On QM/MM and MO/MO cluster calculations of all-atom ADPs for molecules in crystal structures

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1. Supplementary information

1.1. Input files for the program BAERLAUCH

BAERLAUCH-input file for L-alanine with point-charges from B3LYP/3-21G:

```
!This is a comment
title L-Ala at 23K
!Unit cell information
cell     5.9279   12.2597    5.7939   90.0000   90.0000   90.0000
!Space group information; spaces are needed
spgr P 21 21 21
! Number of atoms in the asymmetric unit
! The quantum-chemical calculation requires the presence of a full molecule
mols 13 0 0 0 0 0 0 0 0 0
!
!Sys specifies which part of the asymetric unit will be the system investigated
!E.g. if there are two molecules in the asymmetric unit, one of the two can be studied.
sys 13
!1 creates gaussian output, 2 adf output, 2 does not work yet
output 1
!Element, Integer number, UFF-Force-field name, B3LYP/3-21G point-charge, fractional coordinates
atom  O 1  O_R       -0.635202    0.7268  0.0838  0.6243
atom  O 2  O_R       -0.624844    0.4409  0.1841  0.7612
atom  N 1  N_3       -0.582791    0.6472  0.1375  0.1829
atom  C 1  C_R        0.590107    0.5542  0.1408  0.5999
atom  C 2  C_3        0.161208    0.4662  0.1610  0.3546
atom  C 3  C_3       -0.382163    0.2599  0.0907  0.3034
atom  H 1  H_HB       0.348504    0.7048  0.0591  0.1954
atom  H 2  H_HB       0.357570    0.7808  0.1890  0.2076
atom  H 3  H_HB       0.357229    0.5912  0.1493  0.0177
atom  H 4  H_         0.049463    0.4212  0.2479  0.3406
atom  H 5  H_         0.077246    0.1953  0.1123  0.1330
atom  H 6  H_         0.157056    0.1274  0.1057  0.4303
atom  H 7  H_         0.126617    0.3034  0.0042  0.3050
end
```

BAERLAUCH-input file for L-cysteine with point charges from HF/3-21G:

```
title L-Cys at 30K
cell  8.1435 11.9365 5.4158 90.000 90.000 90.000
spgr P 21 21 21
mols 14 0 0 0 0 0 0 0 0 0
sys 14
output 1
atom  S 1  S_2       -0.367106    0.4146  1.0226  0.6096
atom  O 1  O_R       -0.757923    0.5132  0.7590  0.2702
atom  O 2  O_R       -0.797463    0.7217  0.8798  0.2934
atom  N 1  N_3       -0.561524    0.7380  0.8750  0.7855
atom  C 1  C_R       -0.351957    0.4355  0.8835  0.7433
atom  C 2  C_3        0.194410    0.5920  0.8225  0.6681
atom  C 3  C_3        0.845477    0.6106  0.8197  0.3862
atom  H 1  H_         0.295356    0.3467  0.9877  0.3970
atom  H 2  H_HB       0.363588    0.8442  0.8363  0.7317
atom  H 3  H_HB       0.380758    0.7453  0.9583  0.7422
atom  H 4  H_HB       0.367539    0.7258  0.8736  0.9734
```

```
atom  H 5  H_         0.170928    0.4330  0.8951  0.9428
atom  H 6  H_         0.185798    0.3298  0.8342  0.6850
atom  H 7  H_         0.032119    0.5831  0.7356  0.7349
end
```

BAERLAUCH-input file for L-threonine with point charges from HF/3-21G:

```
title L-THR at 19K
cell  13.626   7.618   5.110  90.000  90.000  90.000
spgr P 21 21 21
mols 17 0 0 0 0 0 0 0 0 0
sys 17
output 1
atom  O 1  O_R      -0.786541    0.4405  0.7101  0.0255
atom  O 2  O_R      -0.770061    0.4945  0.7031  0.4405
atom  O 3  O_3      -0.783461    0.7631  0.6481 -0.0280
atom  N 1  N_3      -0.514018    0.5876  0.5082 -0.1486
atom  C 1  C_3      -0.085807    0.6010  0.6013  0.1053
atom  C 2  C_R       0.863257    0.5028  0.6778  0.1986
atom  C 3  C_3       0.531197    0.6806  0.7417  0.0718
atom  C 4  C_3      -0.602330    0.7067  0.8349  0.3256
atom  H 1  H_HB      0.364915    0.5486  0.3961 -0.1115
atom  H 2  H_HB      0.348698    0.6549  0.4847 -0.2300
atom  H 3  H_HB      0.349854    0.5419  0.5689 -0.2792
atom  H 4  H_        0.113705    0.6272  0.5007  0.2434
atom  H 5  H_HB      0.467228    0.8214  0.7188 -0.0390
atom  H 6  H_       -0.004217    0.6547  0.8372 -0.0733
atom  H 7  H_        0.136213    0.7741  0.9083  0.2890
atom  H 8  H_        0.175975    0.7250  0.7397  0.4774
atom  H 9  H_        0.195393    0.6456  0.9182  0.3864
end
```

