\S2=0.802063\S2-1=0.\S2A=0.7
51888\RMSD=6.558e-09\RMSF=2.054e-05\Dipole=0.8040573,-0.3217693,-1.220
4743\PG=C01 [X(C7H8Cl1)]\\@

meta

1\1\GINC-NODE08\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1(2)\CHS60A\30-Mar-200
8\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76=0
572004280)\\C7H8.Cl meta pi 1K\\0,2\C,0.4091121801,-0.5914979944,-2.8
077924532\C,0.3843453068,-0.6211526541,-1.3109626085\C,1.580150174,-0.
6918369553,-0.5842422957\C,1.5912427594,-0.7071738988,0.8054494536\C,0
.4043605392,-0.6472607411,1.5050534797\C,-0.8096332389,-0.5447194125,0
.8004596348\C,-0.8012271671,-0.5661285956,-0.6073554422\H,-1.742206641
2,-0.5117882724,-1.134312892\H,-1.7433007803,-0.6662342632,1.325999064
5\H,0.3939752193,-0.6545178511,2.5835314126\H,2.53037478,-0.7672390734
,1.3341041572\H,2.5176952295,-0.7367088416,-1.1211907237\H,1.056698846
3,-1.3690207936,-3.2085264994\H,0.7848201735,0.3658922729,-3.167301594
4\H,-0.5852420006,-0.7330426382,-3.2223589773\Cl,-1.1625245969,1.84066
35865,1.1650822024\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-731.669
0148\S2=0.79513\S2-1=0.\S2A=0.751415\RMSD=5.392e-09\RMSF=2.134e-05\Dip
ole=0.6492601,-1.2446144,-0.6320689\PG=C01 [X(C7H8Cl1)]\\@

para

1\1\GINC-DEEPTHOUGHT\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1(2)\CHS60A\28-De
c-2006\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C7H8---Cl
reopt as -1\\0,2\C,-1.3172371016,0.6303828683,-0.7774636549\C,-1.31771
87413,0.6240279514,0.6221180628\C,-0.138906352,0.6009592781,1.32952694
61\C,1.0949359488,0.5540023962,0.6499349039\C,1.0967553601,0.608411657
3,-0.7582052289\C,-0.0909848503,0.6312388573,-1.4512366928\C,-2.603340
0357,0.6076334344,-1.5370371187\H,-2.260110264,0.638346318,1.150473469
5\H,-0.1470720419,0.5931087704,2.4083679036\H,2.0112061146,0.719641457
9,1.1927971375\H,2.0385175547,0.6064720581,-1.2846087744\H,-0.08129360
4,0.6511407465,-2.5314553515\H,-2.9309738914,-0.4209401399,-1.69247047
91\H,-2.4965615471,1.0683189636,-2.5159222323\H,-3.3937598908,1.123260
4069,-0.9969070029\Cl,1.5834718942,-1.7952521906,0.9296412956\\Version
=x86-Linux-G03RevB.04\State=2-A\HF=-731.6704464\S2=0.793404\S2-1=0.\S2
A=0.75131\RMSD=8.170e-09\RMSF=2.215e-05\Dipole=-0.9464199,1.2809915,-0
.5522601\PG=C01 [X(C7H8Cl1)]\\@

3g

ortho

1\1\GINC-NODE05\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1F1(2)\CHS60A\05-Apr-2
007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5F---Cl or
tho pi 1K\\0,2\C,-0.7961164847,-0.566199853,-0.1237233658\C,-0.7893787
627,-0.5727261466,1.2837083798\C,0.4014420429,-0.5724803826,1.97433143
5\C,1.60861876,-0.5977837218,1.2765148066\C,1.6348852625,-0.6332273375
,-0.1115280678\C,0.4366681301,-0.6379223195,-0.7847025806\F,0.43277993
32,-0.7065999477,-2.1081797213\H,2.5600344397,-0.6634530092,-0.6641313
879\H,2.5414216844,-0.5929816942,1.8199920204\H,0.4029894849,-0.553466
9503,3.0527635429\H,-1.7322949075,-0.5499771169,1.8067404453\H,-1.7024
003131,-0.7301448217,-0.6831684143\Cl,-1.2318519692,1.8194977463,-0.43
8010727\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-791.5603228\S2=0.7
86513\S2-1=0.\S2A=0.750938\RMSD=9.790e-09\RMSF=1.207e-05\Dipole=0.6192
432,-1.1234582,0.9895107\PG=C01 [X(C6H5Cl1F1)]\\@

meta

1\1\GINC-NODE14\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1F1(2)\CHS60A\29-Mar-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76
=0572004280)\\C6H5F.Cl meta pi 1K\\0,2\C,-1.4370117443,0.6056607644,-
0.3713035357\C,-1.4441796632,0.5946919274,1.0124380359\C,-0.2493161527
,0.6071286647,1.7149193528\C,0.9473088739,0.6330051205,1.0098090621\C,
0.9953898311,0.6451334906,-0.3589883532\C,-0.2150578063,0.6080529786,-
1.0652201388\H,-0.2056250591,0.7382792561,-2.1354307507\H,1.9436446623
,0.6647888171,-0.870814667\F,2.0867986055,0.6546256739,1.7024130045\H,
-0.2249857435,0.5956454422,2.7933296771\H,-2.3792471497,0.5749232229,1
.5501434719\H,-2.3612225515,0.5938600826,-0.9263069639\Cl,-0.419797155
2,-1.8365391508,-1.6107390792\\Version=x86-Linux-G03RevB.04\State=2-A\
HF=-791.5594876\S2=0.781918\S2-1=0.\S2A=0.750713\RMSD=3.640e-09\RMSF=2

.261e-05\Dipole=-0.5087494,1.0620756,0.3557135\PG=C01 [X(C6H5Cl1F1)]\\
@

para

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1F1(2)\CHS60A\23-Dec-2
006\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5F---Cl fl
orobenzene para complex 1K\\0,2\C,-1.0620297785,-0.5721628705,-0.60684
19817\C,-1.0606067803,-0.5891779462,0.8009505829\C,0.1265782363,-0.599
060954,1.4973486212\C,1.3104753142,-0.6221869025,0.7764837821\C,1.3537
753046,-0.6429574702,-0.6089716064\C,0.1626704795,-0.6329343923,-1.298
6420277\H,0.1612459838,-0.6474988372,-2.377032156\H,2.3069428022,-0.66
7090035,-1.1120894186\F,2.4584436818,-0.631883778,1.445522233\H,0.1588
054385,-0.5902518099,2.5749023404\H,-1.9994108437,-0.5702121595,1.3314
471741\H,-1.9851192865,-0.7243736522,-1.1414857323\Cl,-1.5149196403,1.
8139566888,-0.920435678\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-79
1.5620946\S2=0.786092\S2-1=0.\S2A=0.750912\RMSD=8.023e-09\RMSF=2.762e-
05\Dipole=0.1278312,-1.2201568,0.0999065\PG=C01 [X(C6H5Cl1F1)]\\@

3h

ortho

1\1\GINC-NODE04\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl2(2)\CHS60A\05-Apr-200
7\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Cl---Cl ort
ho pi 1K\\0,2\C,-0.8333252818,-0.4757723034,0.1793148852\C,-0.83282189
09,-0.4805559921,1.5875807369\C,0.3544988062,-0.4802366291,2.284542346
4\C,1.5614036745,-0.5058252588,1.5901508376\C,1.5894355457,-0.54787846
28,0.2011689976\C,0.3992872232,-0.5572967296,-0.4953219952\Cl,0.403996
886,-0.6596196631,-2.2079903243\H,2.5257757629,-0.583305125,-0.3322439
348\H,2.4942546282,-0.4992383243,2.1337208616\H,0.3514341228,-0.459990
9223,3.3630597672\H,-1.7789992511,-0.4552978493,2.1047958541\H,-1.7465
611171,-0.6433039149,-0.3674765011\Cl,-1.3026305688,1.8905919213,-0.08
53314933\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1151.9567441\S2=0
.792393\S2-1=0.\S2A=0.75126\RMSD=8.623e-09\RMSF=2.668e-05\Dipole=0.622
261,-1.1007716,0.9329142\PG=C01 [X(C6H5Cl2)]\\@

meta

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl2(2)\CHS60A\29-Mar-200
8\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76=0
572004280)\\C6H5Cl.Cl 1K pi meta\\0,2\C,-1.7711667239,0.5465857547,-0
.5925019141\C,-1.7706474278,0.5394443268,0.7882092841\C,-0.5709160615,
0.5411708376,1.4869091003\C,0.635962682,0.5540738459,0.7912489318\C,0.
6612982746,0.5616022426,-0.5846997175\C,-0.5519303086,0.5317132023,-1.
2900318485\H,-0.5419487923,0.6719451709,-2.3591064794\H,1.5990914909,0
.5706648335,-1.1159777379\Cl,2.1177913649,0.5686582135,1.677032036\H,-
0.5622434766,0.5322837728,2.5656045151\H,-2.7021967057,0.5317975401,1.
3326092965\H,-2.6977588875,0.5422086448,-1.1440706901\Cl,-0.6407646729
,-1.8919782854,-1.8460827372\\Version=x86-Linux-G03RevB.04\State=2-A\H
F=-1151.9562208\S2=0.788409\S2-1=0.\S2A=0.751034\RMSD=9.349e-09\RMSF=2
.513e-05\Dipole=-0.554808,1.0630258,0.3447815\PG=C01 [X(C6H5Cl2)]\\@

para

1\1\GINC-NODE14\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl2(2)\CHS60A\24-Dec-200
6\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Cl---Cl chl
orobenzene para complex 1K\\0,2\C,-1.4026168006,-0.4944124777,-0.80936
84258\C,-1.4007785624,-0.5147468549,0.5983120133\C,-0.2139180342,-0.52
76875497,1.294304716\C,0.9855423481,-0.5518861902,0.5871579117\C,1.012
6889401,-0.5707796886,-0.8050537337\C,-0.1761500025,-0.5577698136,-1.4
976604412\H,-2.3243731037,-0.6533883688,-1.3446661692\H,-2.3391025338,
-0.494961254,1.1298637525\H,-0.2009464442,-0.521857219,2.3723733101\Cl
,2.4702375807,-0.5684410862,1.4549711754\H,1.9580378495,-0.597704676,-
1.3227646862\H,-0.1737448497,-0.5710337707,-2.5761820493\Cl,-1.8672068
894,1.8709493649,-1.1293697871\\Version=x86-Linux-G03RevB.04\State=2-A
\HF=-1151.958174\S2=0.793152\S2-1=0.\S2A=0.751297\RMSD=3.850e-09\RMSF=
1.145e-05\Dipole=0.1464754,-1.1943838,0.1100984\PG=C01 [X(C6H5Cl2)]\\@

3i

ortho

1\1\GINC-NODE03\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Br1Cl1(2)\CHS60A\05-Apr-
2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Br---Cl\
\0,2\C,-0.9123088693,-0.3548325376,0.6608655597\C,-0.914569778,-0.3535
415131,2.0678080192\C,0.272123498,-0.3548771993,2.7665295288\C,1.47798
6888,-0.3835943746,2.0719806811\C,1.5066706915,-0.4226581637,0.6830417
941\C,0.3182048432,-0.4251773244,-0.0151602896\Br,0.3202619387,-0.5371
774478,-1.8703421682\H,2.4454094037,-0.4585562234,0.1540533879\H,2.411
0714234,-0.3804928533,2.615378404\H,0.2685504926,-0.333437603,3.845029

5449\H,-1.8615777805,-0.3278037686,2.583626956\H,-1.8289573092,-0.5089
968623,0.1157532034\Cl,-1.3607239839,2.0340343918,0.3963378019\\Versio
n=x86-Linux-G03RevB.04\State=2-A\HF=-3263.6090371\S2=0.789209\S2-1=0.\
S2A=0.751081\RMSD=9.826e-09\RMSF=1.632e-05\Dipole=0.5985043,-1.0765231
,0.8866122\PG=C01 [X(C6H5Br1Cl1)]\\@

meta

1\1\GINC-NODE09\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Br1Cl1(2)\CHS60A\30-Mar-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/7
6=0572004280)\\C6H5Br.Cl 1K pi meta\\0,2\C,-2.2293368794,0.4341155613
,-0.9495672963\C,-2.2277778724,0.4268658259,0.4305514936\C,-1.02895431
08,0.4211282049,1.1308587303\C,0.1789262986,0.4309938244,0.4388271184\
C,0.2049427968,0.439784356,-0.9367149832\C,-1.0080624831,0.418674131,-
1.642355008\H,-0.9948414942,0.5609025978,-2.7112958389\H,1.1408382496,
0.4511771775,-1.4709597254\Br,1.7810801007,0.4691033828,1.3988257428\H
,-1.0263620195,0.4136688835,2.2094541014\H,-3.1592018228,0.4227883346,
0.9754729784\H,-3.1549949154,0.4349702801,-1.5025516446\Cl,-1.08715687
18,-2.0077351231,-2.1934483057\\Version=x86-Linux-G03RevB.04\State=2-A
\HF=-3263.6080691\S2=0.787945\S2-1=0.\S2A=0.751011\RMSD=8.401e-09\RMSF
=3.188e-05\Dipole=-0.5327162,1.0585373,0.3486403\PG=C01 [X(C6H5Br1Cl1)
]\\@

para

1\1\GINC-NODE02\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Br1Cl1(2)\CHS60A\24-Dec-
2006\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5Br ---Cl
 chlorobenzene para complex 1K\\0,2\C,-1.9312204925,-0.3764786202,-1.1
214952194\C,-1.9296928059,-0.3959054571,0.2854422141\C,-0.7432750422,-
0.4108021777,0.9820628458\C,0.4568824692,-0.4366176635,0.2776310325\C,
0.4833877107,-0.4598849897,-1.1137800393\C,-0.7046691596,-0.4449226779
,-1.8076001291\H,-2.8538653865,-0.526330065,-1.6579948872\H,-2.8680280
443,-0.3736096588,0.8170458523\H,-0.7355216594,-0.4055064352,2.0601038
504\Br,2.0624754221,-0.474343907,1.2182419755\H,1.4268479059,-0.492029
9989,-1.6344624115\H,-0.700594535,-0.4603358737,-2.8861725078\Cl,-2.36
72914195,2.0004422525,-1.4323854862\\Version=x86-Linux-G03RevB.04\Stat
e=2-A\HF=-3263.6097362\S2=0.79229\S2-1=0.\S2A=0.751248\RMSD=8.531e-09\
RMSF=9.318e-06\Dipole=0.1647106,-1.1862512,0.1241833\PG=C01 [X(C6H5Br1
Cl1)]\\@

3j

ortho

1\1\GINC-NODE12\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1N1O2(2)\CHS60A\06-Apr
-2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5O2N---C
l ortho pi 1K\\0,2\C,-0.4934801168,-0.532010435,0.1318649403\C,-0.5355
786403,-0.5354251137,1.5050149182\C,0.6673167864,-0.5211229898,2.20752
21863\C,1.8764760914,-0.4992701641,1.533503178\C,1.9014454989,-0.48564
60207,0.14599501\C,0.7058972169,-0.4863568043,-0.5794741929\H,0.690777
2302,-0.5681967926,-1.6533567049\H,2.8386971235,-0.464805418,-0.386851
1175\H,2.8028244927,-0.4902751221,2.0865520327\H,0.6496655067,-0.52739
91052,3.286532066\H,-1.4877546437,-0.5544524408,2.0087508559\N,-1.7438
002647,-0.57469542,-0.6151736902\O,-2.7723231922,-0.5164458382,0.01689
60655\O,-1.6690352322,-0.673048759,-1.8166107685\Cl,1.0300469718,2.029
5848683,-0.9590735244\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-896.
7711833\S2=0.769562\S2-1=0.\S2A=0.750275\RMSD=3.836e-09\RMSF=1.589e-04
\Dipole=1.496034,-0.7957091,1.4315438\PG=C01 [X(C6H5Cl1N1O2)]\\@

meta

1\1\GINC-NODE02\Freq\UmPWPW91\6-31+G(d,p)\C6H5Cl1N1O2(2)\CHS60A\26-Dec
-2006\0\\#P MPWPW91/6-31+G(D,P) FREQ=NORAMAN GEOM=CHECKPOINT IOP(3/76=
0572004280)\\C6H5O2N---Cl nitrobenz non-opt freq meta complex\\0,2\C,
0.0719589905,-0.4536106266,0.903790272\C,-0.8778184326,0.1995469635,0.
1499826849\C,-0.6502047297,1.4443157118,-0.4169059421\C,0.5773355959,2
.06007122,-0.2151743708\C,1.5522409069,1.4320724287,0.5353906464\C,1.3
164884219,0.1626222069,1.083645393\H,2.0340902921,-0.2772016603,1.7574
310945\H,2.5088775829,1.9051654906,0.6930042255\H,0.7652717896,3.02981
28113,-0.6483591071\H,-1.4281925436,1.9084045692,-1.0006964036\N,-2.17
28715429,-0.4378638208,-0.0544332869\O,-2.9834308472,0.1539502668,-0.7
278584859\O,-2.3526691586,-1.5133682108,0.4650141722\H,-0.1438579577,-
1.4199161851,1.3278561859\Cl,2.4836886567,-1.1927048326,-0.6994012104\
\Version=x86-Linux-G03RevB.04\State=2-A\HF=-896.7725694\S2=0.780949\S2
-1=0.\S2A=0.750684\RMSD=6.019e-09\RMSF=6.508e-06\Dipole=0.9443069,1.47
72916,0.7255668\..\PG=C01 [X(C6H5Cl1N1O2)]\..\@

para

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31+G(d,p)\C6H5Cl1N1O2(2)\CHS60A\06-Apr
-2007\0\\#P MPWPW91/6-31+G(D,P) OPT IOP(3/76=0572004280)\\C6H5O2N---C

l para pi 1K\\0,2\C,-1.1783979636,-0.5275524334,-1.2027072313\C,-1.222
3260933,-0.5252662235,0.1755214588\C,-0.0236305329,-0.5200243477,0.871
8408085\C,1.2137359103,-0.5164469237,0.2467619833\C,1.2504483303,-0.51
87915137,-1.1316599142\C,0.0564733728,-0.5064074302,-1.8685860162\H,0.
0882624641,-0.6201461414,-2.940769294\H,2.1967894431,-0.5146168507,-1.
6486168789\H,2.1116061543,-0.5145881429,0.8416915231\N,-0.0662961709,-
0.5244012485,2.3315069871\O,-1.1545553331,-0.5313948696,2.8563003662\O
,0.9894544206,-0.5234466007,2.919004521\H,-2.1534305152,-0.5300269384,
0.7169431546\H,-2.0929222222,-0.53002111,-1.7740766117\Cl,0.0621621783
,1.9709337011,-2.3685403784\\Version=x86-Linux-G03RevB.04\State=2-A\HF
=-896.7717304\S2=0.78499\S2-1=0.\S2A=0.75087\RMSD=3.665e-09\RMSF=5.514
e-06\Dipole=0.0412604,-0.8752375,-1.3031981\PG=C01 [X(C6H5Cl1N1O2)]\\@

