Supplementary Material for Organic & Biomolecular Chemistry
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Supplementary data

Structures of all Optimized Stationary Points

1a \(\text{B3LYP/aug-cc-pVDZ} \)
1\1\GINC-PIRX\FOpt\UB3LYP\Aug-CC-pVDZ\C4H8Cl1(2)\BERND\19-Feb-2002\0\)
\#P B3LYP/AUG-CC-PVDZ OPT=TIGHT GEOM=CHECK GUESS=READ
INT=ULTRAFINE\Be
D001 with INT=ULTRAFINE\0,2\C,0.1063168353,0.305635652,-0.55028519350\C,0.1053918322,-1.157928312,-0.5404967856\C,1.3891660007,0.9682412707\C,-1.0097749893\H,-0.7786669558,0.7139466375,-1.0458653312\H,1.5565759958,0.73320935,-2.0741823113,2.0566771132,-0.8980161267\H,2.2479630589,0.603209853,-0.4322274841\Cl,-0.2178927161,0.8953362005,1.2758334388\C,-1.1453929968,-1.9640369835,-0.4846598299\H,1.0592759673,-1.6602096716,-0.361576248,0.9445927668,-0.9623579485\H,-1.4450387789,-2.1570821331,0.5624777398\H,-1.9862773313,-1.4465445235,-0.9648597597\H,3.75661,\S2=0.755661\S2-1=0.\S2A=0.750023\RMSD=7.998e-09\RMSF=8.394e-07\Dipole=0.129
3808,-0.5162435,-0.9249031\PG=C01 [X(C4H8Cl1)]

5 \(\text{B3LYP/aug-cc-pVDZ} \)
1\1\GINC-PIRX\FTS\UB3LYP\Aug-CC-pVDZ\C4H8Cl1(2)\BERND\14-Feb-2002\0\)
\#P B3LYP/AUG-CC-PVDZ OPT=(TS,NOEIGEN,CALCFCC,TIGHT)
GEOM=CHECK INT=ULTRA FINE\Be
D002 go on opt TS\0,2\C,-0.0071294262,0.6852939478,-0.8518735166\C,-0.0064320999,-0.6850764349,-0.858350665\C,1.2114277223,1.5424613492,-0.9458743507\H,-0.9737985869,1.196302198,-0.8545139946\H,1.2261811513,2.0706296165,-1.9136120504\H,1.2009464274,2.3094808941,-0.1597014523\H,2.1309854694,0.9522910993,-0.851715477\Cl,0.0134960969,-0.0002164557,1.7082390061\C,-1.2262245286,-1.5422240545,-0.9270064731\H,0.9601731835,-1.196083693,-0.8700910453\H,-1.2562649575,-2.070148229,-1.8945235273\H,-1.2033271377,-2.3094418815,-0.1412907997\H,-2.441787317,-0.9520791025,-0.8181841239\Version=x86-Linux-G98RevA.7\HF=-617.4312473\S2=0.752677\S2-1=0.\S2A=0.750005\RMSD=5.733e-09\RMSF=3.351e-07\Dipole=-0.0127325,0.0002041,-1.6116141\PG=C01 [X(C4H8Cl1)]
# P3LYP/AUG-CC-PVDZ OPT=(TS,CALCFCC,TIGHT,MAXCYCLE=20)
INT=ULTRAFINE

BeD013 opt=ts INT=ULTRAFINE for TSr1, Start from Be035\0,2\C,0.169235
1105,-0.6674627758-,0.3062828933\C,0.1663992362-,0.6666801318,1.188958
2784\C,1.5756135185-,0.6700454615-,0.9130394153\H,-0.3846397064,-1.539
6166997,-0.6874053715\H,2.1230255883,-1.5492518121,-0.5423370571,1.1,5
284841422,-0.7215298368,-2.008056350,7,2.1255779034,0.2323709552,-0.6
185199636\Cl,-0.7732688294,0.7599737218,-0.9969173641\C,-0.4265872052,
0.3758380091,2.0715553141\H,0.620771710111,-0.5343762325,1.6373908716,\H,
-0.198562056,0.1653981548,3.1240881\H,-0.0518912552,1.3840254445,1.82
92608037\H,-1.5251600281,0.4326289155,1.9660264545,\Version=x86-Linux-
G98RevA.7,\HF=-617.4269386,\S2=0.754273,\S2-
1=0.,\S2A=0.750013,\RMSD=9.425e
-09,\RMSF=2.408e-07,\Dipole=0.4337282,-0.5756197,0.3799538,\PG=C01 [X(C4H
8Cl1)]\ @

