**TITLE:**

Vibrational Spectra of an N719-chromophore/titania interface from empirical-potential molecular-dynamics simulation, solvated by a room-temperature ionic liquid

**AUTHORS AND AFFILIATIONS:**

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Supporting Information

To run the DL-POLY program, three input files are needed - namely CONTROL, FIELD and CONFIG. The contents of these files are given below. To run MPI-enabled DL-POLY on terminal, please use **nohup mpirun -np #** **DL\_POLY.X &** on a terminal.

# is the number of processors required.

1. CONTROL file

DL\_POLY DSSC with RTIL bmim[I]

##l\_scr

##nfold 1 1 1

# Define the State Point

temperature 3.00E+02

pressure 1.00E-03

#pressure is in kbar

#temperature is in kelvin

# Simulation Timesteps and Equilibration

steps 200000000 #total number of steps e.g 120000

equilibration 100000 #equilibrate for this many

scale 5 #rescale atomic velocities every m steps

variable timestep 1.000E-03 #in ps

#mult 1 #multi-step interval

restart

# Ensemble Options

ensemble nvt hoover 1.0

# thermostat barostat relaxation time in ps

# Specify Cut-Offs

cutoff 1.000E+01 #angstrom forces cutoff e.g 9A cutoff

rvdw 0.9000E+01 #short range cutoff (A)

delr 5.0000E-01 #verlet neighbour list shell (A)

# RDF Options

print 1000 #print system data every n timesteps

rdf 100000 #calculate rdf every n steps

zden

 #calculate zdensity profile

print rdf #print radial dist. function

job time 259200 #wall time

close time 3.0000E+02 #job closure time

# Forces Options

spme precision 1.0000E-06

#smooth particle mesh ewald precision

# Statistics Options

stats 1000000 #colect stats every n timesteps

stack 1000000 #rolling average stack

shake 0.0001 #shake tolerance (default 1.000E-8)

steps 200000000

#no vdw

#no elec

# Trajectory Controls

trajectory 1 100000 2

#start at 1, 1 between,

#keytraj -- file output type 1 = coord only, 2=coord +vel, 3=coord+vel+force

finish

1. FIELD file

bmim [NTf2] with anatase (MA) surface and N719 dye (GAFF & AMBER99) + two surface protons

