From: Tom Rescigno <tnrescigno@lbl.gov>
Subject: sample files
Date: June 24, 2013 2:12:51 PM PDT
To: Robert Lucchese <lucchese@mail.chem.tamu.edu>
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http://eriemills.com/tnr/tnr.html

$groups
numel=(30,2,2,0,0,0,1,0,0,0,0)
numel=(30,1,2,1,0,0,0,1,0,0,0) spin=(0,1,1,0,0,0,0,1,1,1,1)
numel=(30,2,1,1,0,0,0,0,1,0,0) spin=(0,0,1,0,0,0,0,0,1,1,1)
numel=(30,1,2,0,1,0,0,0,0,1,0) spin=(0,1,1,1,0,0,0,0,0,1,1)
numel=(30,2,1,0,0,1,0,0,0,1,0) spin=(0,0,1,1,1,0,0,0,0,1,1)
numel=(30,1,2,1,1,0,0,0,0,0,0)
numel=(30,2,1,1,0,1,0,0,0,0,0)
$end
$route
2s+1=1
scf=(pulay,convergence=5) hf
maxsiz=2000000
guess=(chk,alter)
properties=(e1,e2)
kohn=(nsmall=20,ncsfs=68,symmetry=4,nroots=4,
symroot=(1,3,2,4),symnl2=(16,8,8,16),symncsfs=(1,1,1,2),
hqq,freeze,energy=(.40425,.441,.4777,.551,.643,.735,.9187,1.1025))
ci=(nroots=5)
drt=(nsym=8,ngroups=11,nrefs=7)
print=(guess=all,ci=no)
geom=(coord,inau,nocrowd)
phase=(save,nroots=4,compress=(1,3,4,5),prtci)
sym=norotate
$end

$alter
19,20
$end

$drt
1typ1;1 1typ1;6 1typ1;1 1typ1;6 1typ1;1 1typ1;6
1typ1;3 1typ1;4 1typ1;7 1typ1;8 1typ1;1 1typ1;6
1typ1;1 1typ1;7 1typ1;8 1typ2;3 1typ3;4
1typ4;6 1typ5;8 1typ6;7
16typ7;1 2typ11;2 6typ11;3 6typ11;4 2typ11;5
16typ10;6 8typ9;7 8typ8;8
na=17 nb=1 ns=1
$end

$nonstd
1//1,2,3,4;
8//6,22;
9//2,30,40,50;
20//1;
$end

$title
Cl2 Mclean
$end

$geom

cl1(basis=mclean) 0.0 0.0   1.879
cl2(basis=mclean) 0.0 0.0 -1.879
zqc(basis=center) 0. 0. 0.
$end

$mclean cl
/ mclean clorine atom centered
 type=s
105818.8   .000743
15872.0   .005753
 3619.7   .029676
 1030.8   .118010
  339.91   .365230
  124.538   .581221
 type=s
  124.538   .137548
   49.514   .622881
   20.806   .290143
 type=s
6.4648   1.0000000
 type=s
2.5254   1.0000000
 type=s
.5378   1.0000000
 type=s
.1935   1.0000000
 type=p
  589.78   .002760
  139.85   .021536
   44.795   .095916
   16.612   .262315
    6.5995 .726811
 type=p
    6.5995 -1.564924
    2.7141 1.495778
 type=p
   .9528   1.0000000
 type=p
   .3580   1.000000
 type=p
   .1250   1.00000
 type=p
   .05   1.0
 type=d
   .7   1.
 type=d
   .25   1.
$end

$center zq
/diffuse s and p
type=s
.1 1.
type=s
.04 1.
type=s
.016 1.
type=p
.025 1.
type=p
.0125 1.
type=p
.006 1.
$end

$sgroups
numel=(30,2,2,0,0,0,1,0)
numel=(30,1,2,1,0,0,1,0) symtp=(0,0,0,8,8,8,8,8) spin=(0,1,1,0,0,0,1,1)