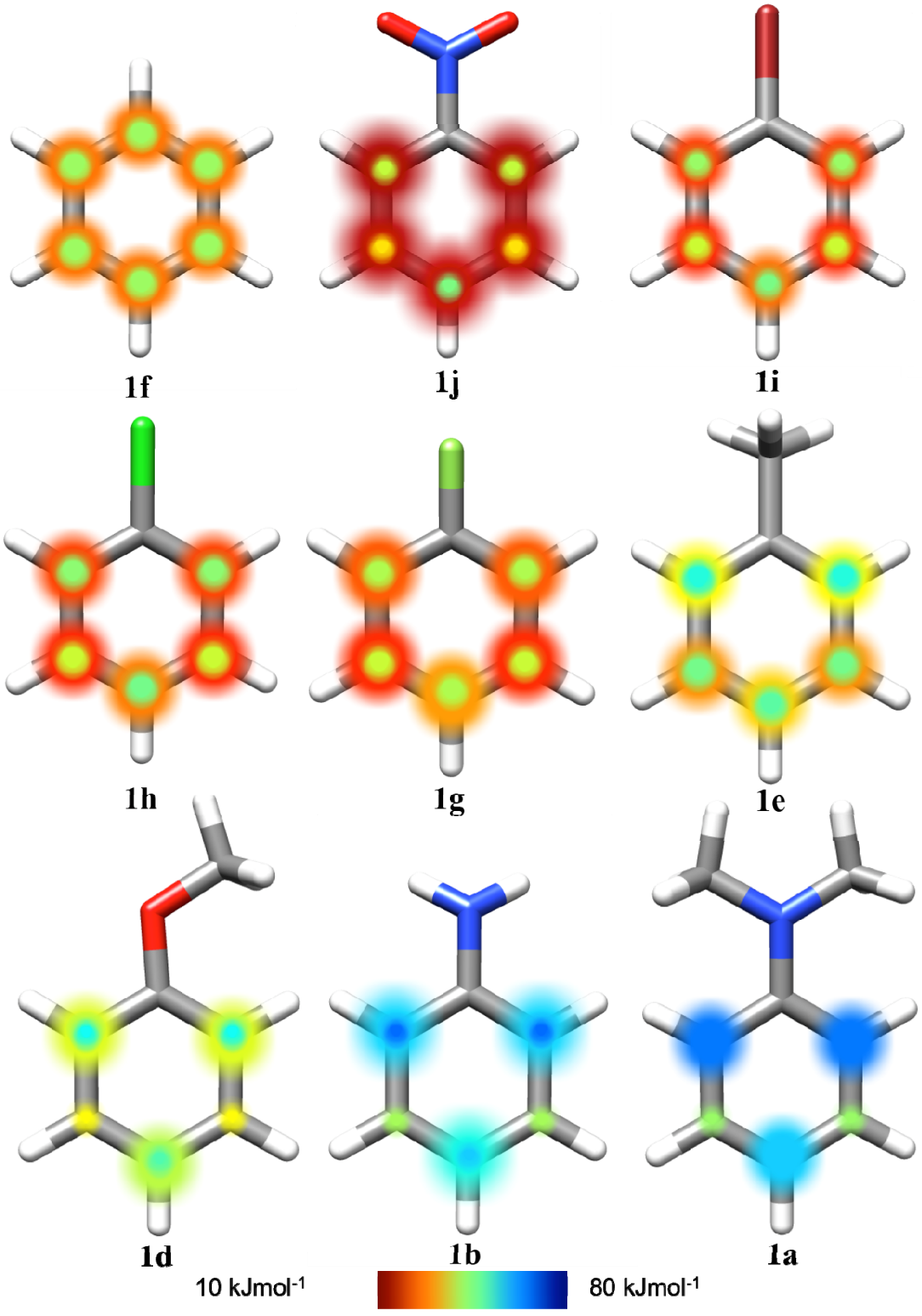
Table S1. ωB97X-D/6-311+G(3df,2p) stabilisation energies for complexes **2a-2j** and **3a-3j**

Table S1. Stabilisation energies calculated at ωB97X-D/6-311+G(3df,2p)//ωB97X-D/6-31+G(d,p) for the η_1-π and η_1-σ complexes of substituted benzenes **1a-1j** with chlorine.

	Stabilisation energy ωB97X-D/6-311+G(3df,2p) (kJ.mol^{-1})					
	□□□□□		*meta*		*para*	
Arene	σ-complex **2**	π-complex **2**	σ-complex **3**	π-complex **2**	σ-complex **3**	π-complex **3**
1a	-	79.2	44.8	-	-	67.8
1b	-	69.1	43.6	-	-	63.5
1c	-	56.1	40.8	-	-	50.8
1d	55.8	51.9	38.7	-	-	52.9
1e	52.5	47.8	46.0	40.4	48.6	44.0
1f[a]	43.7	38.1	43.7	38.1	43.7	38.1
1g	42.2	36.6	40.6	-	43.2	40.5
1h	44.7	35.7	40.6	-	46.5	38.0
1i	45.0	35.6	41.1	33.3	46.5	37.5
1j	41.6	-	35.5	28.7	44.6	26.2

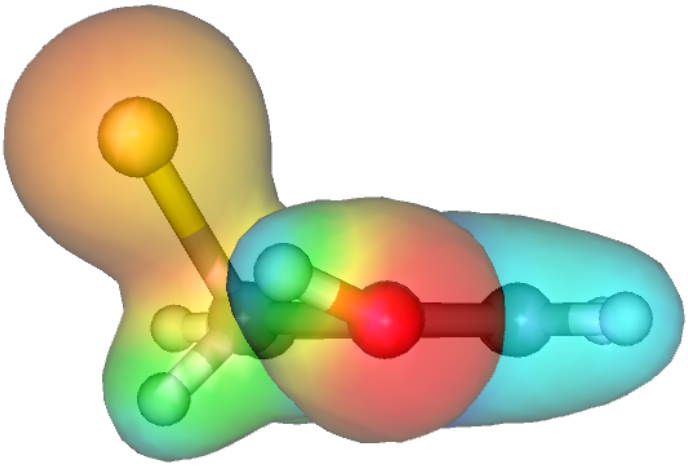
[a]For reference. A hyphen indicates this structure was not identified in this study.

Figure S1. Graphical representation of complex energies for 1a, 1b and 1d-1j

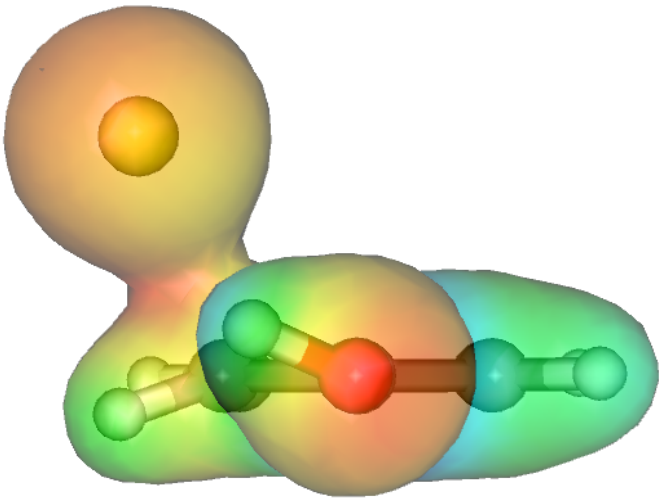


Energy visualisation for σ- (small dots, localised on C-centres) and π-complexes (large, diffuse dots). The colour corresponds to the energy. From this, three observations can be quickly made; 1.) Stability of all complexes increases with increasingly electron rich substituents (a change to cooler colours), 2.) π-complexes were not identified at the meta positions for compounds **1a**, **1b** and **1d**, nor were σ-complexes identified for the *ortho* and *para* positions of **1a** and 3.) The energies of the σ- and π-complexes become more similar (closer in colour) with increasingly electron rich substituents.

Figure S2. Electrostatic Surface Potential maps for complexes 2c (σ) and 3c (π)



2c



3c

ESP maps for the σ and π complexes, **2c** and **3c**, with regions of high electron density marked in red and low electron density in blue. These maps illustrate further evidence for the proposed electrostatic interaction between the electron poor phenolic hydrogen atom (light blue) and the comparatively electron rich chlorine atom (yellow-orange). Molecules and ESP maps have been visualised with Molekel (Varetto, U., Version 5.4.0.8, Swiss National Supercomputing Centre: Manno (Switzerland), http://molekel.cscs.ch/).

MPW1K/6-31+G(d,p) correlations of 2a-2j and 3a-3j data with Swain-Lupton, experimental HOMO and calculated 1a-1j HOMO values

Table 3. Stabilisation energies calculated for the η_1-π and η_1-σ complexes of substituted benzenes **1a-1j** with chlorine, taken as the difference between the calculated energy of the complex and the calculated energies of the components at infinite separation. Calculations were carried out at MPW1K/6-31+G(d,p).

	Stabilisation energy (kJ.mol^{-1})					
	□□□□□		*meta*		*para*	
Arene	σ-complex **2**	π-complex† **3**	σ-complex **2**	π-complex† **3**	σ-complex **2**	π-complex† **3**
1a	n/i	60.6	59.0	n/i	n/i	55.0
1b	58.0	54.3	33.9	n/i	n/i	50.7
1c	46.6	42.0	30.9	n/i	40.2	37.7
1d	44.5	37.1	28.6	n/i	41.1	39.5
1e	42.6	34.9	36.6	27.7	39.8	32.3
1f^{a}	35.6	26.5	35.6	26.5	35.6	26.5
1g	32.0	22.8	31.5	20.5	33.4	27.5
1h	34.2	22.0	31.3	20.2	36.6	25.7
1i	36.9	21.5	32.9	20.2	38.1	25.4
1j	30.5	11.8	25.6	15.4	35.6	13.7

†Counterpoise correction included. ^{a}For reference.

Table S1. Alternative methods for representing the complex as: (a). A weighted average of ortho and para; (b). A weighted average of all calculated complexes and (c). The most stable species.

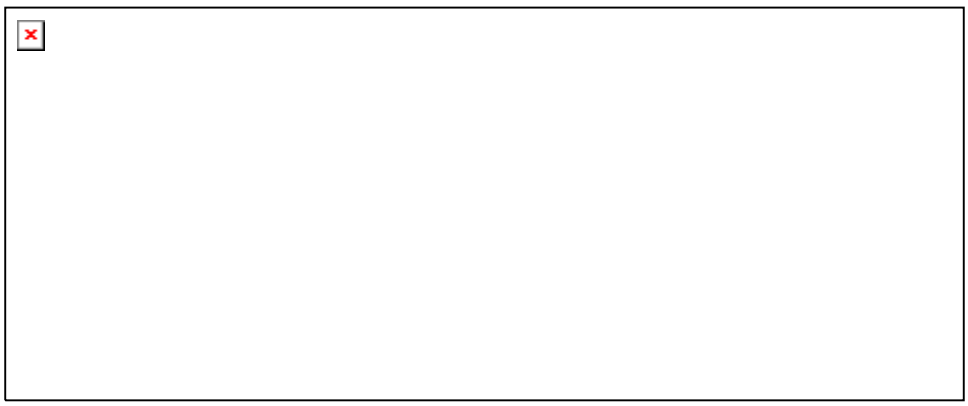
	Stabilisation energy (kJ.mol^{-1})					
	Weighted average (o/m/p)		*Average (non-weighted)*		*Most stable*	
Arene	σ-complex **2**	π-complex† **3**	σ-complex **2**	π-complex† **3**	σ-complex **2**	π-complex† **3**
1a	59.0	58.7	59.0	57.8	59	60.6
1b	46.0	53.1	46.0	52.5	58	54.3
1c	39.0	40.6	39.2	39.9	46.6	42
1d	37.5	37.9	38.1	38.3	44.5	39.5
1e	39.6	31.5	39.7	33.6	42.6	34.9
1f^{a}	35.6	26.5	35.6	26.5	35.6	26.5
1g	32.1	22.8	32.3	25.2	33.4	27.5
1h	33.5	22.0	34.0	23.9	36.6	25.7
1i	35.5	21.8	36.0	23.5	38.1	25.4
1j	29.6	13.6	30.6	12.8	35.6	15.4

Table S2. Correlation values: (a) Swain-Lupton R constants; (b) calculated HOMO (MPW1K); (c) calculated HOMO (ωB97X-D) and (d) Experimental Ionisation Energy (IE).

	Correlation parameters			
Arene	Swain-Lupton R parameters	HOMO (MPW1K/6-31+G(d,p)) (eV)	HOMO (ωB97X-D/6-31+G(d,p)) (eV)	IE (eV)
1a	-3.61	-6.24	-7.21	7.12 ± 0.02
1b	-2.52	-6.66	-7.64	7.720 ± 0.002
1c	-1.89	-7.29	-8.28	8.49 ± 0.02
1d	-1.68	-7.15	-8.12	8.20 ± 0.05
1e	-0.41	-7.63	-8.66	8.828 ± 0.001
1f^{a}	0	-7.99	-8.94	9.24378 ± 0.00007
1g	-0.6	-7.99	-8.98	9.20 ± 0.01
1h	-0.24	-7.92	-8.93	9.07 ± 0.02
1i	-0.18	-7.82	-8.81	9.00 ± 0.03
1j	1	-8.89	-9.91	9.94 ± 0.08

R^2	σ	π	σ	π	σ	π	σ	π
Weighted average	0.795	0.938	0.818	0.937	0.815	0.936	0.855	0.941
Non-weighted average	0.793	0.944	0.812	0.961	0.808	0.959	0.854	0.956
Most stable	0.826	0.956	0.830	0.956	0.820	0.952	0.866	0.959

MPW1K/6-31+G(d,p) PAH structures 4-11



4

1\1\GINC-ABE0578\FOpt\RmPWPW91\6-31+G(d,p)\C10H8\ACROFT\29-Dec-2010\0\
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086479\C,2.4406539001,0.0002307224,1.3569271634\C,2.4090810825,0.00019
26248,-0.0089237822\C,1.1758949109,0.0001920363,-0.6907762848\H,1.1627
441812,0.0001694392,-1.7705962222\H,3.330600703,0.0001734649,-0.571938
578\H,3.385458207,0.0002221718,1.881946975\C,1.2437275956,0.0003488368
,3.5217680945\C,0.070309638,0.0004198388,4.2211928172\C,-1.1630472502,
0.000414996,3.5392441232\C,-1.1946419735,0.0003276006,2.1735581434\H,-
2.1393363413,0.0003172293,1.6483339541\H,-2.0844354264,0.0004877273,4.
1024749447\H,0.0832316343,0.0004927904,5.3010139517\H,2.1908731195,0.0
003444485,4.0425592744\H,-0.9446966399,0.0002094798,-0.5122145499\\Ver
sion=EM64L-G09RevA.02\State=1-A\HF=-385.8096775\RMSD=7.583e-09\RMSF=6.
430e-05\Dipole=0.0000072,0.000018,0.0000007\Quadrupole=3.395813,-6.845
3026,3.4494896,-0.0002245,-0.042808,0.0004647\PG=C01 [X(C10H8)]\\@

5

1\1\GINC-ABE0533\FOpt\RmPWPW91\6-31+G(d,p)\C14H10\ACROFT\29-Dec-2010\0
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2.1236955278\C,2.4531384877,-0.0000755157,1.3554653642\C,2.4113793587,
0.00002596,-0.0025577958\C,1.1656063655,0.0000639423,-0.6837543622\H,1
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1.165242424,-0.0003773797,3.5681092219\C,-1.1782516363,-0.0002252107,2
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,-1.0762176195,-0.0007597637,6.3755608412\C,0.0896206774,-0.0005930239
,5.6778748839\H,1.038878828,-0.0005972555,6.1946272503\H,-1.0622753719
,-0.0008720505,7.4553705416\H,-3.2386068928,-0.0007437516,6.2653400074
\H,-3.3110720155,-0.0004510724,3.8160237012\H,2.216689129,-0.000320698
3,4.0335654618\H,-0.9494879816,0.0000444387,-0.502832198\\Version=EM64
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ipole=-0.0000012,0.0000113,0.0000023\Quadrupole=4.6151949,-9.3465906,4
.7313958,0.0002977,-0.0906206,-0.0013242\PG=C01 [X(C14H10)]\\@

6

1\1\GINC-ABE0532\FOpt\RmPWPW91\6-31+G(d,p)\C12H8\ACROFT\29-Dec-2010\0\
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0106772649,-0.0000500674,1.423779353\C,1.2131048287,-0.0000209072,2.08
02289201\C,2.3881704934,0.0000437276,1.3071393528\C,2.4267311364,0.000
0526648,-0.0778252087\C,1.1697791953,0.0000229379,-0.7334471016\H,1.12
07751607,0.0000378132,-1.8130109823\C,3.7182119337,0.000069581,-0.6624
925085\C,4.8336104357,0.0000673726,0.1403014526\C,4.7554903068,0.00005
01641,1.5558837355\C,3.5183979351,0.0000433217,2.1444135252\C,3.003247
2087,0.0000028509,3.5160606927\C,1.6511373487,-0.0001006872,3.47841558
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2,4.4061822778\H,5.666222803,0.000045027,2.1375577628\H,5.8105302353,0
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rupole=4.7446682,-8.0500446,3.3053764,0.000423,0.0400974,-0.000261\PG=
C01 [X(C12H8)]\\@

7

1\1\GINC-ABE0588\FOpt\RmPWPW91\6-31+G(d,p)\C14H10\ACROFT\30-Dec-2010\0
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2.0794139321\C,2.4315582805,-0.0001330997,1.3289520942\C,2.4019744718,
-0.0004176572,-0.0418128197\C,1.1698227333,-0.0004690965,-0.7043281614
\H,1.1384760472,-0.0006742097,-1.7837932573\H,3.3218121886,-0.00059420
5,-0.6073187784\H,3.3763213133,-0.0000775932,1.8541651748\C,1.28744321
22,0.0004231657,3.5074732041\C,0.1542484883,0.0006712713,4.2391542891\
C,-1.1290772013,0.0005847809,3.6111539211\C,-1.2206817138,0.0002407052
,2.2019674431\C,-2.5019986487,0.000116758,1.6240741451\C,-3.6359657075
,0.000347882,2.398667412\C,-3.5392191061,0.0007126495,3.7942946601\C,-
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4625625554\H,-4.4331633423,0.0009005248,4.3999036288\H,-4.6068889427,0
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8