UNITS kcal

molecules 6

Titanium

 nummols 96

 atoms 1

 Ti 47.8670 2.196 1 0 1 1 TI Ti und

FINISH

Oxygen

 nummols 190

 atoms 1

 O 15.9994 -1.098 1 0 1 1 O O und

FINISH

N719

 nummols 1

 atoms 57

O1 16.0000 -0.6164 1 0 1 1 O1 O und

HO 1.0080 0.4536 1 0 1 2 HO H und

C 12.0010 0.5874 1 0 1 3 C C und

OH 16.0000 -0.6964 1 0 1 4 OH O und

CA 12.0010 0.0398 1 0 1 5 CA C und

CA 12.0010 -0.1964 1 0 1 6 CA C und

HA 1.0080 0.1036 1 0 1 7 HA H und

CA 12.0010 0.1136 1 0 1 8 CA C und

H6 1.0080 0.1036 1 0 1 9 H6 H und

NC 14.0100 -0.6664 1 0 1 10 NC N und

CA 12.0010 0.2636 1 0 1 11 CA C und

CA 12.0010 -0.1964 1 0 1 12 CA C und

HA 1.0080 0.1036 1 0 1 13 HA H und

CA 12.0010 0.2636 1 0 1 14 CA C und

CA 12.0010 -0.1964 1 0 1 15 CA C und

HA 1.0080 0.1036 1 0 1 16 HA H und

CA 12.0010 -0.2254 1 0 1 17 CA C und

C 12.0010 0.9326 1 0 1 18 C C und

O2 16.0000 -0.9464 1 0 1 19 O2 O und

O2 16.0000 -0.9464 1 0 1 20 O2 O und

CA 12.0010 -0.1964 1 0 1 21 CA C und

HA 1.0080 0.1036 1 0 1 22 HA H und

CA 12.0010 0.1136 1 0 1 23 CA C und

H6 1.0080 0.1036 1 0 1 24 H6 H und

NC 14.0100 -0.6664 1 0 1 25 NC N und

Ru 101.07 2.0000 1 0 1 26 Ru Ru und

N2 14.0100 -0.0994 1 0 1 27 N2 N und

CZ 12.0010 0.8866 1 0 1 28 CZ C und

SH 32.0600 0.0736 1 0 1 29 SH S und

N2 14.0100 -0.0994 1 0 1 30 N2 N und

CZ 12.0010 0.8866 1 0 1 31 CZ C und

SH 32.0600 0.0736 1 0 1 32 SH S und

NC 14.0100 -0.6664 1 0 1 33 NC N und

CA 12.0010 0.1136 1 0 1 34 CA C und

H6 1.0080 0.1036 1 0 1 35 H6 H und

CA 12.0010 -0.1964 1 0 1 36 CA C und

HA 1.0080 0.1036 1 0 1 37 HA H und

CA 12.0010 -0.2254 1 0 1 38 CA C und

C 12.0010 0.9326 1 0 1 39 C C und

O2 16.0000 -0.9464 1 0 1 40 O2 O und

HO 1.0080 0.4536 1 0 1 41 HO H und

O2 16.0000 -0.9464 1 0 1 42 O2 O und

CA 12.0010 -0.1964 1 0 1 43 CA C und

HA 1.0080 0.1036 1 0 1 44 HA H und

CA 12.0010 0.2636 1 0 1 45 CA C und

CA 12.0010 0.2636 1 0 1 46 CA C und

CA 12.0010 -0.1964 1 0 1 47 CA C und

HA 1.0080 0.1036 1 0 1 48 HA H und

CA 12.0010 0.0398 1 0 1 49 CA C und

C 12.0010 0.5874 1 0 1 50 C C und

O1 16.0000 -0.6164 1 0 1 51 O1 O und

OH 16.0000 -0.6964 1 0 1 52 OH O und

CA 12.0010 -0.1964 1 0 1 53 CA C und

HA 1.0080 0.1036 1 0 1 54 HA H und

CA 12.0010 0.1136 1 0 1 55 CA C und

H6 1.0080 0.1036 1 0 1 56 H6 H und

NC 14.0100 -0.6664 1 0 1 57 NC N und

 bonds 62

harm 1 3 1140 1.229 1

harm 3 5 938 1.409 2

harm 3 4 900 1.364 3

harm 5 6 938 1.4 4

harm 5 12 938 1.4 5

harm 6 8 938 1.4 6

harm 8 10 880 1.34 7

harm 10 11 880 1.34 8

harm 11 12 938 1.4 9

harm 11 14 938 1.4 10

harm 14 15 938 1.4 11

harm 14 25 880 1.34 12

harm 15 17 938 1.4 13

harm 17 21 938 1.4 14

harm 17 18 938 1.409 15

harm 18 19 1312 1.25 16

harm 18 20 1312 1.25 17

harm 21 23 938 1.4 18

harm 23 25 880 1.34 19

harm 27 28 923.036 1.359 20

harm 28 29 727.824 1.642 21

harm 30 31 923.036 1.359 22

harm 31 32 727.824 1.642 23

harm 33 34 880 1.34 24

harm 33 45 880 1.34 25

harm 34 36 938 1.4 26

harm 36 38 938 1.4 27

harm 38 43 938 1.4 28

harm 38 39 938 1.409 29

harm 39 42 1312 1.25 30

harm 39 40 1312 1.25 31

harm 43 45 938 1.4 32

harm 45 46 938 1.4 33

harm 46 47 938 1.4 34

harm 46 57 880 1.34 35

harm 47 49 938 1.4 36

harm 49 53 938 1.4 37

harm 49 50 938 1.409 38

harm 50 52 900 1.364 39

harm 50 51 1140 1.229 40

harm 53 55 938 1.4 41

harm 55 57 880 1.34 42

harm 26 10 360 1.96 43

harm 26 25 360 1.96 44

harm 26 27 360 1.96 45

harm 26 30 360 1.96 46

harm 26 33 360 1.96 47

harm 26 57 360 1.96 48

harm 2 4 1106 0.96 49

harm 6 7 734 1.08 50

harm 8 9 734 1.08 51

harm 12 13 734 1.08 52

harm 15 16 734 1.08 53

harm 21 22 734 1.08 54

harm 23 24 734 1.08 55

harm 34 35 734 1.08 56

harm 36 37 734 1.08 57

harm 41 52 1106 0.96 58

harm 43 44 734 1.08 59

harm 47 48 734 1.08 60

harm 53 54 734 1.08 61

harm 55 56 734 1.08 62

 angles 98

harm 4 3 5 140 120.00 1

harm 1 3 5 140 120.00 2

harm 1 3 4 160 120.00 3

harm 2 4 3 100 113.00 4

harm 6 5 12 126 120.00 5

harm 3 5 6 126 120.00 6

harm 3 5 12 126 120.00 7

harm 7 6 8 100 120.00 8

harm 5 6 7 100 120.00 9

harm 5 6 8 126 120.00 10

harm 9 8 10 140 120.00 11

harm 6 8 9 100 120.00 12

harm 6 8 10 140 120.00 13

harm 8 10 11 140 120.00 14

harm 12 11 14 126 120.00 15

harm 10 11 12 140 120.00 16

harm 10 11 14 140 120.00 17

harm 5 12 13 100 120.00 18

harm 5 12 11 126 120.00 19

harm 11 12 13 100 120.00 20

harm 15 14 25 140 120.00 21

harm 11 14 15 126 120.00 22

harm 11 14 25 140 120.00 23

harm 16 15 17 100 120.00 24

harm 14 15 16 100 120.00 25

harm 14 15 17 126 120.00 26

harm 15 17 21 126 120.00 27

harm 15 17 18 126 120.00 28

harm 18 17 21 126 120.00 29

harm 17 18 19 140 120.00 30

harm 17 18 20 140 120.00 31

harm 19 18 20 160 126.00 32

harm 22 21 23 100 120.00 33

harm 17 21 22 100 120.00 34

harm 17 21 23 126 120.00 35

harm 24 23 25 140 120.00 36

harm 21 23 24 100 120.00 37

harm 21 23 25 140 120.00 38

harm 14 25 23 140 120.00 39

harm 27 28 29 34.902 180.00 40

harm 30 31 32 34.902 180.00 41

harm 34 33 45 140 120.00 42

harm 35 34 36 100 120.00 43

harm 33 34 35 140 120.00 44

harm 33 34 36 140 120.00 45

harm 37 36 38 100 120.00 46

harm 34 36 37 100 120.00 47

harm 34 36 38 126 120.00 48

harm 36 38 43 126 120.00 49

harm 36 38 39 126 120.00 50

harm 39 38 43 126 120.00 51

harm 38 39 42 140 120.00 52

harm 38 39 40 140 120.00 53

harm 40 39 42 160 126.00 54

harm 44 43 45 100 120.00 55

harm 38 43 44 100 120.00 56

harm 38 43 45 126 120.00 57

harm 43 45 46 126 120.00 58

harm 33 45 43 140 120.00 59

harm 33 45 46 140 120.00 60

harm 47 46 57 140 120.00 61

harm 45 46 47 126 120.00 62

harm 45 46 57 140 120.00 63

harm 48 47 49 100 120.00 64

harm 46 47 48 100 120.00 65

harm 46 47 49 126 120.00 66

harm 47 49 53 126 120.00 67

harm 47 49 50 126 120.00 68

harm 50 49 53 126 120.00 69

harm 49 50 52 140 120.00 70

harm 49 50 51 140 120.00 71

harm 51 50 52 160 120.00 72

harm 41 52 50 100 113.00 73

harm 54 53 55 100 120.00 74

harm 49 53 54 100 120.00 75

harm 49 53 55 126 120.00 76

harm 56 55 57 140 120.00 77

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harm 46 57 55 140 120.00 80

harm 33 26 30 32.8 180.00 81

harm 25 26 27 32.8 180.00 82

harm 57 26 10 32.8 180.00 83

harm 33 26 10 104.8 91.00 84

harm 33 26 25 104.8 91.00 85

harm 57 26 25 104.8 91.00 87

harm 10 26 30 104.8 91.00 88

harm 25 26 30 104.8 91.00 89

harm 33 26 27 104.8 91.00 90

harm 37 26 27 104.8 91.00 91

harm 26 10 8 133.8 123.00 92

harm 26 10 11 133.8 123.00 93

harm 26 25 23 133.8 123.00 94

harm 26 25 14 133.8 123.00 95

harm 26 33 45 133.8 123.00 96

harm 26 33 34 133.8 123.00 97

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 dihedrals 176

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cos 26 25 23 24 0.00 180 1.00 0.00 0.00

