The Journal of Physical Chemistry, submitted, 2010

For the Mark A. Ratner Festschrift

Continuous Symmetry Measures of Density Maps

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Supplementary Information

1. Coordinates of the original clusters and their distorted versions

For each cluster the coordinates of the original symmetric one and the distorted one(s) are given. The distorted specific coordinates are in ***bold italics***.

Table 1. $^{1}Cu_3^{+}$ cluster (D_{3h} point group of symmetry)

$S_0(C_3) = 0$, D_{3h} symmetry

0.000000	1.257365	0.000000
1.088910	-0.628682	0.000000
-1.088910	-0.628682	0.000000

$S_0(C_3) = 0$, C_{2v} symmetry

0.000000	1.112205	0.000000

1.399876 -0.556102 0.000000

-1.399876 -0.556102 0.000000

Table 2. $^{1}Cu_4$ cluster (D_{2h} point group of symmetry)

$S_0(C_i) = 0$, D_{2h} symmetry

0.000000 0.000000 2.113461

0.000000 1.128507 0.000000

0.000000 -1.128507 0.000000

0.000000 0.000000 -2.113461

$S_0(C_i) = 0.1948$, C_s symmetry

0.000000 0.000000 2.113461

0.250000 0.971400 0.000000

0.000000 -1.128507 0.000000

0.000000 0.000000 -2.113461

$S_0(C_i) = 0.7902$, C_s symmetry

0.000000 0.000000 2.113461

0.500000 0.814300 0.000000

0.000000 -1.128507 0.000000

0.000000 0.000000 -2.113461

$S_0(C_i) = 1.7826$, C_s symmetry

0.000000 0.000000 2.113461

0.750000 0.657100 0.000000

0.000000 -1.128507 0.000000

0.000000 0.000000 -2.113461

$S_0(C_i) = 3.1396$, C_s symmetry

0.000000 0.000000 2.113461

1.000000 0.500000 0.000000

0.000000 -1.128507 0.000000

0.000000 0.000000 -2.113461

Table 3. $^{1}Cu_4$ clusters (T_d point group of symmetry)

$S_0(C_s) = 0$, T_d symmetry

0.849289 0.849289 0.849289

-0.849289 -0.849289 0.849289

-0.849289 0.849289 -0.849289

0.849289 -0.849289 -0.849289

$S_0(C_s) = 1.0183$, C_2 symmetry

0.849289 0.849289 ***1.449289***

-0.849289 -0.849289 0.849289

-0.849289 0.849289 -0.849289

0.849289 -0.849289 ***-1.449289***

Table 4. $^{2}Cu_7$ clusters (D_{5h} point group of symmetry)

$S_0(C_5) = 0$, D_{5h} symmetry

0.000000 0.000000 1.257813

0.000000 2.074779 0.000000

1.973232 0.641142 0.000000

-1.973232 0.641142 0.000000

1.219525 -1.678532 0.000000

-1.219525 -1.678532 0.000000

0.000000 0.000000 -1.257813

$S_0(C_5) = 0.3021$, C_s symmetry

0.000000 0.000000 1.257813

0.000000 2.074779 0.000000

1.973232 0.641142 0.000000

-1.973232 0.641142 0.000000

1.219525 -1.678532 0.000000
-1.219525 ***-2.078532*** 0.000000
0.000000 0.000000 -1.257813

Table 5. $^{1}Cu_6$ cluster (D_{4h} point group of symmetry)

$S_0(S_4) = 0$, D_{4h} symmetry
0.000000 1.669096 0.000000
1.669096 0.000000 0.000000
0.000000 -1.669096 0.000000
-1.669096 0.000000 0.000000
0.000000 0.000000 1.808642
0.000000 0.000000 -1.808642

$S_0(S_4) = 1.0183$, C_{2v} symmetry
0.000000 ***2.669096*** 0.000000
1.669096 0.000000 0.000000
0.000000 -1.669096 0.000000
-1.669096 0.000000 0.000000
0.000000 0.000000 1.808642
0.000000 0.000000 -1.808642

2. Input file for the ORCA program for producing electron density maps

An example is given for the non distorted $^{2}Cu_7$ cluster in D_{5h} point group symmetry.

```
! RHF SV
% output
 PrintLevel Normal
 Print[ P_Mos] 1
```

```
 XYZfile true
 end
%scf
 TolE 1e-14
 TolRMSP 1e-14
 TolMaxP 1e-14
 TolErr 1e-14
 TolG 3e-9
 TolX 1e-9
 ConvCheckMode=0
 MaxIter 250
 end
%plots
 dim1  500
 dim2  500
 dim3  500
 min1  -8.45
 max1   8.45
 min2  -8.45
 max2   8.45
 min3  -8.45
 max3   8.45
 Format gOpenMol_bin
 ElDens("Density-Cu7-d5h.plt");
 end
* xyz 0 2
Cu     0.000000    0.000000    1.257813
Cu     0.000000    2.074779    0.000000
Cu     1.973232    0.641142    0.000000
Cu    -1.973232    0.641142    0.000000
Cu     1.219525   -1.678532    0.000000
```

Cu -1.219525 -1.678532 0.000000

Cu 0.000000 0.000000 -1.257813

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