1\1\GINC-ABE0577\FOpt\RmPWPW91\6-31+G(d,p)\C16H10\ACROFT\29-Dec-2010\0
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27111364\C,2.3935851804,0.0001298893,1.3173326741\C,2.4265702427,0.000
0085557,-0.0733423225\C,1.1705478218,-0.0000652335,-0.7271785995\H,1.1
235791019,-0.0001586948,-1.8067561245\C,3.7121789364,-0.0000201022,-0.
6668953748\C,4.8348267906,0.0000701099,0.1248876492\C,4.7688435228,0.0
001942947,1.5391107887\C,3.5379732384,0.0002275629,2.1378887989\C,3.04
82528098,0.0003611206,3.5220086612\C,1.6351333331,0.0003369587,3.48849
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1799,5.8759475095\C,2.9792346083,0.0006698729,5.9088785598\C,3.7182105
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\H,3.490320058,0.0008041351,6.8601673467\H,1.035285118,0.0007620785,6.
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8102770326,-0.0001109381,-1.7430321682\H,-0.9309253122,0.0001427558,1.
9561985245\H,-0.9376399439,-0.0000720077,-0.5048945895\\Version=EM64L-
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ole=0.002942,0.0000106,-0.1240342\Quadrupole=5.7257855,-10.5714361,4.8
456506,0.0002462,0.0208832,0.0016166\PG=C01 [X(C16H10)]\\@

9

1\1\GINC-ABE0534\FOpt\RmPWPW91\6-31+G(d,p)\C18H12\ACROFT\29-Dec-2010\0
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03440854\C,2.441568365,-0.0002616374,1.3628324651\C,2.4045208059,0.000
0078435,0.0014893188\C,1.164226201,0.0003693335,-0.6806475288\H,1.1512
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05053\H,3.3870761742,-0.0005396395,1.8864677016\C,1.2351027536,-0.0004
801086,3.5167102818\C,0.0565013946,-0.0003940058,4.2405559326\C,-1.199
7713177,0.0000331708,3.5587327664\C,-1.1925787451,0.0002847874,2.17617
32393\H,-2.1206186605,0.0005380285,1.625443676\C,-2.4267080996,0.00016
32858,4.3450835341\C,-2.3415389428,-0.0002753298,5.7524024822\C,-3.514
463976,-0.0001987246,6.520430866\C,-4.7523761757,0.0003238232,5.924094
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,-3.4294161864,-0.0005523542,7.598025425\C,-1.0563130775,-0.000754357,
6.3920586593\C,0.0812499347,-0.0007785515,5.6750321481\H,1.0425660824,
-0.0011052512,6.1686864093\H,-1.0238091844,-0.0010775926,7.4722766164\
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,-0.5030378888\\Version=EM64L-G09RevA.02\State=1-A\HF=-693.027389\RMSD
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upole=6.0215564,-11.9274148,5.9058584,-0.004208,-0.2158747,-0.0042964\
PG=C01 [X(C18H12)]\\@

10

1\1\GINC-ABE0586\FOpt\RmPWPW91\6-31+G(d,p)\C16H10\ACROFT\29-Dec-2010\0

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6082042\C,2.4179249349,-0.0001019562,1.4114950228\C,2.4107317636,-0.00
00931825,0.0265995172\C,1.2140898662,-0.0000375452,-0.6705009393\H,1.2
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.000073479,3.5602061034\C,0.0229066861,-0.0000408267,4.2359766071\C,-1
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0134127,2.1448717962\C,-3.6477631054,0.000108593,3.5297402159\C,-2.451
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845318,1.607987277\C,-2.4286364321,0.0001126741,-0.0038342362\C,-1.259
9150654,0.0000692056,-0.679607745\H,-1.2533717627,0.0000810884,-1.7602
89572\H,-3.3685036018,0.0001624492,-0.5372794043\H,0.0163635822,-0.000
0549855,5.3166588376\H,2.1314840779,-0.0001066202,4.093657532\\Version
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-04\Dipole=-0.0000037,0.0000004,-0.0000039\Quadrupole=5.1905895,-10.34
93412,5.1587517,-0.0006225,-0.0276174,-0.0001848\PG=C01 [X(C16H10)]\\@

11

1\1\GINC-ABE0535\FOpt\RmPWPW91\6-31+G(d,p)\C18H12\ACROFT\29-Dec-2010\0
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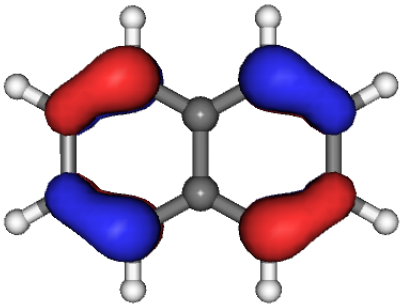
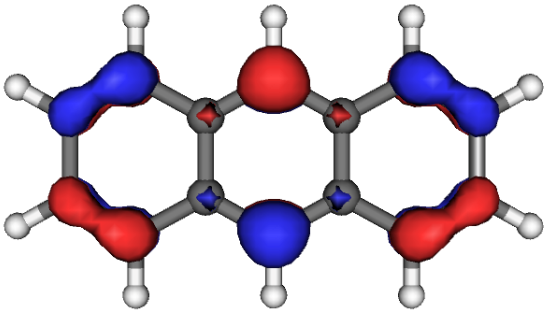
28915007\C,2.4363147165,-0.0000155583,1.3775409804\C,2.4457854869,-0.0
00054985,-0.0352749298\C,1.2020200101,-0.000046293,-0.6985085541\H,1.1
607606968,-0.0000755306,-1.7753253034\C,3.709242046,-0.0001040669,-0.7
330224919\C,3.766932388,-0.0001361366,-2.1555696846\C,4.9469690465,-0.
0001789876,-2.8180169915\C,6.1824787133,-0.0002040333,-2.1183613673\C,
6.1729874539,-0.0001799683,-0.7055458773\C,4.9095298199,-0.0001175421,
-0.0078133327\C,4.8518596773,-0.0000649061,1.4147235769\C,3.6718266426
,-0.0000168816,2.077183068\H,3.6555697641,0.0000241796,3.1577686\H,5.7
644628711,-0.0000541188,1.9871081565\C,7.4167246059,-0.0002235134,-0.0
422843343\C,8.5977695684,-0.0002770371,-0.7387872848\C,8.597986796,-0.
0002906233,-2.1403394988\C,7.406412222,-0.0002568651,-2.8136827057\H,7
.3879605627,-0.0002719791,-3.8944251093\H,9.5320761061,-0.0003299834,-
2.6819279242\H,9.5344796371,-0.0003112336,-0.2013604735\H,7.4579540237
,-0.0002222719,1.0345370114\H,4.9632474836,-0.0001979472,-3.8986026419
\H,2.8543416035,-0.0001233887,-2.7279674378\H,1.2308747812,0.000057527
6,3.1536332546\H,-0.9132796891,0.000070803,1.941170268\H,-0.9157319276
,0.0000043758,-0.539376537\\Version=EM64L-G09RevA.02\State=1-A\HF=-693
.0316591\RMSD=4.131e-09\RMSF=2.681e-05\Dipole=0.0000018,-0.0000009,0.0
000051\Quadrupole=6.2123741,-12.0226277,5.8102536,-0.000543,-0.2279832
,0.0004294\PG=C01 [X(C18H12)]\\@

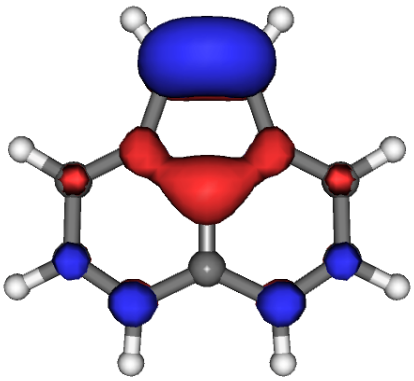
HOMO distributions for PAH structures 4-11



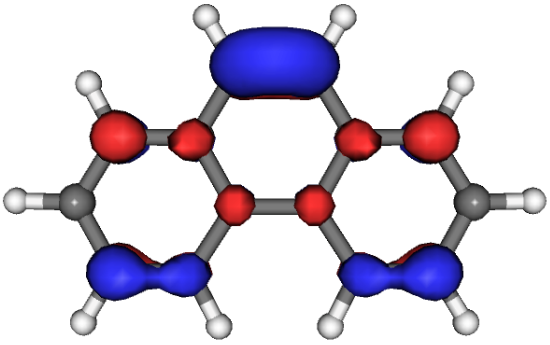
4



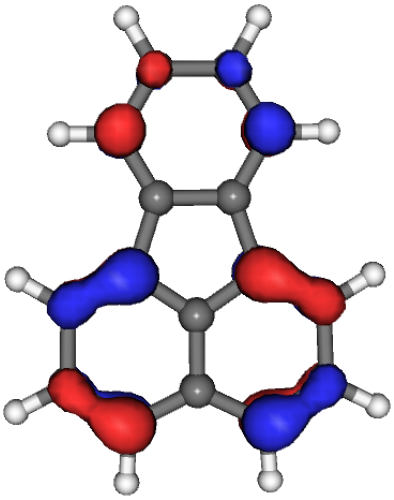
5



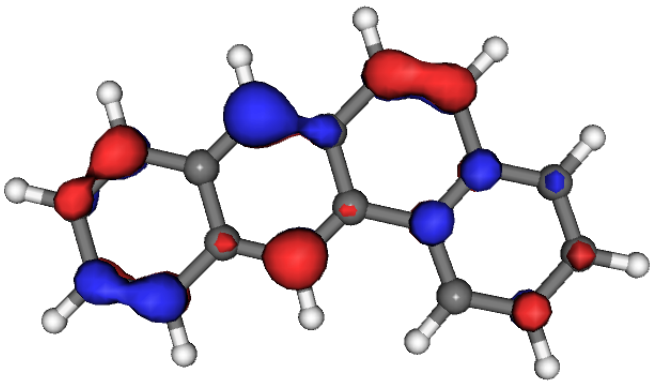
6



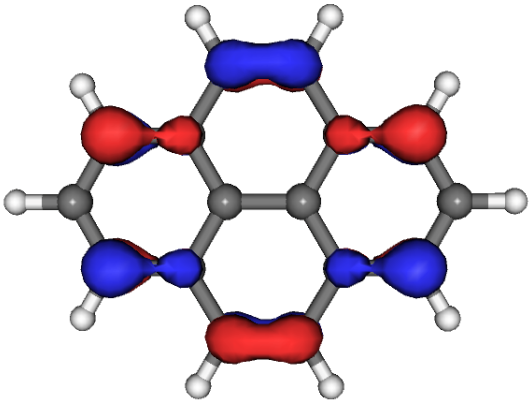
7



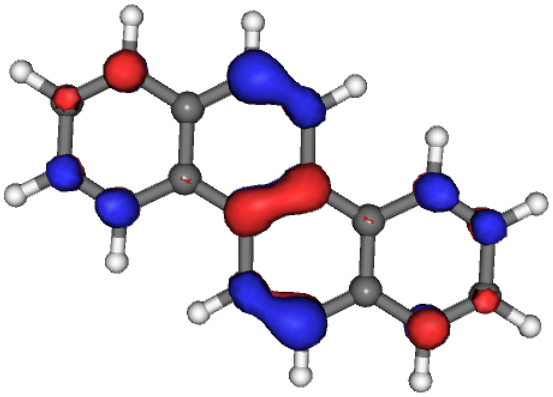
8



9



10



11

Identified MPW1K/6-31+G(d,p) σ-complex structures for 4, 5 and 10

1-Napthalene

1\1\GINC-ABE0444\FOpt\UmPWPW91\6-31+G(d,p)\C10H8Cl1(2)\ACROFT\18-Dec-2
010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=05720
04280)\\C10H8Cl napthalene 1-si mpw1k\\0,2\C,0.0586129403,0.1283154906
,-0.0424051451\C,0.0094261142,0.0468121322,1.4458068471\C,1.1848602821
,-0.0239823141,2.1803451323\C,1.1568550207,-0.0639684551,3.5638800214\
C,-0.0637221382,-0.0285110226,4.2339834497\C,-1.2397763475,0.031573744
2,3.5183464457\C,-1.2291022652,0.0624531966,2.1150290394\C,-2.44253240
12,0.057479524,1.3631932112\C,-2.418503474,-0.0348182769,-0.0277804835
\C,-1.2378543979,-0.0528363124,-0.7202052364\H,-1.2271261874,-0.128454
0808,-1.7964072521\H,-3.3500501706,-0.1070555936,-0.5696799799\H,-3.38
37953526,0.0797068414,1.891472697\H,-2.1895858346,0.0472162174,4.03376
39124\H,-0.0890924024,-0.0530198883,5.3131947285\H,2.0802997428,-0.117
0367082,4.1204697388\H,2.1326901818,-0.0278574824,1.6607394868\H,0.819
6024969,-0.5336793884,-0.4450166671\Cl,0.7216921809,1.7916510835,-0.54
97437983\\Version=EM64L-G09RevA.02\State=2-A\HF=-845.9788349\S2=0.8416
24\S2-1=0.\S2A=0.75623\RMSD=3.887e-09\RMSF=5.161e-06\Dipole=-0.4062545
,-0.7707207,0.4611314\Quadrupole=3.8990949,-6.8089128,2.9098178,-1.512
6729,1.7356585,2.6460769\PG=C01 [X(C10H8Cl1)]\\@

2-Naphthalene

1\1\GINC-ABE0439\FOpt\UmPWPW91\6-31+G(d,p)\C10H8Cl1(2)\ACROFT\18-Dec-2
010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=05720
04280)\\C10H8Cl napthalene 2-si mpw1k\\0,2\C,-0.0683549607,0.082989840
2,-0.0242991346\C,0.0041280502,0.0083103731,1.4500276156\C,1.174472384
8,-0.010131714,2.0993144212\C,2.4407885549,0.0081723471,1.4087082929\C
,2.4402257548,-0.0034796056,-0.0161500831\C,3.6823181808,-0.0157086998
,-0.6927722864\C,4.8654448253,-0.0059955844,0.006880397\C,4.8558595763
,0.0128567042,1.4057185314\C,3.6518787801,0.0173364406,2.0915365989\H,
3.6467471212,0.026638883,3.1724006811\H,5.7872113971,0.0211199998,1.95
14324876\H,5.8056625805,-0.0122578991,-0.5239066565\H,3.6867487057,-0.
0277057683,-1.7732258453\C,1.2263651889,-0.0228217864,-0.7063523083\H,
1.2229658579,-0.0517289996,-1.7857708507\H,1.1883072954,-0.0481601188,
3.1796647732\H,-0.9303422162,-0.0015168052,1.9900633708\H,-0.801300628
1,-0.6080114752,-0.4318784391\Cl,-0.854219401,1.71949943,-0.4867855469
\\Version=EM64L-G09RevA.02\State=2-A\HF=-845.9720453\S2=0.858413\S2-1=
0.\S2A=0.759274\RMSD=8.556e-09\RMSF=1.753e-05\Dipole=0.7177973,-0.7785
219,0.2989572\Quadrupole=1.5785302,-6.0686454,4.4901152,3.692764,-1.56
28649,1.3735562\PG=C01 [X(C10H8Cl1)]\\@

1-Anthracene

1\1\GINC-ABE0453\FOpt\UmPWPW91\6-31+G(d,p)\C14H10Cl1(2)\ACROFT\18-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H8Cl anthracene 1-si mpw1k\\0,2\C,-0.0575607513,-0.1605391
782,-0.0450817984\C,-0.0133922772,-0.0763021669,1.4457226454\C,1.24606
60837,-0.0847250954,2.1209307253\C,1.2642759169,-0.075294276,3.5062161
209\C,0.0803557423,-0.0353281122,4.2613318429\C,-1.1657023794,0.005152
6604,3.580819867\C,-2.3571034943,0.0578068497,4.3327694672\C,-2.319950
395,0.0698683432,5.7009699118\C,-1.0852292042,0.0296209323,6.377753269
2\C,0.0864323839,-0.0216832242,5.6754605405\H,1.0342983686,-0.05243476
67,6.1936987347\H,-1.0680647559,0.0389828176,7.4574295179\H,-3.2386477
026,0.1088849845,6.2669008539\H,-3.3034100889,0.0855151942,3.811457820
3\C,-1.1701209602,-0.0183799994,2.1680509647\H,-2.1219470742,-0.017504
111,1.6537418338\H,2.2150912494,-0.0830362348,4.0214700153\C,2.4483866
734,-0.0384218824,1.3583365423\C,2.4117423705,0.0894528189,-0.03113821
83\C,1.2303178537,0.0880199734,-0.7211261074\H,1.2146258223,0.18871249
34,-1.795138436\H,3.3387798659,0.2045921649,-0.5735253074\H,3.39478435
28,-0.0483573674,1.8777648345\H,-0.8494990939,0.4642672345,-0.44589011
17\Cl,-0.6249704822,-1.8529810492,-0.5532643612\\Version=EM64L-G09RevA
.02\State=2-A\HF=-999.5881964\S2=0.869961\S2-1=0.\S2A=0.761743\RMSD=3.
733e-09\RMSF=2.106e-05\Dipole=0.290255,0.7735464,0.5483403\Quadrupole=
6.2507047,-9.3834499,3.1327452,-0.8413444,-2.1194718,-4.3339466\PG=C01
 [X(C14H10Cl1)]\\@

2-Anthracene

1\1\GINC-ABE0451\FOpt\UmPWPW91\6-31+G(d,p)\C14H10Cl1(2)\ACROFT\18-Dec-

2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H8Cl anthracene 2-si mpw1k\\0,2\C,-0.045276734,0.083300538
8,-0.0535119384\C,0.0176236244,-0.0085159878,1.412229682\C,1.221676317
6,0.0030645297,2.1173130113\C,2.4676030271,0.0022587815,1.3939218177\C
,2.4177406586,-0.0162851026,-0.0520312746\C,1.2686769592,0.0091032246,
-0.7319459312\H,1.2635709741,-0.0009019653,-1.8113346357\H,3.356713730
5,-0.0591988193,-0.5861873382\C,3.6501329044,0.0028385134,2.0783286293
\C,3.6961737211,0.0033535169,3.4946099671\C,2.4725784934,-0.0035012392
,4.2216938732\C,1.2591987743,-0.0049136288,3.5156542062\H,0.32906534,-
0.0075833738,4.0668669731\C,2.5199500172,-0.0078810077,5.6345679222\C,
3.7189874893,-0.0048251935,6.2955025182\C,4.9265148575,0.0020741792,5.
5743539134\C,4.9117405023,0.0058892386,4.2020627129\H,5.8394304662,0.0
114166347,3.6474797401\H,5.8669555671,0.0047661371,6.1047293978\H,3.74
09337975,-0.0071136888,7.3750533051\H,1.5912091669,-0.0123882592,6.187
15734\H,4.5828391345,0.0008133618,1.5303130417\H,-0.9177927034,-0.0278
122888,1.9513362628\H,-0.7524547801,-0.6290145378,-0.470892511\Cl,-0.8
531217788,1.6936098543,-0.520545042\\Version=EM64L-G09RevA.02\State=2-
A\HF=-999.5822188\S2=0.887698\S2-1=0.\S2A=0.765641\RMSD=6.597e-09\RMSF
=1.442e-05\Dipole=0.6612011,-0.7529698,0.5561173\Quadrupole=3.2412763,
-7.8060423,4.564766,3.910901,-3.464885,3.9311643\PG=C01 [X(C14H10Cl1)]
\\@