cos 26 57 55 56 0.00 180 1.00 0.00 0.00

cos 26 57 46 45 0.00 180 1.00 0.00 0.00

cos 26 33 45 46 0.00 180 1.00 0.00 0.00

cos 26 33 34 35 0.00 180 1.00 0.00 0.00

cos 10 26 27 28 0.00 90 1.00 0.00 0.00

cos 10 26 25 14 0.00 180 1.00 0.00 0.00

cos 10 26 25 23 0.00 180 1.00 0.00 0.00

cos 10 26 30 31 0.00 90 1.00 0.00 0.00

cos 10 26 33 45 0.00 90 1.00 0.00 0.00

cos 10 26 33 34 0.00 90 1.00 0.00 0.00

cos 10 26 57 55 0.00 90 1.00 0.00 0.00

cos 10 26 57 46 0.00 90 1.00 0.00 0.00

cos 25 26 27 28 0.00 180 1.00 0.00 0.00

cos 25 26 30 31 0.00 90 1.00 0.00 0.00

cos 25 26 10 11 0.00 180 1.00 0.00 0.00

cos 25 26 10 8 0.00 180 1.00 0.00 0.00

cos 25 26 57 46 0.00 90 1.00 0.00 0.00

cos 25 26 57 55 0.00 90 1.00 0.00 0.00

cos 25 26 33 34 0.00 90 1.00 0.00 0.00

cos 25 26 33 45 0.00 90 1.00 0.00 0.00

cos 33 26 30 31 0.00 180 1.00 0.00 0.00

cos 33 26 27 28 0.00 90 1.00 0.00 0.00

cos 33 26 57 55 0.00 180 1.00 0.00 0.00

cos 33 26 57 46 0.00 180 1.00 0.00 0.00

cos 33 26 10 8 0.00 90 1.00 0.00 0.00

cos 33 26 10 11 0.00 90 1.00 0.00 0.00

cos 33 26 25 14 0.00 90 1.00 0.00 0.00

cos 33 26 25 23 0.00 90 1.00 0.00 0.00

cos 57 26 30 31 0.00 180 1.00 0.00 0.00

cos 57 26 27 28 0.00 90 1.00 0.00 0.00

cos 57 26 10 8 0.00 90 1.00 0.00 0.00

cos 57 26 10 11 0.00 90 1.00 0.00 0.00

cos 57 26 25 23 0.00 90 1.00 0.00 0.00

cos 57 26 25 14 0.00 90 1.00 0.00 0.00

cos 57 26 33 45 0.00 180 1.00 0.00 0.00

cos 57 26 33 34 0.00 180 1.00 0.00 0.00

cos 30 26 27 28 0.00 90 1.00 0.00 0.00

cos 30 26 25 14 0.00 90 1.00 0.00 0.00

cos 30 26 25 23 0.00 90 1.00 0.00 0.00

cos 30 26 33 34 0.00 180 1.00 0.00 0.00

cos 30 26 33 45 0.00 180 1.00 0.00 0.00

cos 30 26 57 55 0.00 180 1.00 0.00 0.00

cos 30 26 57 46 0.00 180 1.00 0.00 0.00

cos 30 26 10 11 0.00 90 1.00 0.00 0.00

cos 30 26 10 8 0.00 90 1.00 0.00 0.00

cos 27 26 30 31 0.00 90 1.00 0.00 0.00

cos 27 26 25 14 0.00 180 1.00 0.00 0.00

cos 27 26 25 23 0.00 180 1.00 0.00 0.00

cos 27 26 33 34 0.00 90 1.00 0.00 0.00

cos 27 26 33 45 0.00 90 1.00 0.00 0.00

cos 27 26 57 55 0.00 90 1.00 0.00 0.00

cos 27 26 57 46 0.00 90 1.00 0.00 0.00

cos 27 26 10 8 0.00 180 1.00 0.00 0.00

cos 27 26 10 11 0.00 180 1.00 0.00 0.00

INVERSIONS 24

plan 5 6 10 26 40.000000 0.00000000

plan 34 36 33 26 40.000000 0.00000000

plan 6 5 8 3 40.000000 0.00000000

plan 36 34 38 35 40.000000 0.00000000

plan 8 6 11 7 40.000000 0.00000000

plan 38 36 43 37 40.000000 0.00000000

plan 11 8 12 14 40.000000 0.00000000

plan 43 38 48 46 40.000000 0.00000000

plan 12 11 10 9 40.000000 0.00000000

plan 48 43 33 39 40.000000 0.00000000

plan 10 12 5 13 40.000000 0.00000000

plan 33 48 34 44 40.000000 0.00000000

plan 14 15 11 25 40.000000 0.00000000

plan 46 47 43 57 40.000000 0.00000000

plan 15 14 17 16 40.000000 0.00000000

plan 47 46 49 48 40.000000 0.00000000

plan 17 15 21 18 40.000000 0.00000000

plan 49 47 53 50 40.000000 0.00000000

plan 21 17 23 22 40.000000 0.00000000

plan 53 49 55 54 40.000000 0.00000000

plan 23 21 25 24 40.000000 0.00000000

plan 55 53 57 56 40.000000 0.00000000

plan 25 23 14 26 40.000000 0.00000000

plan 57 55 46 26 40.000000 0.00000000

FINISH

Protons

 nummols 2

 atoms 2

 HS 1.0080 0.2992 1 0 1 1 HS H und

 OS 15.9994 -1.098 1 0 1 2 OS O und

constraints 1

1 2 0.96

FINISH

bmim

 nummols 12

 atoms 25

 N\* 14.01 -0.764 1 0 1 1 N\* N und

 c2 12.001 0.65 1 0 1 2 c2 C und

 N\* 14.01 -0.764 1 0 1 3 N\* N und

 c2 12.001 0.2 1 0 1 4 c2 C und

 c2 12.001 0.2 1 0 1 5 c2 C und

 CT 12.001 0.274 1 0 1 6 CT C und

 H5 1.008 0.15 1 0 1 7 H5 H und

 CT 12.001 0.354 1 0 1 8 CT C und

 H4 1.008 0.15 1 0 1 9 H4 H und

 H4 1.008 0.15 1 0 1 10 H4 H und

 H1 1.008 0.08 1 0 1 11 H1 H und

 H1 1.008 0.08 1 0 1 12 H1 H und

 H1 1.008 0.08 1 0 1 13 H1 H und

 2C 12.001 -0.16 1 0 1 14 2C C und

 H1 1.008 0.08 1 0 1 15 H1 H und

 H1 1.008 0.08 1 0 1 16 H1 H und

 2C 12.001 -0.16 1 0 1 17 2C C und

 HC 1.008 0.08 1 0 1 18 HC H und

 HC 1.008 0.08 1 0 1 19 HC H und

 CT 12.001 -0.24 1 0 1 20 CT C und

 HC 1.008 0.08 1 0 1 21 HC H und

 HC 1.008 0.08 1 0 1 22 HC H und

 HC 1.008 0.08 1 0 1 23 HC H und

 HC 1.008 0.08 1 0 1 24 HC H und

 HC 1.008 0.08 1 0 1 25 HC H und

 bonds 25

harm 1 6 674 1.475 1

harm 1 5 613.69 1.385 2

harm 1 2 700.762 1.345 3

harm 2 3 700.83 1.345 4

harm 3 8 674 1.475 5

harm 3 4 613.706 1.385 6

harm 4 5 736.148 1.33 7

harm 8 14 620 1.526 8

harm 14 17 620 1.526 9

harm 17 20 620 1.526 10

harm 2 7 659 1.09 11

harm 4 9 659 1.09 12

harm 5 10 659 1.09 13

harm 6 11 659 1.09 14

harm 6 12 659 1.09 15

harm 6 13 659 1.09 16

harm 8 15 659 1.09 17

harm 8 16 659 1.09 18

harm 14 18 659 1.09 19

harm 14 19 659 1.09 20

harm 17 21 659 1.09 21

harm 17 22 659 1.09 22

harm 20 23 659 1.09 23

harm 20 24 659 1.09 24

harm 20 25 659 1.09 25

 angles 45

harm 5 1 6 112.296 119.881 1

harm 2 1 6 130.654 118.729 2

harm 2 1 5 164.162 121.39 3

harm 1 2 7 130.654 121.401 4

harm 1 2 3 182.526 117.199 5

harm 3 2 7 130.66 121.4 6

harm 4 3 8 112.298 119.881 7

harm 2 3 8 130.66 118.729 8