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numel=(30,2,1,1,0,0,1,0) symtp=(0,0,0,7,7,7,7,7) spin=(0,0,1,0,0,0,1,1)
numel=(30,1,2,0,1,0,1,0) symtp=(0,0,0,0,6,6,6,6) spin=(0,1,1,1,0,0,1,1)
numel=(30,2,1,0,0,1,1,0) symtp=(0,0,0,0,0,6,6,6) spin=(0,0,1,1,1,0,1,1)
$end
$groups
numel=(30,2,2,0,0,0,1,0,0,0)
numel=(30,1,2,1,0,0,0,1,0,0,0) spin=(0,1,1,0,0,0,0,1,1,1,1)
numel=(30,2,1,1,0,0,0,0,1,0,0) spin=(0,0,1,0,0,0,0,0,1,1,1)
numel=(30,1,2,0,1,0,0,0,0,1,0) spin=(0,1,1,1,0,0,0,0,0,1,1)
numel=(30,2,1,0,0,1,0,0,0,1,0) spin=(0,0,1,1,1,0,0,0,0,1,1)
$end
$route
2s+1=1
scf=(pulay,convergence=5) hf
maxsiz=2000000
guess=(chk,alter)
properties=(e1,e2)
kohn=(nsmall=20,ncsfs=68,symmetry=4,nroots=4,
symroot=(1,3,2,4),symnl2=(16,8,8,16),symncsfs=(1,1,1,2))
sdrt=(nsym=8,ngroups=8,nrefs=5) ci=(nroots=5)
drt=(nsym=8,ngroups=11,nrefs=5)
print=(guess=all,ci=no)
geom=(coord,inau,nocrowd)
phase=(save,nroots=4,compress=(1,3,4,5),prtci)
sym=norotate
$end

$alter
19,20
$end

$sdrt
1typ1;1 1typ1;6 1typ1;1 1typ1;6 1typ1;1 1typ1;6
1typ1;3 1typ1;4 1typ1;7 1typ1;8 1typ1;1 1typ1;6
1typ1;1 1typ1;7 1typ1;8 1typ2;3 1typ3;4
1typ4;6 1typ5;8 1typ6;7
1typ7;1 63typ8;1
na=17 nb=1 ns=1
$end

$drt
1typ1;1 1typ1;6 1typ1;1 1typ1;6 1typ1;1 1typ1;6
1typ1;3 1typ1;4 1typ1;7 1typ1;8 1typ1;1 1typ1;6
1typ1;1 1typ1;7 1typ1;8 1typ2;3 1typ3;4
1typ4;6 1typ5;8 1typ6;7
1typ7;1 1typ8;8 1typ9;7 1typ10;6 60typ11;1
na=17 nb=1 ns=1
$end

$nonstd
1//1,2;
3//2,12,30;
19//2;
2//6;
6//4;
4//1;
8//7,8,11,19,22;
9//2,8,211,26,90,221;
8//6,22;
9//2,8,222,27,90;
20//1;
$end


$title
Cl2 Mclean
$end

$geom
cl1(basis=mclean) 0.0 0.0   1.879
```

```
cl2(basis=mclean) 0.0 0.0  -1.879
zqc(basis=center)  0.  0.  0.
$end

$mclean cl
/ mclean clorine atom centered
 type=s
105818.8    .000743
15872.0    .005753
 3619.7    .029676
 1030.8    .118010
  339.91   .365230
  124.538  .581221
 type=s
  124.538  .137548
   49.514  .622881
   20.806  .290143
 type=s
6.4648    1.0000000
 type=s
2.5254    1.0000000
 type=s
.5378     1.0000000
 type=s
.1935     1.0000000
 type=p
 589.78   .002760
 139.85   .021536
  44.795  .095916
  16.612  .262315
   6.5995 .726811
 type=p
   6.5995 -1.564924
   2.7141 1.495778
 type=p
  .9528   1.0000000
 type=p
  .3580   1.000000
 type=p
  .1250   1.00000
 type=p
  .05     1.0
 type=d
  .7      1.
 type=d
  .25     1.
$end

$center zq
/diffuse s and p
type=s
.1 1.
type=s
.04 1.
type=s
.016 1.
type=p
.025 1.
type=p
.0125 1.
type=p
.006 1.
$end
```