9-Anthracene

1\1\GINC-ABE0445\FOpt\UmPWPW91\6-31+G(d,p)\C14H10Cl1(2)\ACROFT\18-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C14H12Cl anthracene 9-si mpw1k\\0,2\C,0.0796160392,-0.3264591
272,-0.0395230956\C,0.0227999433,-0.1058011254,1.4329652236\C,1.189482
1013,0.0768773337,2.1585683256\C,1.1565134348,0.2053768043,3.538195147
1\C,-0.0627615812,0.1404175434,4.2109465551\C,-1.2322411794,-0.0301759
951,3.5041325792\C,-1.2188961371,-0.1433341686,2.1012835146\C,-2.41980
41356,-0.2328734723,1.3557506122\C,-2.423875942,-0.1426078312,-0.05768
58675\C,-1.2033018425,-0.1052642432,-0.763914047\C,-1.2087411896,0.077
6665763,-2.1378081822\C,-2.4003351672,0.2068401117,-2.8337164848\C,-3.
6129018139,0.1423079091,-2.1488661969\C,-3.6249961853,-0.0286692912,-0
.782503563\H,-4.562749469,-0.0639391456,-0.2465297597\H,-4.5434026573,
0.2329377644,-2.6892364053\H,-2.3879139847,0.3489583212,-3.9036682911\
H,-0.2689479369,0.0985978875,-2.6716966973\H,-3.3624366729,-0.27820417
92,1.8817369878\H,-2.1805951325,-0.0657165053,4.0210985186\H,-0.091051
7393,0.2304318255,5.2866531512\H,2.073786601,0.3472939379,4.0892134453
\H,2.1371421131,0.0981056839,1.638801682\H,0.8811236227,0.2529877429,-
0.4862833424\Cl,0.6286895451,-2.0625478837,-0.3461910064\\Version=EM64
L-G09RevA.02\State=2-A\HF=-999.5989317\S2=0.85828\S2-1=0.\S2A=0.761164
\RMSD=7.208e-09\RMSF=7.687e-05\Dipole=-0.3964285,0.7987746,0.2213669\Q
uadrupole=4.2943149,-10.3831772,6.0888623,2.59424,1.4568891,-1.452501\
PG=C01 [X(C14H10Cl1)]\\@

1-Pyrene

1\1\GINC-CN49\FOpt\UwB97XD\6-31+G(d,p)\C16H10Cl1(2)\NGS0457\16-Dec-201
0\0\\#P wB97XD/6-31+G(d,p) OPT(EstmFC) FREQ=noraman int=ultrafine\\C16
H10Cl wB97xd pyrene Cl at o-bottom tip\\0,2\C,-0.01151609,-0.013588196
4,0.0081312548\C,-0.0035039825,-0.0312744485,1.4357288688\C,1.21183610
25,-0.0316081004,2.1526408708\C,2.5161478511,-0.1313454322,1.429001624
8\C,2.4295731772,0.0390428546,-0.0445900591\C,1.2492222577,0.057432704
4,-0.6913793566\H,1.2280909209,0.1459747676,-1.7743097831\H,3.36553523
44,0.0983317915,-0.5898271979\H,3.2649280469,0.5293763419,1.869845737\
C,1.1889066593,0.0219739423,3.5554404463\C,-0.0003496712,0.0484342361,
4.2506037041\C,-1.2444846379,0.0203437244,3.5657805993\C,-1.2393147581
,-0.0135515453,2.1440534139\C,-2.4725207485,-0.0270223389,1.4292319014
\C,-3.6803204831,-0.0184232898,2.1514449782\C,-3.6783199328,0.00935908
75,3.5445856409\C,-2.4823165247,0.0313162665,4.2477213835\H,-2.4860537
011,0.0568895483,5.3335936233\H,-4.6205155865,0.0163526428,4.083275394
1\H,-4.6209189104,-0.0313622342,1.6082194859\C,-2.4383194442,-0.039963
9985,0.0050486161\C,-1.2399659321,-0.0237440093,-0.6752886559\H,-1.235
6964716,-0.014718032,-1.7618391598\H,-3.3767787104,-0.0508703663,-0.54
14951798\H,0.0028452454,0.0842330643,5.336028141\H,2.1303486527,0.0182
41716,4.0977137674\Cl,3.2814879501,-1.8148393258,1.7546885594\\Version
=AM64L-G09RevA.02\State=2-A\HF=-1075.7356709\S2=0.853793\S2-1=0.\S2A=0
.759491\RMSD=4.865e-09\RMSF=2.397e-05\Dipole=-0.7916585,0.77632,-0.069
6652\Quadrupole=1.8752681,-9.6564349,7.7811668,4.946405,-0.6039371,-0.
0727455\PG=C01 [X(C16H10Cl1)]\\@

2-Pyrene

1\1\GINC-CN47\FOpt\UwB97XD\6-31+G(d,p)\C16H10Cl1(2)\NGS0457\16-Dec-201
0\0\\#P wB97XD/6-31+G(d,p) OPT(EstmFC) FREQ=noraman int=ultrafine\\C16
H10Cl wB97xd pyrene Cl at mid\\0,2\C,-0.0743265616,-0.147770468,-0.025
8212974\C,-0.0165933873,-0.0238903094,1.4659486803\C,1.2353712879,-0.0
347155608,2.1262403359\C,1.276182932,-0.0065418643,3.5422493047\C,0.06
90254735,0.0599212125,4.2651835174\C,-1.142825473,0.104596126,3.606374
1953\C,-1.1828621705,0.0581977046,2.2054720493\H,-2.1408745191,0.05895
27689,1.692996675\H,-2.0683984424,0.1644584864,4.1694642889\H,0.104401
4518,0.0807727782,5.3508485257\C,2.5503513084,-0.0434938225,4.20359327
69\C,3.7075460668,-0.0774761928,3.4961318358\C,3.6989414025,-0.0574396
314,2.0595555027\C,2.4643942085,-0.039706972,1.3827358446\C,2.43470061
86,0.0294600168,-0.0510551134\C,1.2039835612,0.0677231707,-0.720630771
2\H,1.1819108062,0.1463535099,-1.8029199159\C,3.6597574058,0.079430235
9,-0.7519264778\C,4.8732920099,0.0424677204,-0.0720038203\C,4.90043040
9,-0.0280322151,1.3139786427\H,5.849351063,-0.0493863786,1.8420508966\
H,5.8037429565,0.0712883867,-0.6298766362\H,3.6425958805,0.1372966752,
-1.836288121\H,4.6650972136,-0.1031872062,4.0084439703\H,2.5696304419,
-0.0400618058,5.2897716431\H,-0.8817100952,0.4512632238,-0.448123354\C
l,-0.6578963509,-1.8940026199,-0.4685482777\\Version=AM64L-G09RevA.02\
State=2-A\HF=-1075.7325413\S2=0.809736\S2-1=0.\S2A=0.752571\RMSD=4.537
e-09\RMSF=6.789e-06\Dipole=0.5325016,0.8054514,0.4321308\Quadrupole=5.
128092,-10.34004,5.211948,-3.4354869,-2.9124181,-3.1257335\PG=C01 [X(C
16H10Cl1)]\\@

MPW1K/6-31+G(d,p) lignin precursor/model structures 12-17

12

1\1\GINC-ABE0483\FOpt\RmPWPW91\6-31+G(d,p)\C8H8O2\ACROFT\23-Dec-2010\0
\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572004280
)\\C8H8O2 coumaryl alcohol full OHdb in\\0,1\C,-0.0122019817,0.0340954
611,0.004873324\C,-0.0101201396,0.0181690438,1.4680500957\C,1.16101334
74,0.008572027,2.2239378923\C,1.12668829,-0.033484119,3.6073572382\C,-
0.0904827326,-0.0437908136,4.2742402864\C,-1.2694584994,-0.0081437271,
3.5440557891\C,-1.2209235115,0.0226869642,2.1634860594\H,-2.1482140797
,0.0407345822,1.6081296782\H,-2.2117963769,-0.0075136389,4.0698109399\
O,-0.186437264,-0.0742652941,5.6238031206\H,0.6831166191,-0.0975205605
,6.0159056879\H,2.0524587974,-0.0377020826,4.1674634149\H,2.1205752188
,0.0556069817,1.7304184215\H,-0.8948831393,0.4467726512,-0.4714919534\
C,0.963139513,-0.4455810906,-0.7643973311\O,0.9958007571,-0.4290590476
,-2.1111568846\H,0.215847827,0.0035472668,-2.4549027583\H,1.8461165168
,-0.9196335986,-0.3639576819\\Version=EM64L-G09RevA.02\State=1-A\HF=-4
59.9768389\RMSD=9.741e-09\RMSF=1.375e-05\Dipole=0.1745351,0.1993675,-0
.0272879\Quadrupole=2.9531593,-4.7619059,1.8087466,-0.8658881,9.278007
7,-2.5186602\PG=C01 [X(C8H8O2)]\\@

13

1\1\GINC-ABE0587\FOpt\RmPWPW91\6-31+G(d,p)\C9H10O3\ACROFT\25-Dec-2010\
0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057200428
0)\\C9H11O3 coniferyl alcohol full OHdb in\\0,1\C,-0.0367632747,0.0997
676074,0.0026667701\O,-0.0076224979,-0.0128074135,1.3990066502\C,1.198
1796588,-0.0034190312,2.0239075958\C,1.1120548392,-0.0983040008,3.4164
196547\C,2.2688955694,-0.0723008834,4.1652596\C,3.5023732627,0.0343575
491,3.5386280046\C,3.6062005036,0.1126172132,2.1542613644\C,2.42438305
01,0.1108338301,1.4018837654\H,2.4738760824,0.2280228449,0.3311111227\
C,4.927150973,0.2006644857,1.5350690291\H,5.737039403,0.570381403,2.14
96032546\C,5.2196672387,-0.1649661212,0.2913560377\O,6.4659671455,-0.0
102905259,-0.2159745999\H,6.539940461,-0.4533329209,-1.0556146678\H,4.
4852125608,-0.5964652836,-0.376430767\H,4.4003129668,0.044481937,4.138
8187613\H,2.1918835846,-0.1361650619,5.2397502312\O,-0.090993822,-0.19
61778552,4.0159874346\H,-0.7655978931,-0.1865971534,3.335578139\H,-1.0
817523743,0.068808262,-0.2843410269\H,0.3991584949,1.0435867068,-0.325
4783245\H,0.4910603251,-0.7292532858,-0.4694819609\\Version=EM64L-G09R
evA.02\State=1-A\HF=-574.467308\RMSD=7.925e-09\RMSF=7.640e-06\Dipole=-
0.2818327,-0.3036872,-1.6801351\Quadrupole=-1.0856741,-5.1283393,6.214
0135,-2.6765454,2.5948954,2.7543729\PG=C01 [X(C9H10O3)]\\@

14

1\1\GINC-ABE0014\FOpt\RmPWPW91\6-31+G(d,p)\C10H12O4\ACROFT\25-Dec-2010
\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=05720042
80)\\C9H8O2 sinapyl alcohol full OHdb in\\0,1\C,-0.0435474811,0.084844
653,-0.0071276807\O,-0.0162487252,-0.012367198,1.3903104068\C,1.188321
6057,0.0115182923,2.0181123303\C,1.088525022,-0.0702519531,3.402578070
3\C,2.2499234496,-0.0289847756,4.1679210472\C,3.4836335477,0.079636695
1,3.5389372268\C,3.5823089618,0.1454232625,2.1500619181\C,2.4153257806
,0.12844096,1.387296595\H,2.4688671994,0.239988776,0.3169695189\C,4.90
95522529,0.2346502436,1.5428794657\H,5.7062009356,0.6514924391,2.14451
38392\C,5.217822422,-0.1852699348,0.3203588083\O,6.4627919846,-0.02790
79537,-0.188717395\H,6.5507311165,-0.5101635441,-1.0051174633\H,4.4954
120705,-0.6660282167,-0.32652006\H,4.387948199,0.0975490453,4.12523910
96\O,2.0719296829,-0.1012105026,5.4998631197\C,3.2033351521,-0.0582120
482,6.3220705883\H,2.8362921606,-0.1246993776,7.3401914872\H,3.8720406
206,-0.8977619495,6.1269851345\H,3.751830315,0.8767375666,6.1993804262
\O,-0.1115559368,-0.1685609447,4.0051023886\H,-0.780703059,-0.16807537
52,3.3194331111\H,-1.0880023584,0.0423043317,-0.2949185174\H,0.3848053
482,1.0284978273,-0.3452509501\H,0.4912866149,-0.7448877872,-0.4697880
751\\Version=EM64L-G09RevA.02\State=1-A\HF=-688.9520903\RMSD=6.946e-09
\RMSF=5.110e-06\Dipole=0.2412376,-0.3252371,-1.4288299\Quadrupole=-3.4
055693,-6.8969274,10.3024967,-2.9295377,6.5127815,3.6337167\PG=C01 [X(
C10H12O4)]\\@

15

1\1\GINC-NODE14\SP\RmPWPW91\6-31+G(d,p)\C7H8O1\CHS60A\29-Mar-2008\0\\#

P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C7H8O
electrostat\\0,1\C\C,1,1.4995022\C,2,1.3875459,1,121.6037\C,3,1.38858
81,2,121.57237,1,-179.98925,0\C,4,1.3853394,3,119.84561,2,-0.000499,0\
C,5,1.3887883,4,119.59788,3,-0.0009331,0\C,2,1.3942239,3,117.49245,4,0
.0018755,0\H,7,1.0815541,2,119.36601,3,179.9973,0\H,6,1.0792105,7,121.
2705,2,179.99874,0\O,5,1.3543911,6,117.54271,7,179.99903,0\H,10,0.9540
771,5,110.13446,6,-179.99968,0\H,4,1.0820156,3,119.92254,2,-179.99868,
0\H,3,1.0811682,2,119.54376,7,-179.9974,0\H,1,1.0872392,2,111.20086,3,
-0.1403171,0\H,1,1.0893757,14,107.67745,2,-122.27012,0\H,1,1.0893624,1
4,107.67935,2,122.27266,0\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-
346.7101906\RMSD=3.922e-05\Dipole=0.5308863,-0.0000363,-0.1931711\PG=C
01 [X(C7H8O1)]\\@

16

1\1\GINC-NODE14\SP\RmPWPW91\6-31+G(d,p)\C8H10O2\CHS60A\29-Mar-2008\0\\
#P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C8H1
0O2 electrostat\\0,1\C\C,1,1.4995228\C,2,1.3975761,1,119.98642\C,3,1.3
805843,2,120.581,1,179.97683,0\C,4,1.3984919,3,120.40773,2,-0.001181,0
\C,5,1.3769448,4,119.27671,3,0.0020515,0\C,2,1.3845475,3,118.40817,4,-
0.0013849,0\H,7,1.0804138,2,119.64903,3,-179.99517,0\H,6,1.0792188,5,1
18.68476,4,179.9929,0\O,5,1.3486324,4,120.11498,3,179.99837,0\H,10,0.9
581316,5,108.13331,4,-0.0140829,0\O,4,1.3580064,5,113.85324,6,179.9969
1,0\C,12,1.4013938,4,118.37506,5,179.84664,0\H,13,1.0841202,12,106.354
37,4,-179.88251,0\H,13,1.0901587,12,111.14463,4,-60.997817,0\H,13,1.09
01638,12,111.14676,4,61.239052,0\H,3,1.0796956,4,120.1629,5,179.99706,
0\H,1,1.0870167,2,111.03555,3,179.71706,0\H,1,1.0896091,2,111.43197,3,
-60.252282,0\H,1,1.0895801,2,111.43544,3,59.677898,0\\Version=x86-Linu
x-G03RevB.04\State=1-A\HF=-461.202851\RMSD=9.214e-05\Dipole=1.0364001,
-0.0019605,-0.5946536\PG=C01 [X(C8H10O2)]\\@

17

1\1\GINC-NODE13\SP\RmPWPW91\6-31+G(d,p)\C9H12O3\CHS60A\29-Mar-2008\0\\
#P MPWPW91/6-31+G(D,P) POP=FULL GFOLDPRINT IOP(3/76=0572004280)\\C9H1
2O3 electrostat\\0,1\C\O,1,1.4013729\C,2,1.3584568,1,118.40655\C,3,1.3
872312,2,125.30255,1,0.4067826,0\C,4,1.388952,3,119.64096,2,179.80003,
0\C,5,1.3899475,4,119.30562,3,-0.2390592,0\C,6,1.3908001,5,121.01498,4
,0.221188,0\C,7,1.3915022,6,119.64089,5,-0.0655269,0\O,8,1.3473948,7,1
19.9341,6,-179.72072,0\H,9,0.9579983,8,107.55904,7,179.74816,0\O,7,1.3
460751,6,124.77166,5,-179.81339,0\C,11,1.3988702,7,118.26041,6,-0.1696
631,0\H,12,1.0909888,11,111.54386,7,-61.223879,0\H,12,1.0909849,11,111
.5404,7,61.358243,0\H,12,1.0843642,11,106.03903,7,-179.9365,0\H,6,1.07
83977,5,119.04148,4,-179.74281,0\C,5,1.5000216,4,120.39808,3,178.16242
,0\H,17,1.0877939,5,111.36401,4,28.52089,0\H,17,1.0878836,5,111.33757,
4,148.92055,0\H,17,1.0903365,5,111.14438,4,-91.309494,0\H,4,1.078619,5
,119.73693,6,179.74021,0\H,1,1.0900672,2,111.17707,3,60.970022,0\H,1,1
.0842359,2,106.29656,3,179.82106,0\H,1,1.0900571,2,111.18158,3,-61.338
299,0\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-575.6874727\RMSD=2.8
14e-05\Dipole=0.5791631,-0.0145415,-0.929336\PG=C01 [X(C9H12O3)]\\@