harm 2 3 4 164.17 121.39 9

harm 5 4 9 146.448 125.52 10

harm 3 4 9 112.298 114.326 11

harm 3 4 5 179.96 120.154 12

harm 4 5 10 146.448 125.52 13

harm 1 5 10 112.296 114.326 14

harm 1 5 4 179.958 120.154 15

harm 11 6 12 70 109.5 16

harm 11 6 13 70 109.5 17

harm 12 6 13 70 109.5 18

harm 1 6 11 100 109.5 19

harm 1 6 12 100 109.5 20

harm 1 6 13 100 109.5 21

harm 15 8 16 70 109.5 22

harm 14 8 15 103.41 109.471 23

harm 14 8 16 103.41 109.471 24

harm 3 8 15 100 109.5 25

harm 3 8 16 100 109.5 26

harm 3 8 14 157.916 104.954 27

harm 18 14 19 70 109.5 28

harm 17 14 18 100 109.5 29

harm 17 14 19 100 109.5 30

harm 8 14 18 100 109.5 31

harm 8 14 19 100 109.5 32

harm 8 14 17 143.156 104.954 33

harm 21 17 22 70 109.5 34

harm 20 17 21 100 109.5 35

harm 20 17 22 100 109.5 36

harm 14 17 21 100 109.5 37

harm 14 17 22 100 109.5 38

harm 14 17 20 143.792 104.954 39

harm 23 20 24 70 109.5 40

harm 23 20 25 70 109.5 41

harm 24 20 25 70 109.5 42

harm 17 20 23 100 109.5 43

harm 17 20 24 100 109.5 44

harm 17 20 25 100 109.5 45

 dihedrals 59

cos3 7 4 5 9 0 10.75 0 0.5 0.5

cos3 7 4 5 3 0 10.75 0 0.0 0.0

cos3 1 4 5 9 0 10.75 0 0.5 0.5

cos3 1 4 5 3 0 10.75 0 0.0 0.0

cos3 7 4 1 6 0 3 0 0.5 0.5

cos3 7 4 1 2 0 3 0 0.0 0.0

cos3 5 4 1 6 0 3 0 0.0 0.0

cos3 5 4 1 2 0 3 0 0.0 0.0

cos3 9 5 3 8 0 3 0 0.5 0.5

cos3 9 5 3 2 0 3 0 0.5 0.5

cos3 4 5 3 8 0 3 0 0.0 0.0

cos3 4 5 3 2 0 3 0 0.0 0.0

cos3 4 1 6 11 0 0 0.1314 0.5 0.5

cos3 4 1 6 12 0 0 0.1314 0.5 0.5

cos3 4 1 6 13 0 0 0.1314 0.5 0.5

cos3 2 1 6 11 0 0 0 0.5 0.5

cos3 2 1 6 12 0 0 0 0.5 0.5

cos3 2 1 6 13 0 0 0 0.5 0.5

cos3 6 1 2 10 0 4.649 0 0.5 0.5

cos3 6 1 2 3 0 4.649 0 0.5 0.5

cos3 4 1 2 10 0 4.649 0 0.0 0.0

cos3 4 1 2 3 0 4.649 0 0.0 0.0

cos3 5 3 8 15 0 0 0.1314 0.5 0.5

cos3 5 3 8 16 0 0 0.1314 0.5 0.5

cos3 5 3 8 14 -1.3758 1.0581 0.2095 0.5 0.5

cos3 2 3 8 15 0 0 0 0.5 0.5

cos3 2 3 8 16 0 0 0 0.5 0.5

cos3 2 3 8 14 -0.7715 0 0 0.5 0.5

cos3 8 3 2 10 0 4.649 0 0.5 0.5

cos3 8 3 2 1 0 4.649 0 0.5 0.5

cos3 5 3 2 10 0 4.649 0 0.0 0.0

cos3 5 3 2 1 0 4.649 0 0.0 0.0

cos3 15 8 14 23 0 0 0.3179 0.5 0.5

cos3 15 8 14 25 0 0 0.3179 0.5 0.5

cos3 15 8 14 17 0 0 0.3657 0.5 0.5

cos3 16 8 14 24 0 0 0.3179 0.5 0.5

cos3 16 8 14 25 0 0 0.3179 0.5 0.5

cos3 16 8 14 17 0 0 0.3657 0.5 0.5

cos3 3 8 14 24 0 0 0 0.5 0.5

cos3 3 8 14 25 0 0 0 0.5 0.5

cos3 3 8 14 17 0.1763 -0.16265 0.24362 0.5 0.5

cos3 24 14 17 22 0 0 0.3179 0.5 0.5

cos3 24 14 17 23 0 0 0.3179 0.0 0.0

cos3 24 14 17 20 0 0 0.3657 0.0 0.0

cos3 25 14 17 22 0 0 0.3179 0.5 0.5

cos3 25 14 17 23 0 0 0.3179 0.0 0.0

cos3 25 14 17 20 0 0 0.3657 0.0 0.0

cos3 8 14 17 22 0 0 0.3657 0.5 0.5

cos3 8 14 17 23 0 0 0.3657 0.0 0.0

cos3 8 14 17 20 0.1738 0.1569 0.2787 0.5 0.5

cos3 22 17 20 18 0 0 0.3179 0.5 0.5

cos3 22 17 20 19 0 0 0.3179 0.5 0.5

cos3 22 17 20 21 0 0 0.3179 0.0 0.0

cos3 23 17 20 18 0 0 0.3179 0.5 0.5

cos3 23 17 20 19 0 0 0.3179 0.5 0.5

cos3 23 17 20 21 0 0 0.3179 0.5 0.5

cos3 14 17 20 18 0 0 0.3657 0.0 0.0

cos3 14 17 20 19 0 0 0.3657 0.0 0.0

cos3 14 17 20 21 0 0 0.3657 0.0 0.0

INVERSIONS 5

plan 1 2 5 6 40.000000 0.00000000

plan 2 3 1 7 40.000000 0.00000000

plan 3 4 2 8 40.000000 0.00000000

plan 4 3 5 9 40.000000 0.00000000

plan 5 1 4 10 40.000000 0.00000000

finish

NTf2

nummols 12

atoms 15

 n 14.01 -0.368 1 0 1 1 n N und

 s 32.06 1.3113 1 0 1 2 s S und

 o= 16 -0.717 1 0 1 3 o= O und

 o= 16 -0.717 1 0 1 4 o= O und

 c3 12.001 1.0898 1 0 1 5 c3 C und

 F 19 -0.4277 1 0 1 6 F F und

 F 19 -0.4277 1 0 1 7 F F und

 F 19 -0.4277 1 0 1 8 F F und

 s 32.06 1.3113 1 0 1 9 s S und

 o= 16 -0.717 1 0 1 10 o= O und

 o= 16 -0.717 1 0 1 11 o= O und

 c3 12.001 1.0898 1 0 1 12 c3 C und

 F 19 -0.4277 1 0 1 13 F F und

 F 19 -0.4277 1 0 1 14 F F und

 F 19 -0.4277 1 0 1 15 F F und

 bonds 14

harm 1 2 449.074 1.596 1 224.537

harm 1 9 449.074 1.596 2 224.537

harm 2 5 285.92 1.764 3 142.96

harm 2 3 731.254 1.432 4 365.627

harm 2 4 731.254 1.432 5 365.627

harm 5 6 659.596 1.363 6 329.798

harm 5 7 659.596 1.363 7 329.798

harm 5 8 659.596 1.363 8 329.798

harm 9 12 285.92 1.764 9 142.96

harm 9 10 731.254 1.432 10 365.627

harm 9 11 731.254 1.432 11 365.627

harm 12 13 659.596 1.363 12 329.798

harm 12 14 659.596 1.363 13 329.798

harm 12 15 659.596 1.363 14 329.798

 angles 25

harm 2 1 9 136.424 119.753 1

harm 1 2 5 177.112 112.27 2

harm 1 2 3 249.56 117.054 3

harm 1 2 4 249.56 117.054 4

harm 3 2 5 198.624 115.756 5

harm 3 2 4 280.48 122.877 6

harm 4 2 5 198.624 115.756 7

harm 6 5 7 225.98 110.826 8

harm 6 5 8 225.98 110.826 9

harm 7 5 8 225.98 110.826 10

harm 2 5 6 140.968 119.923 11

harm 2 5 7 140.968 119.923 12

harm 2 5 8 140.968 119.923 13

harm 1 9 12 177.112 112.27 14

harm 1 9 10 249.56 117.054 15

harm 1 9 11 249.56 117.054 16

harm 10 9 12 198.624 115.756 17

harm 10 9 11 280.48 122.877 18

harm 11 9 12 198.624 115.756 19

harm 13 12 14 225.98 110.826 20

harm 13 12 15 225.98 110.826 21

harm 14 12 15 225.98 110.826 22

harm 9 12 13 140.968 119.923 23