Example program run:

```
birger@rottnest:~/L-Alanine_23K_X> baerlauch ala

 PROGRAM BAERLAUCH FOR GENERATING INPUT FOR QM/MM CLUSTER CALCULATIONS

The (default) values for the origin in fractional coordinates are:
 0.500000 0.500000 0.500000
 Change the origin with -o x y z.

The (default) value for the translations to be included is:
 20.000000 AA
 Change the translations included with -t t_in_x t_in_y t_in_z.

The (default) value for the distances to be included is is:
 3.750000 AA
 Change the distances to be included with -d value.


Input file successfully read.
Please input the method for your calculation.
The default is Hartree-Fock [HF].
```

```
Using default value [HF]

Please input the basis set for your calculation.
The default is the Pople basis [6-31G(d,p)].

Using default value [6-31G(d,p)]

Please input the memory required your calculation.
The default is [2048MB].

Using default value [2048MB]

Please input the number of processors.
The default is [nproc=4].
8
Please input the temperature of your X-ray diffraction experiment.
Default (press Enter) is 100 K.
19
Do you want to embed charges for the ONIOM calculation [Y/N]?
Default (press Enter) is Y.

Please input force field type (e.g. UFF, DREIDING or AMBER)!
Default (press Enter) is Universal Force Field UFF

Using default value [UFF]

Thank you for using the program.
```

1.1.1. Details on invariom refinement for L-*alanine*

```
  Weighting: 1/sigma^2, reflections with I > 3sigma I included, 83 parameters.

  Number of data              =   2535
  Rejected based on OBS       =     16
  Rejected based on SIGOBS    =    207
  Rejected based on SINTHL    =      0
  Total number of rejections  =    207
  Included in the refinement  =   2328

                     Residuals after cycle  11

  R{ F } =     0.0187     Rall{ F } =     0.0222     Rw{ F } =     0.0171
  R{F^2} =     0.0260     Rall{F^2} =     0.0265     Rw{F^2} =     0.0340
   GOFw  =     1.2620           GOF =     1.2620     Nref/Nv =    28.0482

           Differences of Mean-Squares Displacement Amplitudes (DMSDA)
                  (1.E4 A**2) along interatomic vectors (*bonds)

 ATOM-->  ATOM    /  DIST  DMSDA ATOM    /  DIST  DMSDA ATOM    /  DIST  DMSDA
 O(1)     C(1)    * 1.2476     0
 O(2)     C(1)    * 1.2670     3
 N(1)     C(2)      1.4912     1
 C(1)     C(2)    * 1.5341     1
 C(2)     C(3)    * 1.5267    -2
```

```
Atom  Invariom            Model compound
========================================
O(1): O1.5c[1.5o1c] from: acetic acid anion
O(2): O1.5c[1.5o1c] from: acetic acid anion
N(1): N1c1h1h1h from: methylammonium
C(1): C1.5o1.5o1c from: acetic acid anion
C(2): C1n1c1c1h from: 2-aminopropane
C(3): C1c1h1h1h from: ethane
H(1): H1n[1c1h1h] from: methylammonium
H(2): H1n[1c1h1h] from: methylammonium
H(3): H1n[1c1h1h] from: methylammonium
H(4): H1c[1n1c1c] from: 2-aminopropane
H(5): H1c[1c1h1h] from: ethane
H(6): H1c[1c1h1h] from: ethane
H(7): H1c[1c1h1h] from: ethane
```