MPW1K/6-31+G(d,p) lignin precursor/model π-complexes for 12-17

12

ipso

1\1\GINC-ABE0480\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\23-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C8H8O2Cl ipso a complex (OHin)\\0,2\C,-0.0439795943,-0.093599
3412,0.0441834966\C,-0.0275380068,-0.1078453227,1.4075245029\C,1.18629
89146,-0.048205849,2.1257978832\C,1.2627517318,-0.0865165787,3.5622884
343\H,2.2466879601,0.059734639,3.992570981\C,0.2353208109,-0.312081972
,4.3979224446\O,0.3103207343,-0.3478184108,5.7306090406\H,1.2058697655
,-0.1880064619,6.0271596825\H,-0.7725818088,-0.499494685,4.0638005848\
C,2.3837191183,0.0637706474,1.387948704\C,2.389484529,0.082210512,0.02
32943346\C,1.1743521177,-0.0499568161,-0.6933032253\O,1.2036650234,0.3
000473903,-1.9820668683\H,0.5148060514,-0.1583109514,-2.4641802278\H,3
.301753736,0.169304776,-0.5442034627\H,3.3206989547,0.1320051253,1.920
9985016\H,-0.9681669414,-0.154897381,1.9331432378\H,-0.9760210343,-0.1
311285074,-0.498662383\Cl,1.1428743559,-2.4402102685,-1.0521796349\\Ve
rsion=EM64L-G09RevA.02\State=2-A\HF=-920.1383751\S2=0.822924\S2-1=0.\S
2A=0.753897\RMSD=5.845e-09\RMSF=9.539e-06\Dipole=-0.0925678,1.4891036,
1.5861613\Quadrupole=6.1056093,-10.0438662,3.9382569,1.1229653,8.20370
66,-3.6078824\PG=C01 [X(C8H8Cl1O2)]\\@

ortho (a)

1\1\GINC-ABE0482\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\23-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C8H8O2Cl ortho a complex (OHin)\\0,2\C,-0.0446304713,-0.01732
68698,0.0576926425\C,-0.0164413356,0.0457865664,1.4597210346\C,1.17598
87661,0.0509707398,2.1497349852\C,1.2565432955,0.0424810837,3.60464708
59\H,2.1385039575,0.485437881,4.0525353236\C,0.3373775789,-0.518200642
6,4.3938090317\O,0.3532382843,-0.5456507892,5.7325325124\H,1.113281977
3,-0.0742733409,6.0711804969\H,-0.5251297622,-1.0365472564,4.002991804
7\C,2.3761275698,0.0895746597,1.3963492344\C,2.3834262031,0.0657043302
,0.0215022193\C,1.1775843117,-0.0073340141,-0.664267706\O,1.1924549455
,-0.0537863269,-1.9934045756\H,0.4042429256,-0.5097805412,-2.301199511
3\H,3.3045260426,0.0718940248,-0.5390559628\H,3.3183434902,0.115687954
9,1.9248323712\H,-0.9556428746,0.1057118477,1.9867893444\H,-0.95270784
68,0.2433729208,-0.4615052599\Cl,-0.6260231992,-2.2473500353,-0.627599
1212\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1403524\S2=0.780271\S
2-1=0.\S2A=0.750591\RMSD=3.768e-09\RMSF=4.096e-06\Dipole=0.8864095,1.4
531533,1.0776993\Quadrupole=3.3595614,-6.6038265,3.2442651,-1.9173131,
4.748039,-0.0987217\PG=C01 [X(C8H8Cl1O2)]\\@

ortho (b)

1\1\GINC-ABE0597\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\23-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C8H8O2Cl ortho b complex (OHin)\\0,2\C,-0.0156515778,-0.19268
76269,0.0360734218\C,0.0151033903,-0.2886429543,1.4102757255\C,1.21398
53029,-0.1587936527,2.1448243731\C,1.253397837,-0.2196201253,3.6015685
692\H,2.2249495097,-0.4090958837,4.0426332064\C,0.2090120087,-0.037503
5005,4.4099775995\O,0.2265820472,-0.1001988906,5.7508487225\H,1.102581
1121,-0.3207142513,6.0645819905\H,-0.7821155327,0.1953651994,4.0523031
746\C,2.3812624295,0.0139927403,1.4309656098\C,2.392902496,0.037727679
5,0.0267180043\C,1.1644809461,0.0099794768,-0.6690645072\O,1.213789633
2,0.1740748088,-1.9912026102\H,0.3592350622,0.0161049359,-2.3881868401
\H,3.2761385857,0.3428679328,-0.5095340723\H,3.3243537529,0.0977695656
,1.9493133728\H,-0.9110524655,-0.4799601385,1.9307258518\H,-0.95508737
98,-0.2787927574,-0.4916009014\Cl,3.0063557368,-2.2352928178,-0.479290
7694\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1361926\S2=0.78857\S2
-1=0.\S2A=0.750994\RMSD=4.079e-09\RMSF=1.314e-06\Dipole=-1.096213,1.09
52251,0.6161931\Quadrupole=3.1102269,-7.1753285,4.0651016,3.7607465,12
.2002666,-4.7641687\PG=C01 [X(C8H8Cl1O2)]\\@

meta (b)

1\1\GINC-ABE0596\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\23-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C8H8O2Cl meta b complex (OHin)\\0,2\C,-0.0077566112,-0.153502
7661,0.0225568128\C,-0.0110496357,-0.2757950743,1.391138177\C,1.177253
956,-0.1877197673,2.1258679691\C,1.2408553254,-0.2439858627,3.56273591
53\H,2.2177378151,-0.4358925004,3.989370449\C,0.1978209016,-0.07548901
26,4.3884390655\O,0.2403794928,-0.1486545951,5.7223489619\H,1.11649457
75,-0.3931866212,6.0195546733\H,-0.7982438392,0.1567563099,4.045244970
5\C,2.3972609768,-0.0712940838,1.3899130753\C,2.3793077922,0.127302024
7,-0.0040885307\C,1.1946254316,0.0636432549,-0.682909536\O,1.206564913
1,0.2179873919,-2.0207248716\H,0.3235789172,0.1588949477,-2.3776904163

\H,3.3007082631,0.278150931,-0.5422116536\H,3.2875044953,0.2075464752,
1.9297317001\H,-0.948306627,-0.4529382568,1.8952673112\H,-0.9381865844
,-0.232993852,-0.523579041\Cl,3.1178173377,-2.2890497756,1.6364041214\
\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1370836\S2=0.816323\S2-1=0
.\S2A=0.753219\RMSD=9.699e-09\RMSF=1.397e-05\Dipole=-1.3303105,1.23796
39,0.1207007\Quadrupole=2.0229985,-8.4555443,6.4325458,4.0536682,9.024
1024,-1.1005515\PG=C01 [X(C8H8Cl1O2)]\\@

para

1\1\GINC-ABE0542\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\25-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C8H8O2Cl si para a complex (OHin)\\0,2\C,-0.0002253937,-0.118
8761135,-0.0400030903\C,-0.0239749622,-0.0120191233,1.3280406025\C,1.1
562191988,0.2400195246,2.0667861839\C,1.1385468311,0.6113419954,3.4694
176558\H,2.0608352865,0.4671903008,4.0175172496\C,0.0766379796,1.12366
76954,4.094602352\O,0.0144239322,1.4642029218,5.3881933652\H,0.8241394
152,1.2252035785,5.8378113019\H,-0.85632141,1.332047737,3.5941705478\C
,2.3659790898,0.3384399822,1.3359114301\C,2.3945177911,0.2318033647,-0
.0294197502\C,1.2078165408,0.0064567766,-0.7275356967\O,1.2897113709,-
0.0942794645,-2.0600962687\H,0.4342503741,-0.2837524467,-2.4407957875\
H,3.3184154072,0.3050676322,-0.58051196\H,3.2827033412,0.5143525427,1.
8778580342\H,-0.9556075233,-0.1478874992,1.8543243011\H,-0.9117800453,
-0.3294649707,-0.5816673031\Cl,1.5336886946,-2.3075962008,2.4376895402
\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1365946\S2=0.773242\S2-1=
0.\S2A=0.750388\RMSD=3.669e-09\RMSF=7.116e-06\Dipole=-0.4701575,1.3899
597,-0.6337422\Quadrupole=3.9022192,-11.3329709,7.4307516,3.3680135,8.
1625853,3.2941459\PG=C01 [X(C8H8Cl1O2)]\\@

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ipso

1\1\GINC-ABE0585\FOpt\UmPWPW91\6-31+G(d,p)\C9H10Cl1O3(2)\ACROFT\25-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H11O3.Cl coniferyl alcohol full OHdb in ipso coomplex\\0,2
\C,-0.0309942445,-0.0398986113,0.0096331013\O,0.0359283687,0.139131817
6,1.404621928\C,1.2265414512,0.0584598914,2.0008352564\C,1.1348908771,
-0.114344353,3.4192746012\C,2.3197187117,-0.0703037936,4.1812826071\C,
3.5285677949,0.0284156674,3.5561573782\C,3.6295174159,0.1127372052,2.1
508044633\C,2.4505260605,0.1526038237,1.3888214271\H,2.5009386456,0.28
27782778,0.3206088887\C,4.9456498848,0.1612756015,1.5629780338\H,5.778
7415083,0.3556469224,2.2240462234\C,5.2267739013,-0.0646431453,0.27404
05729\O,6.4868044949,0.0202853861,-0.1821927431\H,6.53957855,-0.260468
6286,-1.0915005729\H,4.4706385051,-0.3340529279,-0.4507379533\H,4.4340
975784,0.0231738554,4.143602081\H,2.2309600381,-0.1464594634,5.2527503
492\O,-0.0244194856,0.0567713082,4.0331190919\H,-0.7342884784,-0.13018
65029,3.4137352924\H,-1.084749184,-0.0726832992,-0.2393128917\H,0.4356
126585,0.7938347505,-0.5135888401\H,0.4428913577,-0.9785993253,-0.2713
21438\Cl,0.9829117356,-2.56204724,3.0338933028\\Version=EM64L-G09RevA.
02\State=2-A\HF=-1034.6334198\S2=0.805512\S2-1=0.\S2A=0.752165\RMSD=8.
234e-09\RMSF=3.017e-06\Dipole=0.7574608,1.5373532,-2.1950839\Quadrupol
e=2.7798436,-13.9996186,11.2197749,-5.2754281,0.7062226,3.6449148\PG=C
01 [X(C9H10Cl1O3)]\\@

meta (a)

1\1\GINC-ABE0582\FOpt\UmPWPW91\6-31+G(d,p)\C9H10Cl1O3(2)\ACROFT\25-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H11O3.Cl coniferyl alcohol full OHdb in metaa coomplex\\0,
2\C,-0.0400284481,-0.0049718485,0.0282463233\O,-0.0055777581,-0.039199
948,1.43771056\C,1.1790772709,-0.0230415203,2.0725555389\C,1.098624643
6,-0.0157508391,3.4522173136\C,2.2668099629,0.0450614861,4.2063826036\
C,3.5085020851,0.0962854688,3.5957370192\C,3.6326169407,0.0627999802,2
.2121378056\C,2.433911039,-0.0570188672,1.4312656859\H,2.4778525406,0.
2131091372,0.3904290884\C,4.9337529667,0.1524488819,1.6041196394\H,5.7
529157737,0.471276567,2.2333217251\C,5.2155051515,-0.1861159021,0.3394
242192\O,6.4599128251,-0.0546267006,-0.1459852332\H,6.5235804777,-0.44
4496372,-1.0136230359\H,4.474983413,-0.6058126149,-0.3268438464\H,4.39
70047486,0.1612892994,4.2047363875\H,2.1764883938,0.0584171195,5.28176
99883\O,-0.0925433941,-0.0272269903,4.0739133188\H,-0.780187123,-0.106
1149349,3.410678672\H,-1.086190511,-0.079295234,-0.2439103327\H,0.3595
42584,0.9384940779,-0.3439646687\H,0.5106122642,-0.8443976898,-0.38908
53829\Cl,2.5309569833,-2.3149535783,0.7420442717\\Version=EM64L-G09Rev
A.02\State=2-A\HF=-1034.6332433\S2=0.814689\S2-1=0.\S2A=0.752873\RMSD=
3.056e-09\RMSF=1.232e-05\Dipole=-0.0081091,1.1344941,-0.9955385\Quadru
pole=3.4813367,-10.3224564,6.8411197,-1.9415847,0.7262693,-1.344509\PG
=C01 [X(C9H10Cl1O3)]\\@

meta (b)

1\1\GINC-ABE0580\FOpt\UmPWPW91\6-31+G(d,p)\C9H10Cl1O3(2)\ACROFT\25-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H11O3.Cl coniferyl alcohol full OHdb in metab coomplex\\0,
2\C,-0.0629165058,-0.0483689568,-0.026395863\O,-0.0080417861,0.0749855
508,1.3735095551\C,1.1867458835,0.0149436276,1.9861554547\C,1.09156656
55,0.1030108485,3.403857555\C,2.2182676654,0.0108271941,4.1581180404\C
,3.4669956437,-0.2244408996,3.5385750512\C,3.5809103542,-0.1761066126,
2.1154776954\C,2.40385931,-0.1178721694,1.3599003455\H,2.4497310454,-0
.1906006074,0.2860182471\C,4.8975016531,-0.2249140388,1.5353338872\H,5
.7071987156,-0.5390335616,2.1785214391\C,5.1962224147,0.1019870111,0.2
726960629\O,6.4560513474,0.0084160391,-0.1861442297\H,6.5170896032,0.3
293643123,-1.0811905607\H,4.4565498034,0.4625672694,-0.42965247\H,4.35
91978869,-0.0527220694,4.1172151351\H,2.1455867186,0.0536879502,5.2323
445272\O,-0.1116063128,0.2756423812,3.9677464623\H,-0.7765320106,0.299
236007,3.2779318819\H,-1.1119026258,0.0004232282,-0.2927163669\H,0.472
0577362,0.7686228313,-0.5089728429\H,0.3503961171,-1.0036939413,-0.346
221308\Cl,3.8208962933,-2.4961966575,3.8472879291\\Version=EM64L-G09Re
vA.02\State=2-A\HF=-1034.6319299\S2=0.814152\S2-1=0.\S2A=0.753013\RMSD
=5.336e-09\RMSF=9.574e-06\Dipole=-0.8523325,1.8830023,-2.8179986\Quadr
upole=2.5004049,-10.812802,8.3123971,4.9212287,-0.2124891,1.1775799\PG
=C01 [X(C9H10Cl1O3)]\\@

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ipso

1\1\GINC-ABE0013\FOpt\UmPWPW91\6-31+G(d,p)\C10H12Cl1O4(2)\ACROFT\25-De
c-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=05
72004280)\\C10H14O4.Cl sinapyl alcohol ipso complex full OHdb in\\0,2\
C,0.0197844907,0.0859969198,0.0413206212\C,0.0175918189,-0.0705220465,
1.4616808995\C,1.1871743761,-0.1640377356,2.1653260879\C,2.4155825711,
-0.1515185962,1.4806566161\C,2.4321362734,-0.0995681375,0.0791700649\C
,1.2653010012,-0.0067945431,-0.6445635663\O,1.1694284365,0.0229919015,
-1.9666826991\C,2.3514439242,0.1021707884,-2.7218881536\H,2.0378218221
,0.1701160074,-3.756543242\H,2.921298664,0.9910452092,-2.4546222817\H,
2.9655507669,-0.7883048102,-2.5877188047\H,3.3827406493,-0.1129623019,
-0.4273628061\C,3.6849726666,-0.2023582518,2.17068602\H,4.562370498,-0
.4369579398,1.5841877566\C,3.869407698,0.0677700154,3.4665890878\O,5.0
892033417,-0.0206451846,4.0247588696\H,5.0745307868,0.2949626263,4.923
849623\H,3.0645893836,0.3771296872,4.1193111387\H,1.1638482992,-0.2738
026344,3.2360576249\O,-1.2181579308,-0.1131526685,1.9672458693\C,-1.38
06167271,0.0534423902,3.3550204523\H,-2.4486445087,0.104348965,3.52917
92768\H,-0.9673329301,-0.7941534114,3.9005268083\H,-0.910224239,0.9792
627054,3.6812919905\O,-1.092280136,-0.0937815516,-0.6487321988\H,-1.83
794647,0.109348943,-0.0787836029\Cl,-0.0286374336,2.5295289928,0.26051
27948\\Version=EM64L-G09RevA.02\State=2-A\HF=-1149.1229706\S2=0.800404
\S2-1=0.\S2A=0.751873\RMSD=2.469e-09\RMSF=8.435e-06\Dipole=0.9705221,-
1.5095745,1.8731144\Quadrupole=0.6823293,-16.8340553,16.1517259,5.1041
123,-5.7614141,3.6098508\PG=C01 [X(C10H12Cl1O4)]\\@

meta (a)

1\1\GINC-ABE0002\FOpt\UmPWPW91\6-31+G(d,p)\C10H12Cl1O4(2)\ACROFT\25-De
c-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=05
72004280)\\C10H14O4.Cl sinapyl alcohol metaa complex full OHdb in\\0,2
\C,-0.0401111938,0.0009487031,0.0228550117\O,-0.0075714914,-0.01745147
53,1.4330949182\C,1.1799583148,-0.010020186,2.0671361244\C,1.087854362
1,-0.0211283301,3.4377394675\C,2.2652952515,0.0198589739,4.210691502\C
,3.5094577627,0.078568521,3.5927230912\C,3.6208337175,0.0690964669,2.2
096637651\C,2.4313238285,-0.0268167927,1.4226431943\H,2.4802192609,0.2
434899816,0.3832215382\C,4.925423305,0.1721105023,1.6048367399\H,5.738
0321253,0.5220309847,2.225883503\C,5.209398946,-0.1996608155,0.3510598
211\O,6.4483824782,-0.0604444022,-0.1440262579\H,6.5147803843,-0.47978
97056,-0.9977275502\H,4.4725922326,-0.6582921303,-0.2936431112\H,4.406
368035,0.1237505245,4.1872661478\O,2.0733813673,0.0049646989,5.5257992
208\C,3.1909618603,0.0210520206,6.3782492975\H,2.7939104812,-0.0170974
439,7.3855126899\H,3.8277136801,-0.8456265543,6.2058299504\H,3.7690578
442,0.9357720499,6.2518800007\O,-0.0982234044,-0.0417565521,4.05978873
25\H,-0.779424111,-0.1087924681,3.3879298475\H,-1.0855800408,-0.084810
1173,-0.2490685566\H,0.3509540552,0.9441522478,-0.3590914789\H,0.51873
22193,-0.8381572961,-0.3839719333\Cl,2.5438785638,-2.3268326347,0.6544
855818\\Version=EM64L-G09RevA.02\State=2-A\HF=-1149.1239423\S2=0.78863
6\S2-1=0.\S2A=0.75106\RMSD=4.085e-09\RMSF=1.028e-05\Dipole=0.5037822,1
.3219963,-0.2213931\Quadrupole=1.4851922,-12.9467395,11.4615473,-1.840
4168,4.5587287,-2.8343308\PG=C01 [X(C10H12Cl1O4)]\\@

meta(b)