harm 9 12 14 140.968 119.923 24

harm 9 12 15 140.968 119.923 25

 dihedrals 24

cos 9 1 2 5 4.57 0 1.00 0.50 0.50

cos 9 1 2 3 7.12 180 1.00 0.50 0.50

cos 9 1 2 4 7.12 180 1.00 0.50 0.50

cos 2 1 9 12 4.57 0 1.00 0.50 0.50

cos 2 1 9 10 7.12 180 1.00 0.50 0.50

cos 2 1 9 11 7.12 180 1.00 0.50 0.50

cos 1 2 5 6 0.49 0 1.00 0.50 0.50

cos 1 2 5 7 0.49 0 1.00 0.50 0.50

cos 1 2 5 8 0.49 0 1.00 0.50 0.50

cos 3 2 5 6 0.64 0 1.00 0.50 0.50

cos 3 2 5 7 0.64 0 1.00 0.50 0.50

cos 3 2 5 8 0.64 0 1.00 0.50 0.50

cos 4 2 5 6 0.64 0 1.00 0.50 0.50

cos 4 2 5 7 0.64 0 1.00 0.50 0.50

cos 4 2 5 8 0.64 0 1.00 0.50 0.50

cos 1 9 12 13 0.49 0 1.00 0.50 0.50

cos 1 9 12 14 0.49 0 1.00 0.50 0.50

cos 1 9 12 15 0.49 0 1.00 0.50 0.50

cos 10 9 12 13 0.64 0 1.00 0.50 0.50

cos 10 9 12 14 0.64 0 1.00 0.50 0.50

cos 10 9 12 15 0.64 0 1.00 0.50 0.50

cos 11 9 12 13 0.64 0 1.00 0.50 0.50

cos 11 9 12 14 0.64 0 1.00 0.50 0.50

cos 11 9 12 15 0.64 0 1.00 0.50 0.50

 finish

vdw 465

n n lj 0.17 3.257142883

n s lj 0.206155281 3.414285742

n o= lj 0.188944436 3.111785739

n c3 lj 0.136374484 3.332142884

n F lj 0.101833197 3.191071454

n N\* lj 0.17 3.257142883

n c2 lj 0.120913192 3.332142884

n CT lj 0.136374484 3.332142884

n H5 lj 0.050497525 2.841964308

n H4 lj 0.050497525 2.886607166

n H1 lj 0.051662365 3.214928592

n 2C lj 0.136374484 3.332142884

n HC lj 0.051662365 2.956250024

s s lj 0.25 3.5714286

s o= lj 0.229128785 3.268928598

s c3 lj 0.165378354 3.489285742

s F lj 0.12349089 3.348214313

s N\* lj 0.206155281 3.414285742

s c2 lj 0.146628783 3.489285742

s CT lj 0.165378354 3.489285742

s H5 lj 0.061237244 2.999107167

s H4 lj 0.061237244 3.043750024

s H1 lj 0.06264982 3.37207145

s 2C lj 0.165378354 3.489285742

s HC lj 0.06264982 3.113392882

o= o= lj 0.21 2.966428595

o= c3 lj 0.151571765 3.18678574

o= F lj 0.113181271 3.04571431

o= N\* lj 0.188944436 3.111785739

o= c2 lj 0.134387499 3.18678574

o= CT lj 0.151571765 3.18678574

o= H5 lj 0.056124861 2.696607164

o= H4 lj 0.056124861 2.741250022

o= H1 lj 0.057419509 3.069571448

o= 2C lj 0.151571765 3.18678574

o= HC lj 0.057419509 2.81089288

c3 c3 lj 0.1094 3.407142884

c3 F lj 0.081690881 3.266071455

c3 N\* lj 0.136374484 3.332142884

c3 c2 lj 0.096996907 3.407142884

c3 CT lj 0.1094 3.407142884

c3 H5 lj 0.040509258 2.916964309

c3 H4 lj 0.040509258 2.961607167

c3 H1 lj 0.041443697 3.289928592

c3 2C lj 0.1094 3.407142884

c3 HC lj 0.041443697 3.031250024

F F lj 0.061 3.125000025

F N\* lj 0.101833197 3.191071454

F c2 lj 0.072429276 3.266071455

F CT lj 0.081690881 3.266071455

F H5 lj 0.030248967 2.775892879

F H4 lj 0.030248967 2.820535737

F H1 lj 0.030946728 3.148857163

F 2C lj 0.081690881 3.266071455

F HC lj 0.030946728 2.890178595

N\* N\* lj 0.17 3.257142883

N\* c2 lj 0.120913192 3.332142884

N\* CT lj 0.136374484 3.332142884

N\* H5 lj 0.050497525 2.841964308

N\* H4 lj 0.050497525 2.886607166

N\* H1 lj 0.051662365 3.214928592

N\* 2C lj 0.136374484 3.332142884

N\* HC lj 0.051662365 2.956250024

c2 c2 lj 0.086 3.407142884

c2 CT lj 0.096996907 3.407142884

c2 H5 lj 0.03591657 2.916964309

c2 H4 lj 0.03591657 2.961607167

c2 H1 lj 0.036745068 3.289928592

c2 2C lj 0.096996907 3.407142884

c2 HC lj 0.036745068 3.031250024

CT CT lj 0.1094 3.407142884

CT H5 lj 0.040509258 2.916964309

CT H4 lj 0.040509258 2.961607167

CT H1 lj 0.041443697 3.289928592

CT 2C lj 0.1094 3.407142884

CT HC lj 0.041443697 3.031250024

H5 H5 lj 0.015 2.426785734

H5 H4 lj 0.015 2.471428591

H5 H1 lj 0.015346009 2.799750017

H5 2C lj 0.040509258 2.916964309

H5 HC lj 0.015346009 2.541071449

H4 H4 lj 0.015 2.516071449

H4 H1 lj 0.015346009 2.844392874

H4 2C lj 0.040509258 2.961607167

H4 HC lj 0.015346009 2.585714306

H1 H1 lj 0.0157 3.1727143

H1 2C lj 0.041443697 3.289928592

H1 HC lj 0.0157 2.914035732

2C 2C lj 0.1094 3.407142884

2C HC lj 0.041443697 3.031250024

HC HC lj 0.0157 2.655357164

Ti Ti buck 717647.4 0.154 121.0676

Ti O buck 391049.1 0.194 290.3317

Ti n lj 0.3805387 2.5426884

Ti s lj 0.461471 2.6998313

Ti o= lj 0.4229452 2.3973313

Ti c3 lj 0.3052693 2.6176884

Ti F lj 0.2279499 2.476617

Ti N\* lj 0.3805387 2.5426884

Ti c2 lj 0.2706597 2.6176884

Ti CT lj 0.3052693 2.6176884

Ti H5 lj 0.1130369 2.1275099

Ti H4 lj 0.1130369 2.1721527

Ti H1 lj 0.1156443 2.5004742

Ti 2C lj 0.3052693 2.6176884

Ti HC lj 0.1156443 2.2417956

O O buck 271716.3 0.234 696.8883

O n lj 0.2120703 3.0809979

O s lj 0.257173 3.2381408

O o= lj 0.2357029 2.9356408

O c3 lj 0.1701234 3.1559979

O F lj 0.1270341 3.0149265

O N\* lj 0.2120703 3.0809979

O c2 lj 0.1508359 3.1559979

O CT lj 0.1701234 3.1559979

O H5 lj 0.0629943 2.6658194

O H4 lj 0.0629943 2.7104622

O H1 lj 0.0644474 3.0387837

O 2C lj 0.1701234 3.1559979

O HC lj 0.0644474 2.7801051

n O1 lj 0.188944436 3.111785739

s O1 lj 0.229128785 3.268928598

o= O1 lj 0.21 2.966428595

c3 O1 lj 0.151571765 3.18678574

F O1 lj 0.113181271 3.04571431

N\* O1 lj 0.188944436 3.111785739