1.1.2. Details on invariom refinement for L-*cysteine*

```
  Weighting: 1/sigma^2, reflections with I > 3sigma I included, 92 parameters.

  Number of data              =   1516
  Rejected based on OBS       =      2
  Rejected based on SIGOBS    =     44
  Rejected based on SINTHL    =      0
  Total number of rejections  =     44
  Included in the refinement  =   1472

                     Residuals after cycle  11

  R{ F } =     0.0118     Rall{ F } =     0.0125     Rw{ F } =     0.0145
  R{F^2} =     0.0209     Rall{F^2} =     0.0210     Rw{F^2} =     0.0288
   GOFw  =     0.8974           GOF =     0.8974     Nref/Nv =    16.0000

          Differences of Mean-Squares Displacement Amplitudes (DMSDA)
                 (1.E4 A**2) along interatomic vectors (*bonds)

 ATOM-->  ATOM    /  DIST  DMSDA ATOM    /  DIST  DMSDA ATOM    /  DIST  DMSDA
 O(1)     C(3)    * 1.2443    -3
 O(2)     C(3)    * 1.2596     1
 N(1)     C(2)      1.4862     6
 C(1)     C(2)    * 1.5230     8
 C(2)     C(3)    * 1.5344    -1

Atom  Invariom            Model compound
================================================
S(1): S1c1h               from: methanethiol
O(1): O1.5c[1.5o1c]       from: acetic acid anion
O(2): O1.5c[1.5o1c]       from: acetic acid anion
N(1): N1c1h1h1h           from: methylammonium
C(1): C1s[1h]1c1h1h       from:  ethanthiol
C(2): C1n1c1c1h           from: 2-aminopropane
C(3): C1.5o1.5o1c         from: acetic acid anion
H(1): H1s[1c]             from: methanethiol
H(5): H1n[1c1h1h]         from: methylammonium
H(6): H1n[1c1h1h]         from: methylammonium
```

```
H(7): H1n[1c1h1h]         from: methylammonium
H(2): H1c[1s1c1h]         from:  ethanthiol
H(3): H1c[1s1c1h]         from:  ethanthiol
H(4): H1c[1n1c1c]         from: 2-aminopropane
```

1.1.3. Details on invariom refinement for L*-threonine*

```
  Weighting: 1/sigma^2, reflections with I > 3sigma I included, 109 parameters.

  Number of data              =   5988
  Rejected based on OBS       =      0
  Rejected based on SIGOBS    =   1501
  Rejected based on SINTHL    =      0
  Total number of rejections  =   1501
  Included in the refinement  =   4487

                     Residuals after cycle  11

  R{ F } =     0.0207     Rall{ F } =     0.0439     Rw{ F } =     0.0207
  R{F^2} =     0.0359     Rall{F^2} =     0.0432     Rw{F^2} =     0.0405
   GOFw  =     1.5199           GOF =     1.5199     Nref/Nv =    41.1651

           Differences of Mean-Squares Displacement Amplitudes (DMSDA)
                  (1.E4 A**2) along interatomic vectors (*bonds)

 ATOM-->  ATOM    /  DIST  DMSDA ATOM    /  DIST  DMSDA ATOM    /  DIST  DMSDA
 O(1)     C(2)    * 1.2504    -1
 O(2)     C(2)    * 1.2561     1
 O(3)     C(3)    * 1.4255     2
 N(1)     C(1)      1.4900     0
 C(1)     C(2)    * 1.5357     1 C(3)    * 1.5326    -1
 C(3)     C(4)    * 1.5205     2

Atom  Invariom            Model compound
================================================
O(1): O1.5c[1.5o1c]       from: acetic acid anion
O(2): O1.5c[1.5o1c]       from: acetic acid anion
O(3): O1c1h               from: methanol
N(1): N1c1h1h1h           from: methylammonium
C(1): C1n1c1c1h           from: 2-aminopropane
C(2): C1.5o1.5o1c         from: acetic acid anion
C(3): C1o1c1c1h           from: 2-propanol
C(4): C1c1h1h1h           from: ethane
H(1): H1n[1c1h1h]         from: methylammonium
H(2): H1n[1c1h1h]         from: methylammonium
H(3): H1n[1c1h1h]         from: methylammonium
H(4): H1c[1n1c1c]         from: 2-aminopropane
H(5): H1o[1c]             from: methanol
H(6): H1c[1o1c1c]         from: 2-propanol
H(7): H1c[1c1h1h]         from: ethane
H(8): H1c[1c1h1h]         from: ethane
H(9): H1c[1c1h1h]         from: ethane
```