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ORTHONZERO: One Atomic Coordinate of Orthonormal Atomic Coordinate Dataset is Translated to Origin and the Others in the Dataset are Also Done Accordingly

Young-Soo Park[a], Won-Sik Han[b], Tae-Jin Kim[b], Sang Ook Kang[b] and Il-Hwan Suh[b]

[a]LinuxBay Co. 111 HO, Hongin Officetel Bongmyeong-dong, Yuseong-gu, Daejeon 305-710, Korea
[b]Department of Material Chemistry, Korea University, Jochiwon 339-700, Korea

1. The Crystallographic Problem and Method of Solution

Computer programs for the molecular orbital calculation such as DMol3[1,2] and LUMMOX[3] utilize only the orthonormal coordinates. Therefore in order to apply MO calculation to any molecule elucidated by X-ray crystallography, the atomic coordinates must be transformed into orthonormal ones. The program ORTHON[4] can be used for this purpose and how to orthonormalize the atomic coordinates is described in the cited paper.

The program LOMMOX additionally requires that one of atoms in a molecule with the orthonormal coordinates must be translated to origin of the orthonormal coordinate system, which means all other atoms in the molecule are also translated accordingly. The program ORTHONZERO can take care of the translating role. What the ORTHONZERO does is simply to subtract from all atomic coordinates the x, y, z values of the atom to be placed at origin.

2. How to Run the Program

What must be kept in mind is that the input data for the ORTHONZERO is the output of the program ORTHON. So before running the ORTHONZERO, you must run the ORTHON first and then if you have its output file, you are ready to run the ORTHONZERO. Both ORTHON and ORTHONZERO are offered freely by authors.

Follow the following procedure to run the ORTHONZERO:

2.1. Enter orthonzero.exe and then it requires a name of input data file

2.2. Write a name of input data (= the output file of the program ORTHON) and enter, then it requires a name of output file

2.3. Write a name of output file and enter

2.4. It requires the name of an atom to be placed at origin (0 0 0). This program distinguishes between the lower and upper cases.

2.5. Write the name of an atom you want and enter, then the output file with the name given by you is created immediately in the current folder.

3. Software and Hardware Environment

The ORTHONZERO is compiled with Interl Fortran 8.0 complier and will run on windows pc such as winxp/win2003/win2000.

The source program and the manual for ORTHONZERO are shown below.

5. Key words

Molecular orbitals (MO), LUMMOX

References

1) Delley, B., *J. Chem. Phys.*, **92**, 508 (1990).
2) Delley, B., *J. Chem. Phys.*, **113**, 7756 (2000).
3) Akinobu Shiga, LUMMOX, (private communication).
4) Suh, I.-H., Park, Y.-S. and Kim, J.-G., ORTHON: transformation from triclinic axes and atomic coordinates to orthonormal ones, *J. Appl. Crst.*, **33**, 994 (2000).

```
      Program ORTHONZERO
      character input*80,output*80,aname*80
      character atom(20000)*4,tmp*80, am*4
      real x(20000),y(20000),z(20000),ax,ay,az
      real n2,n3,vab,vbc,vac
      real a,b,c,al,be,ga
      integer m, cnt, n
      integer ipos, jpos, kpos, lpos
     PRINT*,'            '
     PRINT*,'            ************************************************'
     PRINT*,'            * Program ORTHONZERO by Young-Soo Park *'
     PRINT*,'            * *'
     PRINT*,'            * ihsuh@korea.ac.kr *'
     PRINT*,'            ************************************************'
     PRINT*,'  '
     PRINT*,'     This program brings one of atoms in input data'
     PRINT*,'     to origin (0 0 0) and the coordinates of the rest'
     PRINT*,'     atoms are also transformed accordingly.'
     PRINT*,'     The input data must be an output of the program'
     PRINT*,'     ORTHON which is available from ihsuh@korea.ac.kr.'
     PRINT*,'     An atom to be placed at origin must be chosen by '
     PRINT*,'     you.'
     print*,''
     print*,' (1) The ORTHONZERO requires the name of input data,'
     print*,'     which must be an output of the program ORTHON.'
     print*,''
     print*,' (2) The ORTHONZERO requires the name of output data.'
     print*,''
     print*,' (3) The ORTHONZERO requires the name of an atom to be '
     print*,'     placed at origin (0 0 0). This program distinguishes'
     print*,'     between the lower and upper cases.'
     print*,''
      type 300
300    format(' [Enter Input file...?] : ',$)
      accept 555,input
      print*,' '
      type 310
310    format(' [Enter Output file..?] : ',$)
      accept 555,output
      print*,' '
      type 320
320    format(' [Enter Origin Atom Name..?] : ',$)
      accept 555,aname
555    format(a80)
      open(unit=11,file=input)
      open(unit=12,file=output)
```

```
      cnt=0
      ipos=0
      jpos=0
      kpos=0
     do 20 m=0,20000
     read(11,FMT=*,END=888) tmp
     if(tmp.eq.'Orthonormal') then
      cnt=1
      kpos=m+5
      read(11,FMT=*,END=888) tmp
      read(11,FMT=*,END=888) tmp
      exit
     endif
20    continue
222   do 30 n=0,kpos-8
      read(11,FMT=333,END=280) atom(n), x(n), y(n),z(n)
      if(atom(n).eq.aname) then
        cnt=2
        am=atom(n)
        ax=x(n)
        ay=y(n)
        az=z(n)
      endif
30    continue
280   rewind(11)
     do 40 m=0,kpos
      read(11,FMT=111) tmp
      write(12,FMT=111) tmp
40    continue
     do 50 m=1,kpos-8
      write(12,FMT=333) atom(m), x(m)-ax, y(m)-ay, z(m)-az
50   continue
333  format(a4,1x,3(f12.5))
111  format(a80)
888  if(cnt.eq.0) then
        close(11)
        close(12)
        print*,' '
        stop ' !! Invalid input file format !!'
      endif
      if(cnt.eq.1) then
        close(11)
        close(12)
        print*,' '
        stop '     !! Can not find origin atom name !!'
      endif
```

```
close(11)
close(12)
print*,' '
stop '     !! Program terminated successfully !!'
end.
```