c2 O1 lj 0.134387499 3.18678574

CT O1 lj 0.151571765 3.18678574

H5 O1 lj 0.056124861 2.696607164

H4 O1 lj 0.056124861 2.741250022

H1 O1 lj 0.057419509 3.069571448

2C O1 lj 0.151571765 3.18678574

HC O1 lj 0.057419509 2.81089288

Ti O1 lj 0.422945174 2.397331298

O O1 lj 0.235702944 2.935640798

n HO lj 0 2.521428592

s HO lj 0 2.67857145

o= HO lj 0 2.376071448

c3 HO lj 0 2.596428592

F HO lj 0 2.455357163

N\* HO lj 0 2.521428592

c2 HO lj 0 2.596428592

CT HO lj 0 2.596428592

H5 HO lj 0 2.106250017

H4 HO lj 0 2.150892874

H1 HO lj 0 2.4792143

2C HO lj 0 2.596428592

HC HO lj 0 2.220535732

Ti HO lj 0 1.80697415

O HO lj 0 2.34528365

n C lj 0.120913192 3.332142884

s C lj 0.146628783 3.489285742

o= C lj 0.134387499 3.18678574

c3 C lj 0.096996907 3.407142884

F C lj 0.072429276 3.266071455

N\* C lj 0.120913192 3.332142884

c2 C lj 0.086 3.407142884

CT C lj 0.096996907 3.407142884

H5 C lj 0.03591657 2.916964309

H4 C lj 0.03591657 2.961607167

H1 C lj 0.036745068 3.289928592

2C C lj 0.096996907 3.407142884

HC C lj 0.036745068 3.031250024

Ti C lj 0.270659735 2.617688442

O C lj 0.150835854 3.155997942

n OH lj 0.189124298 3.165178597

s OH lj 0.229346899 3.322321455

o= OH lj 0.210199905 3.019821453

c3 OH lj 0.151716051 3.240178597

F OH lj 0.113289011 3.099107168

N\* OH lj 0.189124298 3.165178597

c2 OH lj 0.134515427 3.240178597

CT OH lj 0.151716051 3.240178597

H5 OH lj 0.056178288 2.750000022

H4 OH lj 0.056178288 2.79464288

H1 OH lj 0.057474168 3.122964305

2C OH lj 0.151716051 3.240178597

HC OH lj 0.057474168 2.864285737

Ti OH lj 0.423347787 2.450724155

O OH lj 0.235927317 2.989033655

n CA lj 0.120913192 3.332142884

s CA lj 0.146628783 3.489285742

o= CA lj 0.134387499 3.18678574

c3 CA lj 0.096996907 3.407142884

F CA lj 0.072429276 3.266071455

N\* CA lj 0.120913192 3.332142884

c2 CA lj 0.086 3.407142884

CT CA lj 0.096996907 3.407142884

H5 CA lj 0.03591657 2.916964309

H4 CA lj 0.03591657 2.961607167

H1 CA lj 0.036745068 3.289928592

2C CA lj 0.096996907 3.407142884

HC CA lj 0.036745068 3.031250024

Ti CA lj 0.270659735 2.617688442

O CA lj 0.150835854 3.155997942

n HA lj 0.050497525 2.931250023

s HA lj 0.061237244 3.088392882

o= HA lj 0.056124861 2.785892879

c3 HA lj 0.040509258 3.006250024

F HA lj 0.030248967 2.865178594

N\* HA lj 0.050497525 2.931250023

c2 HA lj 0.03591657 3.006250024

CT HA lj 0.040509258 3.006250024

H5 HA lj 0.015 2.516071449

H4 HA lj 0.015 2.560714306

H1 HA lj 0.015346009 2.889035732

2C HA lj 0.040509258 3.006250024

HC HA lj 0.015346009 2.630357164

Ti HA lj 0.113036852 2.216795582

O HA lj 0.062994262 2.755105082

n H6 lj 0.050497525 2.886607166

s H6 lj 0.061237244 3.043750024

o= H6 lj 0.056124861 2.741250022

c3 H6 lj 0.040509258 2.961607167

F H6 lj 0.030248967 2.820535737

N\* H6 lj 0.050497525 2.886607166

c2 H6 lj 0.03591657 2.961607167

CT H6 lj 0.040509258 2.961607167

H5 H6 lj 0.015 2.471428591

H4 H6 lj 0.015 2.516071449

H1 H6 lj 0.015346009 2.844392874

2C H6 lj 0.040509258 2.961607167

HC H6 lj 0.015346009 2.585714306

Ti H6 lj 0.113036852 2.172152724

O H6 lj 0.062994262 2.710462224

n NC lj 0.17 3.257142883

s NC lj 0.206155281 3.414285742

o= NC lj 0.188944436 3.111785739

c3 NC lj 0.136374484 3.332142884

F NC lj 0.101833197 3.191071454

N\* NC lj 0.17 3.257142883

c2 NC lj 0.120913192 3.332142884

CT NC lj 0.136374484 3.332142884

H5 NC lj 0.050497525 2.841964308

H4 NC lj 0.050497525 2.886607166

H1 NC lj 0.051662365 3.214928592

2C NC lj 0.136374484 3.332142884

HC NC lj 0.051662365 2.956250024

Ti NC lj 0.38053875 2.542688442

O NC lj 0.212070286 3.080997942

n Ru lj 0.272873597 2.798571442

s Ru lj 0.330907842 2.9557143

o= Ru lj 0.303282047 2.653214298

c3 Ru lj 0.218899977 2.873571442

F Ru lj 0.163456416 2.732500013

N\* Ru lj 0.272873597 2.798571442

c2 Ru lj 0.194082457 2.873571442

CT Ru lj 0.218899977 2.873571442

H5 Ru lj 0.081055537 2.383392867

H4 Ru lj 0.081055537 2.428035724

H1 Ru lj 0.082925268 2.75635715

2C Ru lj 0.218899977 2.873571442

HC Ru lj 0.082925268 2.497678582

Ti Ru lj 0.610817514 2.084117

O Ru lj 0.340402245 2.6224265

n N2 lj 0.17 3.257142883

s N2 lj 0.206155281 3.414285742

o= N2 lj 0.188944436 3.111785739

c3 N2 lj 0.136374484 3.332142884

F N2 lj 0.101833197 3.191071454

N\* N2 lj 0.17 3.257142883

c2 N2 lj 0.120913192 3.332142884

CT N2 lj 0.136374484 3.332142884

H5 N2 lj 0.050497525 2.841964308

H4 N2 lj 0.050497525 2.886607166

H1 N2 lj 0.051662365 3.214928592

2C N2 lj 0.136374484 3.332142884

HC N2 lj 0.051662365 2.956250024

Ti N2 lj 0.38053875 2.542688442

O N2 lj 0.212070286 3.080997942

n CZ lj 0.120913192 3.332142884

s CZ lj 0.146628783 3.489285742

o= CZ lj 0.134387499 3.18678574

c3 CZ lj 0.096996907 3.407142884

F CZ lj 0.072429276 3.266071455

N\* CZ lj 0.120913192 3.332142884

c2 CZ lj 0.086 3.407142884

CT CZ lj 0.096996907 3.407142884

H5 CZ lj 0.03591657 2.916964309

H4 CZ lj 0.03591657 2.961607167

H1 CZ lj 0.036745068 3.289928592

2C CZ lj 0.096996907 3.407142884

