symmetry

MDPI

Supplementary material

Supplementary material for "The eigenproblem translated for alignment of molecules"

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Received: date; Accepted: date; Published: date

Summary: The datafile for CID 444173, the Matlab program implementing the Cartesian alignment of the molecule are given here.

1. The input data

The used part of the Conformer3D_CID_444173.sdf file (as downloaded from PubChem database) is:

```
444173
  -OEChem-07121900543D

 20 20  0     1  0  0  0  0  0999 V2000
    0.7428   -1.4498   -0.0709 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1425    1.1688    1.3882 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.1461    1.0581   -1.4377 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7540   -0.3648   -0.3408 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.7344   -0.2934    0.3835 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7774    1.0064    0.0187 C   0  0  1  0  0  0  0  0  0  0  0  0
    0.7504    0.9905   -0.0675 C   0  0  1  0  0  0  0  0  0  0  0  0
   -1.3475   -0.3060   -0.5320 C   0  0  1  0  0  0  0  0  0  0  0  0
    1.3187   -0.2968    0.5474 C   0  0  1  0  0  0  0  0  0  0  0  0
   -0.6710   -1.5130    0.1111 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1917    1.8546   -0.5382 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1810    1.8612    0.4392 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1666   -0.3445   -1.6130 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.1212   -0.3396    1.6245 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9099   -1.5934    1.1787 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0338   -2.4357   -0.3549 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1129    1.1270    1.4362 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.9648    0.1979   -1.8521 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1405    0.4212   -0.7630 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.9381    0.1134   -0.4754 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  9  1  0  0  0  0
  1 10  1  0  0  0  0
  2  6  1  0  0  0  0
  2 17  1  0  0  0  0
  3  7  1  0  0  0  0
  3 18  1  0  0  0  0
  4  8  1  0  0  0  0
```

```
  4 19  1  0  0  0  0
  5  9  1  0  0  0  0
  5 20  1  0  0  0  0
  6  7  1  0  0  0  0
  6  8  1  0  0  0  0
  6 11  1  0  0  0  0
  7  9  1  0  0  0  0
  7 12  1  0  0  0  0
  8 10  1  0  0  0  0
  8 13  1  0  0  0  0
  9 14  1  0  0  0  0
 10 15  1  0  0  0  0
 10 16  1  0  0  0  0
M  END
```

2. The Cartesian coordinates file

From the Conformer3D_CID_444173.sdf data file was generated the s444173xyz.txt file containing only the Cartesian coordinates. The content of the s444173xyz.txt file is (tab delimited):

```
0.7428 -1.4498   -0.0709
-1.1425   1.1688 1.3882
1.1461 1.0581 -1.4377
-2.754 -0.3648   -0.3408
2.7344 -0.2934   0.3835
-0.7774   1.0064 0.0187
0.7504 0.9905 -0.0675
-1.3475   -0.306 -0.532
1.3187 -0.2968   0.5474
-0.671 -1.513 0.1111
```

3. The Matlab program for Cartesian alignment of the molecule

The program implementing the minimizing (minimizing and maximizing are interchangeable) of the magnitude of the imaginary roots is:

```
mol = dlmread('s444173x.txt','\t');
[NumRows,NumCols] = size(mol);
for i=1:NumRows
    for j=1:NumRows
       d_x(i,j)=mol(i,1)-mol(j,1);         d_y(i,j)=mol(i,2)-mol(j,2);
d_z(i,j)=mol(i,3)-mol(j,3);

d_r(i,j)=sqrt(d_x(i,j)*d_x(i,j)+d_y(i,j)*d_y(i,j)+d_z(i,j)*d_z(i,j));
    end
end
fr1 = @(t)sum_eig_rotat_x(d_x,d_y,t);
rot_1 = fminbnd(fr1,0,pi);
d1x = rotat_x(d_x,d_y,rot_1); d1y = rotat_y(d_x,d_y,rot_1); d1z = d_z;

fr2 = @(u)sum_eig_rotat_x(d1x,d1z,u);
rot_2 = fminbnd(fr2,0,pi);

d2x = rotat_x(d1x,d1z,rot_2); d2y = d1y; d2z = rotat_y(d1x,d1z,rot_2);

fr3 = @(v)sum_eig_rotat_x(d2y,d2z,v);
rot_3 = fminbnd(fr3,0,pi);
```

```
d3x = d2x; d3y = rotat_x(d2y,d2z,rot_3); d3z = rotat_y(d2y,d2z,rot_3);

display(s2a(eig(d_x)));
display(s2a(eig(d_y)));
display(s2a(eig(d_z)));

display(rot_1);
display(rot_2);
display(rot_3);

display(s2a(eig(d3x)));
display(s2a(eig(d3y)));
display(s2a(eig(d3z)));

function f = rotat_x(u,v,t)
    f = u*cos(t) - v*sin(t);
end

function f = rotat_y(u,v,t)
    f = u*sin(t) + v*cos(t);
end

function f = sum_eig_rotat_x(u,v,t)
    f = -s2a(eig(rotat_x(u,v,t)));
end

function f = s2a(u)
    NumRows = size(u);
    f = 0;
    for i=1:NumRows
       f = f + u(i)*u(i);
    end
end
```

It should be noted that the program uses four functions ('rotat_x', 'rotat_y', 'sum_eig_rotat_x ' and 's2a') which can be defined in external files for Matlab versions below R2016b or inside of the script file (at the end of it) for Matlab versions staring from R2016b.

5. The program output

The above given source code (named 'eigen.m') provides the initial magnitudes of the roots (before alignment), the rotations required, and the resulted magnitudes after alignment minimizing the magnitude of the roots for Ox coordinates first and Oy coordinates second.

For convenience, the results are:

```
 >> eigen
ans =
 -468.0896

ans =
 -185.4316

ans =
  -97.2449
```

```
rot_1 =
    1.5708

rot_2 =
    1.5708

rot_3 =
    1.5708

ans =
  -97.2449

ans =
 -185.4316

ans =
 -468.0896
```

Please note that 1.5708 is about $\pi/2$ - the molecule were already aligned in the Conformer3D_CID_444173.sdf file by maximizing the magnitude of the Ox Cartesian coordinate axis roots, second maximized magnitude being Oy while the final result maximizes the magnitude by Oz axis, and then maximizes on Oy axis.