1\1\GINC-ABE0589\FOpt\UmPWPW91\6-31+G(d,p)\C10H12Cl1O4(2)\ACROFT\25-De

c-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=05
72004280)\\C10H14O4.Cl sinapyl alcohol metab complex full OHdb in\\0,2
\C,-0.0632636422,-0.0728818269,-0.0279498064\O,-0.0101825963,0.0741410
115,1.3696641295\C,1.1809092803,0.0137283391,1.9914716563\C,1.07614725
23,0.1114847155,3.3854651099\C,2.2195121609,0.0268241377,4.1536834192\
C,3.4636408935,-0.1965327563,3.5226312314\C,3.5651092429,-0.1986891744
,2.1018995611\C,2.4034489372,-0.1402812498,1.3499781638\H,2.4455336604
,-0.2437607135,0.2790863326\C,4.8881084303,-0.2877457009,1.5189525555\
H,5.6689126683,-0.7282715969,2.122683863\C,5.2027992496,0.1563215082,0
.3012264223\O,6.4457243312,0.0159619852,-0.1950082351\H,6.5298229634,0
.4669127962,-1.0300176437\H,4.4841663215,0.6542449501,-0.3368550819\H,
4.3668496276,-0.0482974627,4.088528212\O,2.0619428743,0.1287317086,5.4
721727775\C,3.1897406325,0.0207853036,6.3092593855\H,2.8050774806,0.05
88831901,7.3215634307\H,3.7066219297,-0.9222675411,6.1467174303\H,3.87
1506128,0.858196829,6.1565519132\O,-0.1193714582,0.2797085636,3.972852
3484\H,-0.7903111231,0.2872497957,3.2892190008\H,-1.1116104414,-0.0164
562377,-0.2958228991\H,0.4802613266,0.7294217353,-0.5250858554\H,0.338
1036137,-1.0381137188,-0.3323794808\Cl,3.7816765328,-2.558574113,3.894
6471253\\Version=EM64L-G09RevA.02\State=2-A\HF=-1149.1186674\S2=0.7903
11\S2-1=0.\S2A=0.751142\RMSD=7.228e-09\RMSF=9.765e-06\Dipole=-0.311061
7,1.8860951,-2.3142085\Quadrupole=-0.8155719,-12.8917157,13.7072876,6.
2436447,4.5573956,-1.3594429\PG=C01 [X(C10H12Cl1O4)]\\@

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ortho (a)

1\1\GINC-NODE10\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\27-Mar-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76
=0572004280)\\C7H8O.Cl ortho_b 1K\\0,2\C,-0.4202466933,0.495799642,-3
.182390568\C,-0.3877197413,0.5044936586,-1.6865561562\C,0.787946923,0.
4754630703,-0.9850376215\C,0.8012699438,0.449105456,0.4291881223\C,-0.
4333935087,0.5050896558,1.1275506953\C,-1.6258791651,0.5594168654,0.42
22176835\C,-1.596817308,0.5555803491,-0.95615768\H,-2.5316585066,0.582
3642799,-1.4984564982\H,-2.5556681657,0.5843804184,0.9679179598\O,-0.4
667089012,0.4971814074,2.4596989352\H,0.3195864305,0.0595411425,2.7947
098132\H,1.6982137125,0.7501507665,0.9469485689\H,1.7346927192,0.45931
03108,-1.5033498742\H,0.5823389319,0.5338714483,-3.5988910427\H,-0.901
104027,-0.4087255948,-3.5532356971\H,-0.9803193756,1.3452500421,-3.570
4069622\Cl,1.3892133405,-1.7148991915,1.0778991412\\Version=x86-Linux-
G03RevB.04\State=2-A\HF=-806.8734484\S2=0.789452\S2-1=0.\S2A=0.751052\
RMSD=9.352e-09\RMSF=9.536e-06\Dipole=-0.5068484,1.1861398,-0.9052974\P
G=C01 [X(C7H8Cl1O1)]\\@

ortho (b)

1\1\GINC-NODE12\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\28-Mar-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76
=0572004280)\\C7H8O.Cl ortho 1K\\0,2\C,0.4221574139,0.5229598892,-3.1
049296371\C,0.3905601221,0.5174140039,-1.608210317\C,1.5849556023,0.40
32850511,-0.8745453159\C,1.604258151,0.4018018119,0.5066950227\C,0.411
4595794,0.506283967,1.2075077321\C,-0.8122583395,0.5381595864,0.502964
414\C,-0.7861192582,0.6086902255,-0.9053242831\H,-1.7272058766,0.69123
09049,-1.4277602429\H,-1.7053623037,0.7956529868,1.0481051286\O,0.3408
649921,0.5764684365,2.5384781835\H,1.1975820301,0.427859515,2.93418038
82\H,2.5433144373,0.3365706179,1.0381181661\H,2.5220443095,0.323488247
5,-1.4077789935\H,1.1339203075,1.254031167,-3.4847889481\H,0.71683619,
-0.4526336043,-3.4902520951\H,-0.5547849698,0.7592811337,-3.5175454558
\Cl,-1.3966672757,-1.7493409218,0.8032324053\\Version=x86-Linux-G03Rev
B.04\State=2-A\HF=-806.8696783\S2=0.788328\S2-1=0.\S2A=0.751007\RMSD=8
.512e-09\RMSF=1.006e-05\Dipole=1.4404282,1.2347482,-0.5048605\PG=C01 [
X(C7H8Cl1O1)]\\@

meta (a)

1\1\GINC-NODE09\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\27-Mar-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76
=0572004280)\\C7H8O.Cl meta_b 1K pi\\0,2\C,-0.3248641404,0.5416404188
,-2.610879443\C,-0.3359247098,0.533149356,-1.1189350131\C,0.8658547535
,0.5212094923,-0.3768187872\C,0.8550975963,0.5774297501,1.023862992\C,
-0.3430366861,0.5688729627,1.6924639038\C,-1.5482988653,0.5447392132,0
.9695681995\C,-1.5353183143,0.5294509012,-0.4062432724\H,-2.4717922697
,0.5163596222,-0.9446102579\H,-2.4759134979,0.537692987,1.5210462714\O
,-0.4514270222,0.5944592392,3.0335028788\H,0.4112497284,0.5515855863,3
.4408843947\H,1.7917313278,0.594859437,1.5619533296\H,1.8015426919,0.6
580494829,-0.8956158027\H,0.685424666,0.6224524245,-3.0002309829\H,-0.
7538108692,-0.3803994135,-2.9994493426\H,-0.9132680006,1.3729970355,-2
.9967241861\Cl,1.1608937999,-1.8898955083,-0.881963996\\Version=x86-Li
nux-G03RevB.04\State=2-A\HF=-806.8689085\S2=0.7811\S2-1=0.\S2A=0.75063
4\RMSD=6.408e-09\RMSF=1.449e-05\Dipole=-0.2110006,1.3337903,0.3078539\

PG=C01 [X(C7H8Cl1O1)]\\@

meta (b)

1\1\GINC-NODE13\FOpt\UmPWPW91\6-31G(d)\C7H8Cl1O1(2)\CHS60A\27-Mar-2008
\0\\#P MPWPW91/6-31G(D) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76=05720
04280)\\C7H8O.Cl meta 1K\\0,2\C,0.3848091728,0.5434091418,-2.63922463
37\C,0.3945469204,0.5258102599,-1.1478279753\C,1.5684631677,0.51992755
06,-0.4168133476\C,1.5532879496,0.5243349396,0.9694887932\C,0.34393495
5,0.5456148187,1.6719854002\C,-0.8421305676,0.554971203,0.9757071546\C
,-0.828120707,0.4946475879,-0.4256249497\H,-1.7489508799,0.6761053096,
-0.9579560147\H,-1.7765376315,0.5721561102,1.5129949024\O,0.2933786029
,0.5756419355,3.0178972548\H,1.180066853,0.5546946956,3.3794647048\H,2
.4882037747,0.5174452813,1.5145577089\H,2.5176592423,0.5177983074,-0.9
322759055\H,1.393007818,0.6090373796,-3.0404720699\H,-0.0799443858,-0.
3637799464,-3.0239676345\H,-0.1863589739,1.3907591853,-3.019014451\Cl,
-1.2695835285,-1.8430379303,-0.7942736428\\Version=x86-Linux-G03RevB.0
4\State=2-A\HF=-806.8409088\S2=0.798757\S2-1=0.\S2A=0.751621\RMSD=7.91
8e-09\RMSF=1.538e-05\Dipole=1.2773693,1.3092126,0.2671332\PG=C01 [X(C7
H8Cl1O1)]\\@

para

1\1\GINC-NODE14\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\CHS60A\28-Mar-2
008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/76
=0572004280)\\C7H8O.Cl para 1K\\0,2\C,-0.0309347113,0.713868756,-2.49
47141334\C,-0.0283800904,0.4508530031,-1.0217211718\C,1.1694290684,0.5
611004425,-0.2767800445\C,1.1599045132,0.6220113436,1.0950549593\C,-0.
0562054379,0.597915589,1.7787394659\C,-1.2612755645,0.5237459626,1.075
1901585\C,-1.2432373484,0.460826179,-0.2924991994\H,-2.1726475557,0.39
99832215,-0.8385973597\H,-2.1865661861,0.5089700697,1.6289944197\O,-0.
1312149226,0.6482885855,3.1147368691\H,0.7410079802,0.6652961072,3.504
1529814\H,2.0895428091,0.6807071825,1.6437805616\H,2.1091790635,0.5792
281837,-0.8078550688\H,0.8766009981,0.3426910064,-2.9606435107\H,-0.87
80374008,0.234140126,-2.975228518\H,-0.096615734,1.7879349703,-2.67459
68481\Cl,0.1359678136,-1.9980698356,-1.2127954011\\Version=x86-Linux-G
03RevB.04\State=2-A\HF=-806.8707508\S2=0.781153\S2-1=0.\S2A=0.750675\R
MSD=8.031e-09\RMSF=1.931e-06\Dipole=0.4566175,1.6063288,0.6689808\PG=C
01 [X(C7H8Cl1O1)]\\@

16

ortho (a)

1\1\GINC-NODE06\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\CHS60A\28-Mar-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/7
6=0572004280)\\C8H10O2.Cl ortho pi 1K\\0,2\C,-0.8843237892,-0.4555357
381,-3.2337105831\C,-0.8241764906,-0.4511726933,-1.7392614154\C,0.3707
772427,-0.5430506581,-1.0728287234\C,0.4108318051,-0.4770420392,0.3328
649324\C,-0.8045200651,-0.3705871135,1.0665662434\C,-2.0110273465,-0.2
880497121,0.3832395561\C,-2.0145980086,-0.328750418,-0.9896557946\H,-2
.9558357534,-0.2574637408,-1.5153576071\H,-2.9217462936,-0.193239346,0
.9523569474\O,-0.7799420307,-0.3965297061,2.388372093\H,0.1340160467,-
0.3528537854,2.6825369277\O,1.4667769314,-0.7827791777,1.0847367906\C,
2.7589209045,-0.5933818841,0.5441992149\H,3.4492746846,-0.7399807863,1
.3657978757\H,2.9634483507,-1.3275789891,-0.2328124159\H,2.8455953669,
0.4198433189,0.1580257248\H,1.2941093471,-0.6330155108,-1.6220223782\H
,-1.6301620917,-1.1606469172,-3.5963943988\H,-1.1574767583,0.530991558
1,-3.6074050526\H,0.0744369001,-0.7217485621,-3.6698884563\Cl,0.611667
9695,2.0538579629,0.561871246\\Version=x86-Linux-G03RevB.04\State=2-A\
HF=-921.3669477\S2=0.770379\S2-1=0.\S2A=0.750286\RMSD=8.854e-09\RMSF=9
.304e-06\Dipole=0.2452197,-1.6734794,-0.9288018\PG=C01 [X(C8H10Cl1O2)]
\\@

ortho (b)

1\1\GINC-NODE04\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\CHS60A\28-Mar-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/7
6=0572004280)\\C8H10O2.Cl ortho_b 1K pi\\0,2\C,-0.3001990431,-0.47750
04562,-3.2675194856\C,-0.3222412988,-0.4697387716,-1.7710430746\C,0.90
20574849,-0.4634829876,-1.0635388463\C,0.9283912106,-0.4608722665,0.30
77752558\C,-0.2758247052,-0.4687388867,1.0316691299\C,-1.493915033,-0.
3919176478,0.3434351081\C,-1.495203195,-0.451330014,-1.0649458618\H,-2
.4429184264,-0.4364494944,-1.5801462631\H,-2.4038194522,-0.518216807,0
.9064803811\O,-0.2645254551,-0.540690269,2.3560649891\H,0.6446510661,-
0.4883296682,2.6602852681\O,2.0286145078,-0.477375549,1.0932889411\C,3
.2885586556,-0.42088497,0.4756767148\H,4.0191071792,-0.414701506,1.275
9016113\H,3.4528754959,-1.2931204317,-0.1568127471\H,3.3908017728,0.48
81602794,-0.1161905239\H,1.8254968449,-0.4646799433,-1.6225928094\H,-1
.3038952786,-0.5681392066,-3.6730111333\H,0.1325857187,0.444725458,-3.
6543206707\H,0.2947946957,-1.3049504283,-3.6519341594\Cl,-1.7124786172

,2.0192367232,0.7099091743\\Version=x86-Linux-G03RevB.04\State=2-A\HF=
-921.3623215\S2=0.773313\S2-1=0.\S2A=0.750341\RMSD=7.892e-09\RMSF=1.08
8e-05\Dipole=1.7994486,-1.3682052,-0.8741459\PG=C01 [X(C8H10Cl1O2)]\\@

meta (a)

1\1\GINC-NODE07\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\CHS60A\27-Mar-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/7
6=0572004280)\\C8H10O2.Cl meta 1K pi\\0,2\C,-0.9022908099,-0.43797530
77,-2.8912462224\C,-0.9157918081,-0.4407025584,-1.3993413057\C,0.32152
881,-0.3877592128,-0.6969941299\C,0.3359748126,-0.4464012389,0.7093922
631\C,-0.8611755418,-0.4373507659,1.4235411458\C,-2.0533851446,-0.4424
345007,0.7327632383\C,-2.0761225195,-0.4501591698,-0.6678409844\H,-3.0
290683085,-0.4644694141,-1.1749744487\H,-2.9722356559,-0.4407575215,1.
2989288968\O,-0.8537301381,-0.4497052386,2.7687572045\H,0.0544130886,-
0.4016102706,3.0703972644\O,1.439262897,-0.478892533,1.4653876993\C,2.
7085580923,-0.4654202122,0.8466208861\H,3.4302098332,-0.4324714578,1.6
537813567\H,2.8607669812,-1.37387927,0.2649992598\H,2.8150591513,0.413
5967788,0.2159360523\H,1.2307926118,-0.5890866131,-1.2398072822\H,-1.9
0973917,-0.5098460846,-3.2911123619\H,-0.4501511152,0.4815062569,-3.26
13410728\H,-0.3219787531,-1.2722720671,-3.2844463907\Cl,0.8390525835,1
.9451346844,-0.9686405794\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-
921.3651273\S2=0.784171\S2-1=0.\S2A=0.750806\RMSD=2.789e-09\RMSF=3.497
e-05\Dipole=0.4188339,-1.3488425,-0.1128507\PG=C01 [X(C8H10Cl1O2)]\\@

meta (b)

1\1\GINC-NODE03\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\CHS60A\29-Mar-
2008\0\\#P MPWPW91/6-31+G(D,P) OPT INT=ULTRAFINE SCF=VERYTIGHT IOP(3/7
6=0572004280)\\C8H10O2.Cl meta_b pi 1K\\0,2\C,-0.3100584119,-0.475170
3904,-2.8642944054\C,-0.2698061927,-0.4407145122,-1.3742341423\C,0.927
6164141,-0.4955905054,-0.6810229369\C,0.9345718567,-0.4865816392,0.705
6274481\C,-0.2739728092,-0.442247532,1.4402340548\C,-1.4615367235,-0.3
838879893,0.7715112238\C,-1.4755631211,-0.3172530079,-0.6346420282\H,-
2.4126412458,-0.4588820881,-1.1482288277\H,-2.3825352711,-0.3416434313
,1.3297824875\O,-0.2351807338,-0.4693158478,2.780494923\H,0.6796742885
,-0.4996632925,3.0639531722\O,2.0298657765,-0.530565746,1.4788460356\C
,3.2995729256,-0.539814282,0.8697582201\H,4.0202057353,-0.5457081013,1
.6784966438\H,3.4304350957,-1.4323897594,0.2601414667\H,3.4416139361,0
.3511771213,0.2607018322\H,1.8547081659,-0.5506937275,-1.2288222227\H,
-0.9440233592,-1.2873013481,-3.2181285777\H,-0.725836466,0.456551829,-
3.2446175772\H,0.6818440307,-0.6102877047,-3.2863845015\Cl,-1.77799228
71,2.0238501414,-1.0552497747\\Version=x86-Linux-G03RevB.04\State=2-A\
HF=-921.3660647\S2=0.787572\S2-1=0.\S2A=0.750926\RMSD=3.503e-09\RMSF=5
.318e-06\Dipole=2.0361667,-1.6183543,-0.0200048\PG=C01 [X(C8H10Cl1O2)]
\\@

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ipso

1\1\GINC-ABE0595\FOpt\UmPWPW91\6-31+G(d,p)\C9H12Cl1O3(2)\ACROFT\22-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H12O3Cl ferulic acid ortho a (Cl on opposite H of OH)\\0,2
\C,-0.0005928897,-0.0485762847,-0.067733108\O,0.0261704203,0.173772674
2,1.3234058462\C,1.1991916608,0.1000484854,1.9554507322\C,2.4449159302
,0.1191934474,1.3714969455\C,3.584452029,0.0759195813,2.1752189813\C,3
.4704702824,0.0342643603,3.5646173866\C,2.2305360042,0.0152804994,4.17
26874846\C,1.0581449315,-0.0024615561,3.367947149\O,-0.1130776747,0.20
30114536,3.9440177862\H,-0.8023711652,0.0367417375,3.2964110747\O,2.00
52350038,0.0112452804,5.4783507886\C,3.0991601669,-0.1397773424,6.3476
754543\H,3.6326991533,-1.0658142931,6.1386660903\H,3.7803325578,0.7078
166294,6.274647517\H,2.6803436275,-0.1795608434,7.3458768565\H,4.36599
88771,0.0114017575,4.1633775833\C,4.9376405702,0.0348531286,1.54072303
03\H,4.9474973504,0.5615225288,0.5895627483\H,5.6935208532,0.47635881,
2.1853672645\H,5.230071328,-0.9979159635,1.3486193925\H,2.5484734114,0
.1577294399,0.2994605284\H,0.4556936733,-1.0076712556,-0.3043888251\H,
-1.0464174489,-0.0598713421,-0.349627709\H,0.5078227934,0.7543772771,-
0.5993900049\Cl,0.9870573468,-2.5008316369,3.1411195416\\Version=EM64L
-G09RevA.02\State=2-A\HF=-1035.8557452\S2=0.778777\S2-1=0.\S2A=0.75057
\RMSD=1.911e-09\RMSF=7.098e-06\Dipole=1.1755278,1.6234771,-0.939555\Qu
adrupole=4.2584175,-13.7898168,9.5313993,-2.0798679,7.7314641,-0.29234
45\PG=C01 [X(C9H12Cl1O3)]\\@

meta (a)