HC CZ lj 0.036745068 3.031250024

Ti CZ lj 0.270659735 2.617688442

O CZ lj 0.150835854 3.155997942

n SH lj 0.206155281 3.414285742

s SH lj 0.25 3.5714286

o= SH lj 0.229128785 3.268928598

c3 SH lj 0.165378354 3.489285742

F SH lj 0.12349089 3.348214313

N\* SH lj 0.206155281 3.414285742

c2 SH lj 0.146628783 3.489285742

CT SH lj 0.165378354 3.489285742

H5 SH lj 0.061237244 2.999107167

H4 SH lj 0.061237244 3.043750024

H1 SH lj 0.06264982 3.37207145

2C SH lj 0.165378354 3.489285742

HC SH lj 0.06264982 3.113392882

Ti SH lj 0.461471018 2.6998313

O SH lj 0.257172996 3.2381408

n O2 lj 0.188944436 3.111785739

s O2 lj 0.229128785 3.268928598

o= O2 lj 0.21 2.966428595

c3 O2 lj 0.151571765 3.18678574

F O2 lj 0.113181271 3.04571431

N\* O2 lj 0.188944436 3.111785739

c2 O2 lj 0.134387499 3.18678574

CT O2 lj 0.151571765 3.18678574

H5 O2 lj 0.056124861 2.696607164

H4 O2 lj 0.056124861 2.741250022

H1 O2 lj 0.057419509 3.069571448

2C O2 lj 0.151571765 3.18678574

HC O2 lj 0.057419509 2.81089288

Ti O2 lj 0.422945174 2.397331298

O O2 lj 0.235702944 2.935640798

OS Ti buck 391049.1 0.194 290.3317

OS OS buck 271716.3 0.234 696.8883

OS O buck 271716.3 0.234 696.8883

OS n lj 0.2120703 3.0809979

OS s lj 0.257173 3.2381408

OS o= lj 0.2357029 2.9356408

OS c3 lj 0.1701234 3.1559979

OS F lj 0.1270341 3.0149265

OS N\* lj 0.2120703 3.0809979

OS c2 lj 0.1508359 3.1559979

OS CT lj 0.1701234 3.1559979

OS H5 lj 0.0629943 2.6658194

OS H4 lj 0.0629943 2.7104622

OS H1 lj 0.0644474 3.0387837

OS 2C lj 0.1701234 3.1559979

OS HC lj 0.0644474 2.7801051

OS O1 lj 0.235702944 2.935640798

OS HO lj 0 2.34528365

OS C lj 0.150835854 3.155997942

OS OH lj 0.235927317 2.989033655

OS CA lj 0.150835854 3.155997942

OS HA lj 0.062994262 2.755105082

OS H6 lj 0.062994262 2.710462224

OS NC lj 0.212070286 3.080997942

OS Ru lj 0.340402245 2.6224265

OS N2 lj 0.212070286 3.080997942

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c2 HS lj 0.041472883 2.594471442

CT HS lj 0.046776062 2.594471442

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H4 HS lj 0.017320508 2.148935724

H1 HS lj 0.017720045 2.47725715

2C HS lj 0.046776062 2.594471442

HC HS lj 0.017720045 2.218578582

Ti HS lj 0.130523714 1.805017

O HS lj 0.072739508 2.3433265

O1 HS lj 0.064807407 2.374114298

HO HS lj 0.0 1.78375715

C HS lj 0.041472883 2.594471442

OH HS lj 0.064869099 2.427507155

CA HS lj 0.041472883 2.594471442

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H6 HS lj 0.017320508 2.148935724

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Ru HS lj 0.093594872 2.0609

N2 HS lj 0.058309519 2.519471442

CZ HS lj 0.041472883 2.594471442

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O2 HS lj 0.064807407 2.374114298

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HS HS lj 0.02 1.7818

O1 O1 lj 0.21 2.966428595

HO O1 lj 0 2.376071448

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OH O1 lj 0.210199905 3.019821453

CA O1 lj 0.134387499 3.18678574

HA O1 lj 0.056124861 2.785892879

H6 O1 lj 0.056124861 2.741250022

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Ru O1 lj 0.303282047 2.653214298

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O2 O1 lj 0.21 2.966428595

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CA C lj 0.086 3.407142884

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H6 C lj 0.03591657 2.961607167

NC C lj 0.120913192 3.332142884

Ru C lj 0.194082457 2.873571442

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CZ C lj 0.086 3.407142884

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O2 C lj 0.134387499 3.18678574

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H6 OH lj 0.056178288 2.79464288

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CZ OH lj 0.134515427 3.240178597

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Ru CA lj 0.194082457 2.873571442

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CZ CA lj 0.086 3.407142884

SH CA lj 0.146628783 3.489285742

O2 CA lj 0.134387499 3.18678574

HA HA lj 0.015 2.605357164

H6 HA lj 0.015 2.560714306

NC HA lj 0.050497525 2.931250023

Ru HA lj 0.081055537 2.472678582

N2 HA lj 0.050497525 2.931250023

CZ HA lj 0.03591657 3.006250024

SH HA lj 0.061237244 3.088392882

O2 HA lj 0.056124861 2.785892879

H6 H6 lj 0.015 2.516071449

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Ru H6 lj 0.081055537 2.428035724

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O2 H6 lj 0.056124861 2.741250022

NC NC lj 0.17 3.257142883

Ru NC lj 0.272873597 2.798571442

N2 NC lj 0.17 3.257142883

CZ NC lj 0.120913192 3.332142884

SH NC lj 0.206155281 3.414285742

O2 NC lj 0.188944436 3.111785739

Ru Ru lj 0.438 2.34

N2 Ru lj 0.272873597 2.798571442

CZ Ru lj 0.194082457 2.873571442

SH Ru lj 0.330907842 2.9557143

O2 Ru lj 0.303282047 2.653214298

N2 N2 lj 0.17 3.257142883

CZ N2 lj 0.120913192 3.332142884

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O2 N2 lj 0.188944436 3.111785739