Manual for ORTHONZERO

Program ORTHONZERO by Young-Soo Park
The program is available from:ihsuh@korea.ac.kr

This program brings one of atoms in input data to origin (0 0 0) and the coordinates of the rest atoms are also transformed accordingly.

The input data must be the output of the program ORTHON. The ORTHON is available from:ihsuh@korea.ac.kr. An atom to be placed at origin must be chosen by you.

(1) The ORTHONZERO requires the name of input data, which must be an output of the program ORTHON.

An example of the input data (an output of the program ORTHON):

a=15.00048 b=15.00048 c=15.00048
alpha=78.89523 beta=78.89523 gamma=78.89523

P	0.83563	0.75000	0.66436
N	0.83206	0.66793	0.75000
C1	0.86059	0.70605	0.55539
C2	0.94236	0.72508	0.50901
C3	0.80220	0.65462	0.52095
C4	0.78483	0.67788	0.43055
C5	0.74128	0.62225	0.39567
C6	0.71374	0.54397	0.45084
C7	0.72925	0.52216	0.53925
C8	0.77329	0.57667	0.57510
C9	0.98562	0.69943	0.41763
C10	1.01173	0.76647	0.34402
C11	1.05028	0.74356	0.26007
C12	1.06333	0.65501	0.24648
C13	1.03955	0.58628	0.31750
C14	0.99906	0.60909	0.40385

Orthonormal Data :
a=1.00000 b=1.00000 c=1.00000
alpha=90.00000 beta=90.00000 gamma=90.00000

P	16.62114	12.61903	9.65076
N	16.57791	11.61457	10.89480
C1	16.55375	11.71306	8.06781
C2	17.70132	11.88292	7.39408
C3	15.42978	10.87416	7.56753
C4	14.97524	11.00164	6.25434
C5	14.06048	10.09987	5.74766
C6	13.58059	9.07877	6.54908
C7	14.00567	8.96790	7.83336
C8	14.92735	9.85549	8.35413
C9	18.01212	11.28813	6.06666
C10	18.38480	12.09995	4.99737
C11	18.65434	11.56316	3.77788
C12	18.55500	10.22743	3.58047
C13	18.20490	9.38458	4.61213
C14	17.91291	9.92560	5.86648

(2) The ORTHONZERO requires a name for output data.

(3) The ORTHONZERO requires the name of an atom to be placed at the origin (0 0 0). This program distinguishes between the lower and upper cases.

In an example of an output data given below, P (phosphorus) is placed at the origin (0 0 0):

a=15.00048 b=15.00048 c=15.00048
alpha=78.89523 beta=78.89523 gamma=78.89523

P	0.83563	0.75000	0.66436
N	0.83206	0.66793	0.75000
C1	0.86059	0.70605	0.55539
C2	0.94236	0.72508	0.50901

C3	0.80220	0.65462	0.52095
C4	0.78483	0.67788	0.43055
C5	0.74128	0.62225	0.39567
C6	0.71374	0.54397	0.45084
C7	0.72925	0.52216	0.53925
C8	0.77329	0.57667	0.57510
C9	0.98562	0.69943	0.41763
C10	1.01173	0.76647	0.34402
C11	1.05028	0.74356	0.26007
C12	1.06333	0.65501	0.24648
C13	1.03955	0.58628	0.31750
C14	0.99906	0.60909	0.40385

Orthonormal Data :

a=1.00000 b=1.00000 c=1.00000

alpha=90.00000 beta=90.00000 gamma=90.00000

P	0.00000	0.00000	0.00000
N	−0.04323	−1.00446	1.24404
C1	−0.06739	−0.90597	−1.58295
C2	1.08018	−0.73611	−2.25668
C3	−1.19136	−1.74487	−2.08323
C4	−1.64590	−1.61739	−3.39642
C5	−2.56066	−2.51916	−3.90310
C6	−3.04055	−3.54026	−3.10168
C7	−2.61547	−3.65113	−1.81740
C8	−1.69379	−2.76354	−1.29663
C9	1.39098	−1.33090	−3.58410
C10	1.76366	−0.51908	−4.65339
C11	2.03320	−1.05587	−5.87288
C12	1.93386	−2.39160	−6.07029
C13	1.58376	−3.23445	−5.03863
C14	1.29177	−2.69343	−3.78428