1\1\GINC-ABE0583\FOpt\UmPWPW91\6-31+G(d,p)\C9H12Cl1O3(2)\ACROFT\22-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H12O3Cl ferulic acid meta a (Cl on opposite H of OH)\\0,2\
C,-0.0175937254,-0.0826945247,0.0082294477\O,-0.0055006774,0.023335681

9,1.41587927\C,1.1694939727,0.0010021521,2.0666499198\C,2.4287284972,-
0.0999887896,1.4450323055\C,3.6043313191,-0.0395104984,2.2409075601\C,
3.4849592322,0.0093392646,3.6079756271\C,2.2232097803,0.0437213849,4.2
191148705\C,1.0593642113,0.0441908688,3.4398982608\O,-0.1372779613,0.0
989900751,4.0450016271\H,-0.8121380036,0.0391621947,3.3667511944\O,2.0
272001291,0.0822054027,5.5332965049\C,3.1373845484,0.0508040936,6.3951
14978\H,3.7187322675,-0.8592940028,6.2538962681\H,3.7738527581,0.92301
82816,6.2505415545\H,2.7306201216,0.066222758,7.3991274469\H,4.3746937
483,0.0232115034,4.2153422928\C,4.9355152207,-0.0696381936,1.568304046
9\H,5.0344937233,0.7503275903,0.8577038236\H,5.7441869623,0.0076975671
,2.2894187287\H,5.0501124295,-1.0010836352,1.0159577069\H,2.5130277655
,0.0718930013,0.3853554384\H,0.5015172712,-0.9825559476,-0.3121484789\
H,-1.0621188841,-0.1367414229,-0.2746058852\H,0.4307692722,0.799628371
8,-0.4477650235\Cl,2.5015364186,-2.4615692977,0.8971517947\\Version=EM
64L-G09RevA.02\State=2-A\HF=-1035.8553744\S2=0.775508\S2-1=0.\S2A=0.75
0424\RMSD=1.292e-09\RMSF=7.433e-06\Dipole=0.4988664,1.5295006,0.289078
8\Quadrupole=4.6432112,-10.2208086,5.5775974,2.2060087,9.5224818,-5.65
96508\PG=C01 [X(C9H12Cl1O3)]\\@

meta (b)

1\1\GINC-ABE0580\FOpt\UmPWPW91\6-31+G(d,p)\C9H12Cl1O3(2)\ACROFT\22-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H12O3Cl ferulic acid meta b (Cl on opposite H of OH)\\0,2\
C,-0.0164949243,0.0338657507,-0.0099602884\O,-0.0002979326,0.072994536
,1.396848331\C,1.1771339539,0.0311781651,2.0434448801\C,2.4283516409,0
.0027663833,1.4165754013\C,3.5701902315,-0.0466817312,2.1756037457\C,3
.4549617001,-0.1149810999,3.589593784\C,2.1898292969,-0.0181269094,4.2
124201228\C,1.0476064657,0.027740852,3.4308417478\O,-0.1616531287,0.08
24716848,4.0144122007\H,-0.8261575238,0.0920162464,3.3247063021\O,2.00
80246056,0.0079283032,5.5286811504\C,3.1260936967,-0.0819348411,6.3814
676041\H,3.6975664412,-0.9846232844,6.1777947186\H,3.7614761807,0.7990
23216,6.2862564457\H,2.7227978007,-0.1201870606,7.3863531347\H,4.34026
12617,0.0456741371,4.1811390457\C,4.9278574862,-0.0765011013,1.5576849
063\H,4.8720133143,0.0170818017,0.4767790276\H,5.5499167048,0.73354705
18,1.9368316543\H,5.4244953339,-1.0151438368,1.7992785245\H,2.49919847
36,0.0212531753,0.3414505415\H,0.4497360719,-0.8782084728,-0.378510789
6\H,-1.0611094751,0.047383839,-0.2970811762\H,0.484955251,0.9041940585
,-0.4302386998\Cl,3.8904102053,-2.4865054042,3.8445345565\\Version=EM6
4L-G09RevA.02\State=2-A\HF=-1035.8540121\S2=0.77561\S2-1=0.\S2A=0.7504
39\RMSD=4.909e-09\RMSF=4.192e-06\Dipole=-0.2839957,1.5152424,-1.460443
5\Quadrupole=1.1560541,-10.3952334,9.2391793,4.9210109,7.6602461,0.986
637\PG=C01 [X(C9H12Cl1O3)]\\@

para

1\1\GINC-ABE0570\FOpt\UmPWPW91\6-31+G(d,p)\C9H12Cl1O3(2)\ACROFT\27-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C10H14O4.Cl sinapyl model para complex full OHdb in\\0,2\C,-
0.0097195188,0.0254682768,0.0200848682\O,-0.0060582997,-0.0497802409,1
.4249463489\C,1.1881375414,-0.0915157653,2.0563702921\C,2.4171982703,-
0.1819140521,1.4632216447\C,3.5896594214,-0.1584160065,2.261277165\C,3
.4539393298,-0.1369725501,3.6705110477\C,2.2204117828,-0.0485074661,4.
2644022483\C,1.0682574889,-0.0224929834,3.454080337\O,-0.1273564237,0.
080615872,4.0207633576\H,-0.7865507122,0.1132752784,3.322532893\O,1.98
77929065,0.0205503933,5.5799825011\C,3.0950914372,0.0814849715,6.44084
32051\H,3.6918110718,-0.8292394058,6.3816314567\H,3.7202651431,0.94518
41119,6.2159963196\H,2.6896312198,0.1787694007,7.4410043286\H,4.351320
5361,-0.1530503046,4.2658374986\C,4.8823942238,-0.6250858115,1.6665585
769\H,4.978841643,-0.3008623497,0.6353811891\H,5.7294264714,-0.2373552
089,2.223495708\H,4.9183407995,-1.7154061568,1.6943567119\H,2.52266600
39,-0.2281845747,0.3922371202\H,0.4097511047,-0.8794103371,-0.41838521
71\H,-1.0481127154,0.118728718,-0.2749939939\H,0.5484098741,0.89581947
71,-0.3213858441\Cl,4.0341362583,2.2101782105,1.9073473425\\Version=EM
64L-G09RevA.02\State=2-A\HF=-1035.851599\S2=0.789957\S2-1=0.\S2A=0.750
965\RMSD=5.919e-09\RMSF=9.244e-06\Dipole=-0.64936,-1.6300483,-0.250890
9\Quadrupole=1.2889034,-9.5125788,8.2236754,-6.2725249,10.6261539,3.58
10845\PG=C01 [X(C9H12Cl1O3)]\\@

MPW1K/6-31+G(d,p) lignin precursor/model σ-complexes for 12, 13, 15 and 16

12

ipso

1\1\GINC-ABE0546\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\29-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H14O4.Cl coumaryl model ipso complex full OHdb in\\0,2\C,-
0.0087994255,-0.0521085878,0.0140630873\C,-0.0032660039,-0.0335772933,
1.3609694115\C,1.2121817446,-0.0365171248,2.1123892268\C,1.2571385215,
-0.0509185042,3.5359786728\H,2.2448429879,-0.0025715203,3.9817583436\C
,0.1991468212,-0.129979345,4.373205509\O,0.2726717493,-0.1376951949,5.
711815244\H,1.1821637356,-0.076311721,6.00110735\H,-0.8236864811,-0.20
0310335,4.0412799491\C,2.4305127451,0.0075385252,1.3768935438\C,2.4656
782315,-0.0029513753,0.0271590198\C,1.2380540223,-0.1242316626,-0.7783
668452\O,1.2961495606,0.7476735158,-1.837747861\H,0.5512250103,0.59947
90875,-2.4198694243\H,3.3916637974,0.0513010163,-0.522995752\H,3.36036
59516,0.0658231378,1.9251740256\H,-0.9502310009,0.0033133735,1.8778149
058\H,-0.9374908922,-0.0449233217,-0.5382902069\Cl,1.2461227197,-1.869
9082331,-1.53261893\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.141351
8\S2=0.852261\S2-1=0.\S2A=0.757986\RMSD=7.755e-09\RMSF=4.321e-06\Dipol
e=-0.1059228,0.5419102,1.0688506\Quadrupole=4.7795431,-7.1740887,2.394
5456,-0.407824,8.7215423,-1.9018558\PG=C01 [X(C8H8Cl1O2)]\\@

ortho (a)

1\1\GINC-ABE0545\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\29-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H14O4.Cl coumaryl model orthoa complex full OHdb in\\0,2\C
,-0.0041508221,0.053564651,-0.0384500395\C,0.0390659415,0.16738925,1.4
085265207\C,1.2116851282,0.0971659741,2.1097233879\C,1.2537523352,0.12
09128398,3.571248302\H,2.1202440611,0.5803032169,4.0330531798\C,0.3140
683399,-0.4247772391,4.3432971806\O,0.286637794,-0.4220922277,5.685253
9338\H,1.0330711376,0.0628525657,6.034208222\H,-0.5346410979,-0.953395
1916,3.9362083711\C,2.4352198194,0.0347386951,1.3906085214\C,2.4619528
636,0.0131635348,-0.0002040015\C,1.2906009525,0.0271333893,-0.71163617
89\O,1.3168122356,0.0144622012,-2.0509776856\H,0.499148306,-0.36109423
,-2.3837103519\H,3.3955503301,-0.0276970381,-0.5393020324\H,3.36444836
13,-0.0065144106,1.9386563946\H,-0.9005104206,0.3108574367,1.918964137
6\H,-0.7145065388,0.7250753614,-0.5093929505\Cl,-0.9070200254,-1.62371
7575,-0.5560020476\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1397881
\S2=0.834088\S2-1=0.\S2A=0.754506\RMSD=8.204e-09\RMSF=8.066e-05\Dipole
=0.6382513,0.9002663,0.6593742\Quadrupole=1.69358,-4.1526298,2.4590498
,-1.5533557,5.6430402,1.6874693\PG=C01 [X(C8H8Cl1O2)]\\@

ortho (b)

1\1\GINC-ABE0544\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\29-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H14O4.Cl coumaryl model orthob complex full OHdb in\\0,2\C
,0.0030894684,-0.0833839371,-0.0090215427\C,0.0109830162,-0.1967538169
,1.3816448703\C,1.227270771,-0.122463852,2.1158912015\C,1.25207871,-0.
1342098596,3.5757469758\H,2.2225713988,-0.2927211391,4.0315626412\C,0.
1984841734,0.0521403598,4.3706215614\O,0.2108404519,0.0365950313,5.714
8975993\H,1.0926933578,-0.1427546299,6.0378582114\H,-0.7963057046,0.24
6392714,4.0016002817\C,2.4021761514,-0.024989344,1.4256622631\C,2.4744
240311,-0.0878963576,-0.0360175854\C,1.1749919717,0.032033624,-0.70705
31838\O,1.2582034764,0.2118224217,-2.032669241\H,0.3884358803,0.215414
4603,-2.4281293401\H,3.2082942886,0.5860455773,-0.4655088879\H,3.34163
59386,0.03499178,1.9543579585\H,-0.9270651967,-0.3296118003,1.89595963
77\H,-0.940500749,-0.0734242946,-0.5379491013\Cl,3.2323013642,-1.75703
6848,-0.5283897699\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1374598
\S2=0.847091\S2-1=0.\S2A=0.756005\RMSD=4.368e-09\RMSF=7.631e-06\Dipole
=-0.7722648,0.7180546,0.3274391\Quadrupole=2.386314,-5.4015922,3.01527
82,2.1970327,11.5367957,-3.7872872\PG=C01 [X(C8H8Cl1O2)]\\@

meta (a)

1\1\GINC-ABE0543\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\29-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H14O4.Cl coumaryl model metaa complex full OHdb in\\0,2\C,
0.0376897379,0.0222084474,-0.0658782291\C,-0.0296953106,-0.2170620674,
1.380994542\C,1.2540641413,-0.0827397348,2.1152583995\C,1.2887446683,-
0.0354597681,3.5385636758\H,2.2681684423,0.087531243,3.9876772122\C,0.
2236432367,-0.1354812508,4.3612832561\O,0.2746761613,-0.0709364035,5.6
984688536\H,1.1750076345,0.0514982472,5.9968291238\H,-0.7844563815,-0.
294806626,4.0151321435\C,2.4402037012,-0.0277334302,1.3822697635\C,2.4
526608309,0.0294878526,0.0076739284\C,1.2223715646,0.083674775,-0.7103
049382\O,1.3503764807,0.2325713595,-2.0460820714\H,0.4925201315,0.2063

853806,-2.4647323974\H,3.3750147455,0.0703973516,-0.549130244\H,3.3784
151327,-0.0066840602,1.9182707703\H,-0.8216893158,0.3618038427,1.84478
77832\H,-0.8970500549,0.0690744829,-0.605621383\Cl,-0.6973420416,-1.96
96390463,1.6475215821\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1443
142\S2=0.858634\S2-1=0.\S2A=0.757796\RMSD=5.146e-09\RMSF=3.015e-05\Dip
ole=0.4813319,0.866699,0.1815701\Quadrupole=2.1955299,-6.69834,4.50281
01,-2.1170235,9.2135421,0.806646\PG=C01 [X(C8H8Cl1O2)]\\@

meta (b)

1\1\GINC-ABE0542\FOpt\UmPWPW91\6-31+G(d,p)\C8H8Cl1O2(2)\ACROFT\29-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C10H14O4.Cl coumaryl model metab complex full OHdb in\\0,2\C,
0.0158665198,-0.1083609668,-0.0193991687\C,0.0002144656,-0.1975741405,
1.3566879871\C,1.1714629306,-0.147305954,2.1078704927\C,1.2142369964,-
0.142038388,3.5394601511\H,2.1859725316,-0.3119320859,3.9893863363\C,0
.1665978633,0.0602651447,4.3599953921\O,0.2129391421,0.0366039966,5.69
89603317\H,1.0922913271,-0.1879777108,6.0012189214\H,-0.830216514,0.27
74487256,4.01056402\C,2.4709085917,-0.1593003936,1.391652645\C,2.41887
52713,0.0959965549,-0.0493855408\C,1.2444966879,0.0762513845,-0.716324
543\O,1.247850958,0.2448466346,-2.0581325033\H,0.3556227548,0.30603975
8,-2.3895848607\H,3.3443873269,0.2302055489,-0.5855296891\H,3.20921233
68,0.4606884617,1.8888528762\H,-0.9507083645,-0.3084139258,1.855641421
3\H,-0.909828155,-0.167304359,-0.5748206936\Cl,3.2649426655,-1.8676671
917,1.6697702572\\Version=EM64L-G09RevA.02\State=2-A\HF=-920.1393378\S
2=0.869961\S2-1=0.\S2A=0.759489\RMSD=6.155e-09\RMSF=1.903e-05\Dipole=-
0.9554816,0.7459206,0.2539271\Quadrupole=2.2289829,-5.9383455,3.709362
6,2.3053252,9.0735016,-1.1917006\PG=C01 [X(C8H8Cl1O2)]\\@

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meta (a)

1\1\GINC-ABE0586\FOpt\UmPWPW91\6-31+G(d,p)\C9H10Cl1O3(2)\ACROFT\25-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H11O3.Cl coniferyl alcohol full OHdb in metaa coomplex\\0,
2\C,-0.044475421,0.273438185,0.0511152831\O,0.0004610777,-0.2459575311
,1.3583684558\C,1.1499662404,-0.1194947992,2.0659674354\C,1.0209271398
,-0.1388711723,3.4222911686\C,2.1596461704,-0.0509863298,4.247616636\C
,3.4146233759,0.0994956103,3.6863133474\C,3.6095030171,0.1230749077,2.
3102816966\C,2.4586703403,-0.1491456284,1.4220436839\H,2.4954550343,0.
4410828634,0.5135083876\C,4.9068993506,0.3761627261,1.7702390774\H,5.6
90474529,0.6271539503,2.4721348711\C,5.2487452947,0.3141087524,0.47143
19697\O,6.5053988786,0.6033104826,0.0831899824\H,6.6174153915,0.427134
6679,-0.8465651364\H,4.5591230252,0.0212594845,-0.3070843296\H,4.26998
87561,0.2301679809,4.3324709065\Cl,2.6751796423,-1.9094587152,0.640870
6405\H,2.0191531881,-0.0671634005,5.316644473\O,-0.1901275598,-0.20793
67411,4.0071516548\H,-0.8486022721,-0.2969921743,3.3161014109\H,-1.068
2213666,0.1547663835,-0.2853806825\H,0.2154701477,1.3325603364,0.04179
64208\H,0.6129545656,-0.2823939309,-0.6151170818\\Version=EM64L-G09Rev
A.02\State=2-A\HF=-1034.6329958\S2=0.875583\S2-1=0.\S2A=0.760468\RMSD=
3.969e-09\RMSF=1.764e-05\Dipole=0.0334394,0.9518496,-1.206611\Quadrupo
le=1.7792383,-7.8922326,6.1129944,-1.3968471,0.5840907,-2.7132199\PG=C
01 [X(C9H10Cl1O3)]\\@

meta (b)

