

Supplementary Material for Organic & Biomolecular Chemistry

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## Supplementary data

### Structures of all Optimized Stationary Points

#### 1a (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,0.1063168353,0.3005635652,-0.5502851935
\C,0.1053918322,-1.157928312,-0.5404967856\C,1.3891660007,0.9682412707
,-1.0097749893\H,-0.7786669558,0.7139466375,-1.0458655312\H,1.55655799
58,0.73320935,-2.0718423113\H,1.327841017,2.0566771132,-0.8980161267\H
,2.2479630589,0.603209853,-0.4322274841\Cl,-0.2178927161,0.8953362005,
1.2758334388\C,-1.1453929968,-1.9640369835,-0.4846598299\H,1.059275967
3,-1.6602096716,-0.361576248\H,-1.0103688266,-2.9449592768,-0.96235794
85\H,-1.4450387789,-2.1570821331,0.5624777398\H,-1.9862773313,-1.44654
45235,-0.9684597597\ \Version=x86-Linux-G98RevA.7\HF=-617.4354366\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 (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,CALCFC,TIGHT)
GEOM=CHECK INT=ULTRA
FINE\ \BeD002 go on opt TS\ \0,2\C,-0.0071294262,0.6852939478,-0.8581736
166\C,-0.0064320999,-0.6850764349,-0.858350665\C,1.2114277223,1.542461
3492,-0.9458743507\H,-0.9737985869,1.196302198,-0.8545139946\H,1.22618
11513,2.0706296165,-1.9136120504\H,1.2009464274,2.3094808941,-0.159701
4523\H,2.1309854694,0.9522910993,-0.851715477\Cl,0.0134960692,-0.00021
64557,1.7082390061\C,-1.2262245286,-1.5422240545,-0.9270064731\H,0.960
1731835,-1.196083693,-0.8700910453\H,-1.2562649575,-2.070148229,-1.894
5235273\H,-1.2033271377,-2.3094418815,-0.1412907997\H,-2.1441787317,-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)]\ \@
```

#### 6 (B3LYP/aug-cc-pVDZ)

```
1\1\GINC-XINYE\FTS\UB3LYP\Aug-CC-pVDZ\C4H8Cl1(2)\BERND\02-
Mar-2002\0\
```

```
#P B3LYP/AUG-CC-PVDZ OPT=(TS,CALCF,C,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\H,1.5
284841422,-0.7215298368,-2.0080563507\H,2.1255779034,0.2323709552,-0.6
185199636\Cl,-0.7732688294,0.7599737218,-0.9969173641\C,-0.4265872052,
0.3758380091,2.0715553141\H,0.6207717011,-1.5534762325,1.6373908716\H,
-0.1985622056,0.1653981548,3.1240881\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\
```

```
#P B3LYP/AUG-CC-PVDZ OPT=(TS,CALCF,C,TIGHT,MAXCYCLE=20)
INT=ULTRAFINE\
```

```
BeD015 opt=ts INT=ULTRAFINE for TSr2 B3LYP/aug-cc-pVDZ with Be037
Star
```

```
tstructure\ \0,2\C,-0.078360336,-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\H,1.855112242,-1.20245
54975,-0.6279780317\H,1.232961555,-0.3043845844,-2.033421451\H,1.88470
81094,0.5823308363,-0.6261969953\Cl,-1.0220524652,1.1625342188,-0.9204
082298\C,0.6910019223,-1.3244973331,1.9524993919\H,-0.7244119328,0.408
208635,1.7158501477\H,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\
```

```
#P B3LYP/AUG-CC-PVDZ OPT=(TIGHT,MAXCYCLE=20)
```

```
INT=ULTRAFINE\ \BeD011 opt
```

```
INT=ULTRAFINE for "cis"-Minimum, B3LYP/aug-cc-pVDZ start with Be033-s
tructure\ \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
```

499646,0.2190371088,-0.7149364126\Cl,-1.0666718968,0.9196257896,-0.877  
 1349253\C,0.9176679249,0.029539143,1.9777337036\H,-1.0159677719,-1.033  
 7635396,1.6498357741\H,0.7588090426,-0.1455413104,3.0485373708\H,1.941  
 6747672,-0.288981184,1.7262454448\H,0.8793767668,1.1215132793,1.807044  
 966\ \ Version=x86-Linux-G98RevA.7\ HF=-617.4338852\ S2=0.755768\ S2-  
 1=0.\ S  
 2A=0.750023\ RMSD=8.440e-09\ RMSF=1.354e-06\ Dipole=0.6480024,-  
 0.7295618,  
 0.481643\ PG=C01 [X(C4H8Cl1)]\ \@

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,CALCFC,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,-1.6930489248,0.6524841734\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.\ S2A=0.750005\ RMSD=  
 2.843e-09\ RMSF=2.090e-07\ Dipole=0.4220817,-0.2300537,1.5944929\ PG=C01  
 [X(C4H8Cl1)]\ \@