7 (B3LYP/aug-cc-pVDZ)
1\1\GINC-XINYE\FTS\UB3LYP\Aug-CC-pVDZ\C4H8Cl1(2)\BERND\04-
Mar-2002\0\0\0\0\0\0\0\0\0\1
# P B3LYP/AUG-CC-PVDZ OPT=(TS,CALCFCC,TIGHT,MAXCYCLE=20)
INT=ULTRAFINE

BeD015 opt=ts INT=ULTRAFINE for TSr2 B3LYP/aug-cc-pVDZ with Be037
Star
\structure\0,2\C,-0.078363036,-0.2946028067,-0.2999556864\C,-0.079312
202,-0.2943111386,1.1928844687\C,1.3114692432,-0.2990888484,-0.9398902
896\H,-0.6541156699,-1.1521616872,-0.6882939478,1.8551122242,-1.20245
54975,-0.6279780317,1.232961555,-0.3043845844,-2.033421451,1.88470
81094,0.5823308363,-0.6261969953,1.2202524652,1.625342188,-0.9204
80229\C,0.6910019223,-1.3244973331,1.9524993919,\H,-0.7244193289,0.408
208635,1.7158501477,0.4016908032,-1.3284567719,3.0108368001,\H,0.5285
282427,-2.3416009231,1.5522890286\H,1.7816267933,-1.1495609659,1.91062
70479\Version=x86-Linux-G98RevA.7,\HF=-617.4278661,\S2=0.754186,\S2-
1=0.,\S2A=0.750013,\RMSD=9.186e-09,\RMSF=3.849e-07,\Dipole=0.5458122,-
0.762521
6,0.3726464,\PG=C01 [X(C4H8Cl1)]\ @

1b (B3LYP/aug-cc-pVDZ)
1\1\GINC-EDDY\FOpt\UB3LYP\Aug-CC-pVDZ\C4H8Cl1(2)\BERND\02-
Mar-2002\0\0\0\0\0\0\0\0\0\1
# P B3LYP/AUG-CC-PVDZ OPT=(TIGHT,MAXCYCLE=20)
INT=ULTRAFINE

BeD011 opt=ts INT=ULTRAFINE for "cis"-Minimum, B3LYP/aug-cc-pVDZ start with Be033-s
structure\0,2\C,-0.1087531458,-0.6766990349,-0.304058274\C,-0.11021056
8,-0.6752689913,1.1587919809,\C,1.2361867184,-0.6541322415,-1.008717058
5,\H,-0.7673060597,-1.4511690976,-0.7068597399,\H,1.7964236194,1.564602
1148,-0.7453894418,\H,1.1007163389,-0.6307648165,-2.0956863432\H,1.8303
8 (B3LYP/aug-cc-pVDZ)
1 \ 1 \ GINC-Z4 \ FTS \ UB3LYP \ Aug-CC-pVDZ \ C4H8Cl1(2) \ BERND \ 11-Mar-2002 \ 0 \ \ #P
B3LYP/AUG-CC-PVDZ OPT=(TS,NOEIGEN,CALCFCC,TIGHT)
INT=ULTRAFINE \ \ BeD019:
  opt=ts TSc calcfc ULTRAFINE B3LYP/aug-cc-pVDZ start from Be040b-resul
t"\  0.2 \ Cl,-0.447830637,0.4037392276,-1.6917672856 \ C,-0.4549160656,0.43
89285857,0.9653321378 \ C,0.8729479606,0.4389262527,0.6138485544 \ C,-1.27
95619585,-0.7331409524,1.3829572083 \ H,-0.9533615766,1.409715394,0.9955
20372 \ C,1.7962103668,-0.733146353,0.5687965751 \ H,1.3210564905,1.409710
6356,0.3934787006 \ H,-0.7861979914,-1.6930459169,1.1983486026 \ H,-2.2408
591893,-0.7245179865,0.8516448637 \ H,-1.5067956954,-0.6586261437,2.4595
47955 \ H,1.2761244904,-1.6930459169,0.6524841734 \ H,2.3687319459,-0.7245
429134,-0.3685429733 \ H,2.5263405354,-0.6586162124,1.3919553067 \ Versio
n=SGI-G98RevA.6 \ HF=-617.4294737 \ S2=0.752678 \ S2-1=0.7500 \ RMSD=
2.843e-09 \ RMSF=2.090e-07 \ Dipole=0.4220817,-0.2300537,1.5944929 \ PG=C01
[X(C4H8Cl1)] \ \ @