1\1\GINC-ABE0558\FOpt\UmPWPW91\6-31+G(d,p)\C9H10Cl1O3(2)\ACROFT\25-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C9H11O3.Cl coniferyl alcohol full OHdb in metab coomplex\\0,
2\C,-0.0558514037,-0.0822356813,-0.0042056029\O,-0.002526354,0.0182833
92,1.395471962\C,1.2000131278,-0.0279567576,2.0027627814\C,1.108955502
6,0.088586511,3.4331919851\C,2.2167442285,0.0012215107,4.1909765198\C,
3.5107485019,-0.3172065308,3.5915067915\C,3.6024649313,-0.1747640261,2
.124289259\C,2.4166977491,-0.1366936901,1.3782398028\H,2.4624638633,-0
.1763663615,0.3019469371\C,4.9084418118,-0.1487930259,1.5510429358\H,5
.7418695867,-0.3346355088,2.2151323272\C,5.2102708076,0.0888307876,0.2
604306467\O,6.4917134667,0.0594089657,-0.1573201859\H,6.5522785361,0.2
982434989,-1.0775410683\H,4.4662801149,0.3142078202,-0.4908449971\H,4.
3376781752,0.1612232968,4.1015399318\H,2.1414243742,0.0795779804,5.263
2339847\O,-0.1005409923,0.3028968304,3.9775009614\H,-0.7506950656,0.33
86524372,3.2745830737\H,-1.1054204145,-0.0489708495,-0.2715978448\H,0.
4644873003,0.7518975623,-0.4742392185\H,0.3759088288,-1.0238645693,-0.
3414448064\Cl,3.9262518166,-2.1524947044,4.0220950404\\Version=EM64L-G
09RevA.02\State=2-A\HF=-1034.6330373\S2=0.858837\S2-1=0.\S2A=0.757848\
RMSD=6.593e-09\RMSF=1.330e-05\Dipole=-0.6146262,1.1557289,-2.5678824\Q
uadrupole=0.435067,-8.3563232,7.9212562,3.4168859,0.9292093,0.2289804\
PG=C01 [X(C9H10Cl1O3)]\\@

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ipso

1\1\GINC-ABE0441\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\ACROFT\31-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C7H8O.Cl coumaryl model ipso complex full OHdb in\\0,2\C,0.01
90736025,-0.0751586527,-0.0111479913\C,-0.0077003357,0.0132732894,1.47
71436542\C,1.189457258,-0.002316094,2.2283108609\C,1.189174625,0.02492
60854,3.5857238442\C,-0.0645150563,-0.0078674763,4.353672104\C,-1.2823
634748,0.1367706681,3.5342181365\C,-1.2314553715,0.1113331584,2.177577
9123\H,-2.1513493025,0.1842545601,1.6145082707\H,-2.2229671958,0.21869
86432,4.0592854231\O,0.0235962962,0.8346395915,5.4303778241\H,-0.74902
08834,0.7329768971,5.9856855133\H,2.1006055252,0.0404422058,4.16202964
91\H,2.1343690068,-0.0151453104,1.7035762559\H,0.9283869979,0.36066253
11,-0.4193067001\H,-0.0167740437,-1.116146616,-0.3383239052\H,-0.83353
79872,0.4332651726,-0.4560455651\Cl,-0.1882462338,-1.7814512776,5.0884
157681\\Version=EM64L-G09RevA.02\State=2-A\HF=-806.8672797\S2=0.839738
\S2-1=0.\S2A=0.754732\RMSD=5.434e-09\RMSF=3.915e-06\Dipole=-0.4018379,
0.5572336,-0.9566631\Quadrupole=3.4006897,-6.3122412,2.9115516,-1.5753
632,-2.7390001,1.9874917\PG=C01 [X(C7H8Cl1O1)]\\@

ortho (a)

1\1\GINC-ABE0428\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\ACROFT\31-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C7H8O.Cl coumaryl model ortha complex full OHdb in\\0,2\C,0.0
150268304,-0.0260796622,-0.0172484841\C,-0.0273987705,-0.00039447,1.47
92437426\C,1.1852394825,-0.1090224561,2.2102343113\C,1.1972480531,-0.0
672192913,3.602922011\C,0.0262043736,0.0652856965,4.2995037885\C,-1.26
70611458,0.1434964878,3.6153628531\C,-1.1985053692,0.144166536,2.15502
31279\H,-2.1320878348,0.2495142803,1.6229013958\H,-1.8980697098,0.9329
931291,4.0150988505\O,0.0422751536,0.1301604317,5.6392542371\H,-0.8006
17447,-0.1693133726,5.9851675413\H,2.1211294187,-0.1408053343,4.155505
5792\H,2.115940859,-0.2254938327,1.6750738892\H,0.6584051693,0.7626605
583,-0.4045987795\H,0.4124683414,-0.975105794,-0.3751439238\H,-0.97527
3966,0.1046650779,-0.4445336765\Cl,-2.3109005204,-1.3634248887,4.22517
04622\\Version=EM64L-G09RevA.02\State=2-A\HF=-806.8737494\S2=0.828024\
S2-1=0.\S2A=0.753672\RMSD=7.961e-09\RMSF=3.050e-05\Dipole=0.3127661,0.
5657972,-0.6661757\Quadrupole=0.3465758,-3.1918217,2.845246,-3.0185951
,-1.9347233,0.2362115\PG=C01 [X(C7H8Cl1O1)]\\@

ortho (b)

1\1\GINC-ABE0425\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\ACROFT\31-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C7H8O.Cl coumaryl model orthob complex full OHdb in\\0,2\C,-0
.0150098548,0.0056653422,-0.009026221\C,0.0171876249,0.0011585822,1.48
84131822\C,1.1902582679,0.0315942845,2.1763912577\C,1.2519663833,-0.06
10638511,3.6404179198\C,-0.0460869181,0.0957590158,4.3080229649\C,-1.2
190237051,0.0574875066,3.6049522009\C,-1.203736539,-0.016292246,2.2094
34295\H,-2.1390875808,-0.0509024091,1.6709897309\H,-2.1630692209,0.112
976843,4.1302916861\O,0.0403217114,0.2384090969,5.638754149\H,-0.83015
78577,0.2693429051,6.0312835042\H,2.0073520218,0.5771232053,4.08736838
18\H,2.1341066514,0.0527211233,1.652371959\H,0.9860298591,0.0758601474
,-0.4255680321\H,-0.4713319486,-0.9082006077,-0.3878552996\H,-0.599084
4676,0.8430261047,-0.3882931486\Cl,1.9439841483,-1.7648254621,4.096969
2436\\Version=EM64L-G09RevA.02\State=2-A\HF=-806.8711852\S2=0.831034\S
2-1=0.\S2A=0.753963\RMSD=9.382e-09\RMSF=5.977e-06\Dipole=-1.1394882,0.
8472398,-0.3825748\Quadrupole=2.3613734,-5.0011578,2.6397844,1.5381945
,-4.4863312,1.6451674\PG=C01 [X(C7H8Cl1O1)]\\@

meta (a)

1\1\GINC-ABE0419\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\ACROFT\31-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C7H8O.Cl coumaryl model metaa complex full OHdb in\\0,2\C,0.0
393700354,-0.0154410918,0.0055794672\C,0.0601180457,-0.0226687862,1.49
36464417\C,1.2225262772,0.003506283,2.2197069034\C,1.2271288155,0.0365
28234,3.6159811547\C,0.001763604,0.0942140567,4.3224573036\C,-1.182114
1451,0.080242114,3.6610077198\C,-1.2338556333,-0.1022744739,2.20690890
64\H,-1.9894519901,0.5232093562,1.7398663441\H,-2.121145652,0.13420434
27,4.1928562995\O,0.1108477421,0.1944374808,5.6655979961\H,-0.75323273
65,0.1652997578,6.0706682199\H,2.1483784537,0.048005548,4.1760036447\H
,2.1677360188,0.0165417888,1.6959445603\H,1.043731526,0.0603624394,-0.
4017972024\H,-0.4224938816,-0.9242095238,-0.3800590363\H,-0.5453284437
,0.824114929,-0.3735095149\Cl,-1.984647181,-1.8104809539,1.8550523661\
\Version=EM64L-G09RevA.02\State=2-A\HF=-806.8714119\S2=0.834009\S2-1=0

.\S2A=0.754181\RMSD=5.511e-09\RMSF=3.473e-05\Dipole=0.132865,0.8123308
,0.0274112\Quadrupole=1.1885272,-4.4215539,3.2330267,-2.9305432,-5.058
6233,-1.3835495\PG=C01 [X(C7H8Cl1O1)]\\@

meta (b)

1\1\GINC-ABE0417\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\ACROFT\31-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C7H8O.Cl coumaryl model metab complex full OHdb in\\0,2\C,-0.
0197326527,0.0256065904,0.0054436023\C,-0.047917691,0.0009047549,1.493
3182909\C,1.2298622196,-0.2023993026,2.2120695451\C,1.1907604549,-0.03
35000618,3.6669967461\C,0.0088471942,0.0793265821,4.3288009964\C,-1.20
8139272,0.135151767,3.6165062144\C,-1.2029542814,0.1207070236,2.214757
4299\H,-2.142671339,0.2252108004,1.6913635089\H,-2.1441478627,0.216735
4132,4.151037809\O,0.0311910727,0.157936239,5.6797456175\H,-0.84711983
88,0.3087856389,6.0197017311\H,2.1164065091,-0.068364273,4.2186563954\
H,2.0423253918,0.3563657768,1.7558234813\H,0.633540994,0.8193951627,-0
.3598682162\H,0.3682488983,-0.9128805781,-0.3900213353\H,-1.0124767708
,0.1886641955,-0.404983081\Cl,1.8194814092,-1.9678780068,1.8442887522\
\Version=EM64L-G09RevA.02\State=2-A\HF=-806.869421\S2=0.841906\S2-1=0.
\S2A=0.754963\RMSD=7.929e-09\RMSF=7.846e-06\Dipole=-1.1105003,0.970618
3,-0.042589\Quadrupole=3.115826,-4.9150358,1.7992098,0.8683662,-3.2921
787,-0.7252957\PG=C01 [X(C7H8Cl1O1)]\\@

para

1\1\GINC-ABE0414\FOpt\UmPWPW91\6-31+G(d,p)\C7H8Cl1O1(2)\ACROFT\31-Dec-
2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=0572
004280)\\C7H8O.Cl coumaryl model para complex full OHdb in\\0,2\C,0.04
12614778,-0.0503357733,-0.0098671115\C,-0.0472769842,-0.0956390138,1.5
010808745\C,1.2406814675,0.1087251896,2.1822828214\C,1.3529634559,0.82
66325238,3.3287892479\C,0.2302372461,1.4718271379,3.8796934386\C,-1.00
48924088,1.421423658,3.2144601452\C,-1.1413468676,0.7113519718,2.06008
61447\H,-2.0901001176,0.683355995,1.5457320195\H,-1.850599164,1.966610
8697,3.6125859376\O,0.4123345945,2.1540684759,5.024967124\H,-0.4089439
152,2.5414945264,5.3203382646\H,2.3025155683,0.9292807919,3.8314611487
\H,2.1047491097,-0.3800015172,1.7576963438\H,0.7928713291,-0.746790030
9,-0.3714376926\H,-0.9133395222,-0.3099793846,-0.4594589061\H,0.315483
162,0.9562992783,-0.3223526277\Cl,-0.5360900614,-1.9383107385,1.870285
2927\\Version=EM64L-G09RevA.02\State=2-A\HF=-806.8700635\S2=0.828093\S
2-1=0.\S2A=0.7537\RMSD=4.271e-09\RMSF=1.908e-05\Dipole=-0.2502065,1.30
22732,-0.0258691\Quadrupole=2.3784822,-4.5333228,2.1548406,-4.9195091,
-3.0768424,2.2815445\PG=C01 [X(C7H8Cl1O1)]\\@

16

ipso

1\1\GINC-ABE0584\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\ACROFT\29-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C10H14O4.Cl coniferyl model ipso complex full OHdb in\\0,2\C
,0.0197583245,0.094750177,0.0263323314\C,-0.0152380613,0.0198967185,1.
5163768139\C,1.1870071361,0.0736980662,2.2549061351\C,1.169983005,0.06
41122704,3.6168836506\C,-0.0967084099,0.1207208836,4.3747089907\C,-1.2
88894624,-0.1252563444,3.5692775482\C,-1.2340440976,-0.1147244076,2.20
99123393\H,-2.1466573604,-0.233736139,1.6439848133\H,-2.212083238,-0.2
511301893,4.1117462283\O,-0.1009963144,-0.5782335612,5.536505911\H,0.7
252373307,-0.4123867454,5.9941422195\O,2.2292830877,0.0393493796,4.431
750104\C,3.5140903342,0.0980696711,3.8654118575\H,4.2112339421,0.08536
6398,4.6945834519\H,3.6957880749,-0.7633081569,3.2234538432\H,3.640984
728,1.0178099806,3.2960652222\H,2.1254789869,0.0965046892,1.7225312377
\H,-0.8856541109,-0.3170989773,-0.4125506666\H,0.1045563681,1.12997032
94,-0.3090302575\H,0.8720639013,-0.4468698626,-0.380665537\Cl,-0.21625
51273,2.0164627364,4.9029625201\\Version=EM64L-G09RevA.02\State=2-A\HF
=-921.3636348\S2=0.827194\S2-1=0.\S2A=0.753685\RMSD=8.901e-09\RMSF=1.0
22e-05\Dipole=1.1991724,-0.7240429,-1.1926426\Quadrupole=6.8405644,-7.
5895187,0.7489543,0.5273019,3.2653308,-1.6235514\PG=C01 [X(C8H10Cl1O2)
]\\@

ortho (b)

1\1\GINC-ABE0561\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\ACROFT\29-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C10H14O4.Cl coniferyl model orthob complex full OHdb in\\0,2
\C,0.0380707379,-0.0128464525,0.0240502822\C,-0.0427420538,0.031552711
6,1.5184911578\C,1.1728288835,0.1419819918,2.259320426\C,1.1504560262,
0.1066088427,3.6412096864\C,-0.052236309,0.0005890501,4.3232801787\C,-
1.3284186236,0.0790270447,3.6269932041\C,-1.2283813976,-0.0429472012,2
.169101941\H,-2.1537443342,-0.1230500588,1.6196194196\H,-2.0735299362,
-0.5665860453,4.0787186794\O,-0.0908116651,-0.1050906029,5.652886724\H
,0.808420953,-0.067413713,5.986477608\O,2.2374463403,0.1282747368,4.45

45985361\C,3.5099022847,0.1739356417,3.8653531551\H,4.2230471959,0.169
0883475,4.6816007296\H,3.6806335328,-0.696053156,3.2312694979\H,3.6393
999814,1.0845071242,3.2808107977\H,2.106280991,0.2218173626,1.72540970
91\H,-0.9460411461,-0.1336259698,-0.4198537922\H,0.4714065095,0.907393
2657,-0.3668566192\H,0.6654960214,-0.8374152666,-0.3126308051\Cl,-2.11
80377235,1.7820035385,4.018208125\\Version=EM64L-G09RevA.02\State=2-A\
HF=-921.362331\S2=0.82272\S2-1=0.\S2A=0.753084\RMSD=3.646e-09\RMSF=9.1
44e-06\Dipole=1.7198341,-0.813215,-0.7473388\Quadrupole=4.1291533,-4.9
92807,0.8636538,3.2807822,3.2960657,-0.7516858\PG=C01 [X(C8H10Cl1O2)]\
\@

meta (b)

1\1\GINC-ABE0555\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\ACROFT\29-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C10H14O4.Cl coniferyl model metab complex full OHdb in\\0,2\
C,0.0245222998,-0.0088537614,0.0284430249\C,0.0167098091,0.0466399249,
1.5161503645\C,1.1769497842,0.0532482663,2.2543063193\C,1.1380903799,0
.0620263519,3.6467550222\C,-0.1057485651,0.0077396114,4.337803344\C,-1
.2669552094,0.0051501274,3.6430806634\C,-1.270945337,0.1754490545,2.20
16254292\H,-2.0802705103,-0.341270215,1.7005766775\H,-2.2049372657,-0.
0426999075,4.1718383986\O,-0.0985764157,-0.0715901125,5.679701821\H,0.
8104760669,-0.0790226256,5.9819725505\O,2.2090653228,0.0689586728,4.46
16437218\C,3.4956828871,0.1254258605,3.8966836827\H,4.1893269534,0.156
9337057,4.7284410177\H,3.6951831748,-0.7585666579,3.2925332556\H,3.613
7457258,1.0223889359,3.290575357\H,2.1256332365,0.0244742309,1.7409862
264\H,-0.5615694974,-0.8542017432,-0.3340737889\H,-0.4230111195,0.8932
658265,-0.3885809353\H,1.0341654913,-0.1058341207,-0.361606985\Cl,-1.9
057922709,2.0155626872,1.8224091943\\Version=EM64L-G09RevA.02\State=2-
A\HF=-921.3653885\S2=0.82074\S2-1=0.\S2A=0.753144\RMSD=4.293e-09\RMSF=
1.079e-05\Dipole=1.964897,-1.0359679,-0.2004381\Quadrupole=5.778632,-5
.5500451,-0.2285869,3.3955851,1.8765343,2.5936106\PG=C01 [X(C8H10Cl1O2
)]\\@

para

1\1\GINC-ABE0551\FOpt\UmPWPW91\6-31+G(d,p)\C8H10Cl1O2(2)\ACROFT\29-Dec
-2010\0\\#P MPWPW91/6-31+G(d,p) OPT(EstmFC) int=ultrafine IOp(3/76=057
2004280)\\C10H14O4.Cl coniferyl model para complex full OHdb in\\0,2\C
,0.0705165599,0.0955857899,0.0357594912\C,-0.0941713917,0.1132443604,1
.5412801393\C,1.1727041008,-0.0287177703,2.2724100647\C,1.2486682086,-
0.7517702022,3.4144849378\C,0.1255879896,-1.4772417644,3.9025056854\C,
-1.0669798717,-1.4800067952,3.1771248596\C,-1.1765511652,-0.754768574,
2.028304649\H,-2.0969037825,-0.7572136471,1.4648025306\H,-1.8884474648
,-2.0769947083,3.5422711437\O,0.2284231616,-2.1812584336,5.0348716381\
H,1.1159407893,-2.0681686816,5.3823210266\O,2.3414896561,-0.9001039553
,4.1968367843\C,3.5032710061,-0.1878489992,3.8544291374\H,4.2346155693
,-0.4116441969,4.6221270766\H,3.8847580382,-0.5097338145,2.8859196191\
H,3.3087625565,0.8836964459,3.8350177581\H,2.0215849004,0.5174126227,1
.8943409922\H,0.411579439,-0.8914259072,-0.2736425088\H,-0.8734538164,
0.3119138291,-0.4567816978\H,0.8007969578,0.8354498606,-0.2809001376\C
l,-0.7105526001,1.9286411712,1.8965802356\\Version=EM64L-G09RevA.02\St
ate=2-A\HF=-921.3653152\S2=0.817806\S2-1=0.\S2A=0.752809\RMSD=6.731e-0
9\RMSF=6.629e-06\Dipole=1.3408223,-0.6990934,-0.128228\Quadrupole=6.38
1805,-7.6154521,1.2336471,3.5980567,3.348085,1.4912731\PG=C01 [X(C8H10
Cl1O2)]\\@