CZ CZ lj 0.086 3.407142884

SH CZ lj 0.146628783 3.489285742

O2 CZ lj 0.134387499 3.18678574

SH SH lj 0.25 3.5714286

O2 SH lj 0.229128785 3.268928598

O2 O2 lj 0.21 2.966428595

close

1. CONFIG file

DSSC with rtil simulation

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Ti 2

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Ti 3

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Ti 4

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Ti 5

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Ti 6

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Ti 7

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 -0.1907985258 -1.566507096 -3.613590472

 -14134.86492 -4726.183602 -159.9446044

Ti 8

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 -0.9767300375 -2.154699428 3.754166780

 3345.709097 -8138.435880 -8351.409497

Ti 9

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 -1571.153564 8349.393533 9585.885399

Ti 10

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 -0.8277525976 1.156512301 2.060535687

 -9623.227966 -1186.655522 3284.200339

Ti 11

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 3322.753934 -2742.985967 3977.406899

Ti 12

 6.690433129 -9.729117530 -0.7768123231

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 21909.59406 8821.146828 -1017.806817

Ti 13

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Ti 14

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 -4.600817908 -1.756714231 0.8397535345

 -19141.23310 8598.328171 -5510.288036

Ti 15

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 -2.870318146 -0.8353019465E-01 -0.4038307708

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Ti 16

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Ti 17

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 12649.66370 -1891.132808 8900.764879

Ti 18

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Ti 19

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Ti 20

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Ti 21

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Ti 22

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Ti 23

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Ti 24

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Ti 25

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Ti 26

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Ti 29

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Ti 30

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Ti 31

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 0.6834653600 -1.833841563 1.246331371

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Ti 32

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Ti 33

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Ti 34

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 -4840.944092 -7790.093227 7972.927445

Ti 35

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 1.269028113 3.546146178 1.674464111

 855.9515152 4739.708094 2291.909579

Ti 36

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 1.841735858 -2.427446751 -0.5483185953

 6.686481283 1889.876202 -8445.567720

Ti 37

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 -2.261312493 1.106568529 -5.869640669

 -3335.228078 -3892.999675 5953.825396

Ti 38

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Ti 39

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Ti 40

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Ti 41

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 -3219.187297 3766.647243 -267.6729825

Ti 42

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Ti 43

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Ti 44

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Ti 45

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Ti 46

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Ti 47

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Ti 48

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Ti 49

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Ti 53

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Ti 54

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Ti 55

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Ti 56

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Ti 57

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Ti 58

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Ti 59

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Ti 60

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Ti 61

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 1245.556677 -1458.033001 7666.186882

Ti 62

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Ti 63

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Ti 64

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Ti 65

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Ti 66

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Ti 67

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Ti 68

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Ti 69

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Ti 70

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 -2619.186884 4928.827343 3705.699500

Ti 71

 -4.423613988 2.084386704 -4.183570977

 -2.011139960 0.3075295123 1.527526158

 14099.25395 -8829.792925 3479.821213

Ti 72

 -4.453208969 3.527688603 -1.476177639

 -1.384487320 4.362075777 -4.957463980

 -2323.439620 4132.660677 -15255.38237

Ti 73

 1.180883732 7.044168032 -4.213226633

 -0.4796105119 -2.370183179 2.216984640

 10446.71921 7501.996480 -1002.377417

Ti 74

 1.175277027 -1.608580749 -1.278120440

 -1.241554311 1.140783407 -0.5766790449

 8294.760108 482.8929606 -268.4957517

Ti 75

 -0.5438442169 2.031943274 -4.089936547

 -4.570408833 1.741246423 3.593627756

 -14876.52050 5094.052477 -4606.020069

Ti 76

 -0.6729574078 3.556953889 -1.424548364

 -0.6444240089 1.106598328 0.5690532434

 5417.048591 3923.967063 -2094.862850

Ti 77

 5.002271503 7.026521563 -3.977725678

 0.8489170228 -0.7501769893 -1.091090757

 2162.546847 -202.5166313 -10025.59541

Ti 78

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 -0.3470313940E-01 1.039470080 0.1938122331E-01

 4374.867786 10779.55904 -4180.648782

Ti 79

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 -7928.586324 7281.001790 14573.14371

Ti 80

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 1.231595662 -1.888831022 1.434504481

 -13000.30034 4707.575008 -14910.59424

Ti 81

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 9900.548548 15.69466933 1515.794951

Ti 82

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 -2.210483646 -1.221051109 -2.057735622

 3837.867676 -2450.338881 6900.363307

Ti 83

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 -1.556692822 0.2405286052 2.872985114

 3056.911597 3637.755334 -13998.18866

Ti 84

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 -0.4620807271E-01 -1.001253831 -0.9020687640E-01

 17789.54582 10673.43174 701.1891466

Ti 85

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 3.295636380 -0.4905865746 -0.7832046169E-01

 -3104.028327 10862.01743 9537.182492

Ti 86

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 10697.69831 13786.23380 -15123.29969

Ti 87

 -6.244918096 -0.2981807008 -4.925203241

 -0.3087500615 -0.7826239832 0.7166385291

 4857.678595 3902.590920 1538.456674

Ti 88

 -8.327022181 4.864365033 -4.971601216

 1.669818064 0.6241472615 -2.616707838

 3838.439687 1884.057277 -9660.697505

Ti 89

 -2.495270446 -0.2472730938 -4.857398659

 -2.104417059 -1.797280474 -3.009984732

 1791.881348 1806.078500 4575.441518

Ti 90

 -4.487766916 4.886308935 -5.123723307

 2.429645567 1.087220928 0.9571808167

 6433.640613 -8929.886036 -2854.330776

Ti 91

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 -3.457966240 -4.305332992 -0.5386734534E-01

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Ti 92

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 -2669.147790 4674.506812 1347.579408

Ti 93

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 -0.9208521612 -4.713828072 0.2556612991

 11094.35583 8849.531801 922.8080002

Ti 94

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 1.596214626 1.592049836 1.359811412

 -8926.203953 8443.341225 -8708.065573

Ti 95

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 -4.835049735 0.1105747249 -0.4864188379E-01

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Ti 96

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 16348.24729 -13472.00658 2124.073302

O 97

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 -2.549704338 6.429859146 1.482949746

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O 98

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O 101

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 706.1663358 5613.480316 -1420.195987

O 102

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O 103

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O 105

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O 110

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O 121

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s 799

 3.826413928 9.495792795 -8.232388127

 -1.000289532 0.3958392888 -0.4677708661

 1777.949303 104.9102601 -12175.98763

o= 800

 4.502914402 9.424339375 -9.508945320

 0.7289552316 0.5846481275 -6.179164107

 -5945.398593 -2910.911516 -374.9508750

o= 801

 4.686388679 10.13532564 -7.257888467

 -0.9150881836 -0.3808786549 -1.341448577

 -1298.423635 -2208.540030 15733.60000

c3 802

 2.219782226 -9.912550328 -8.375262422

 0.6350592165 1.441549587 0.7064328985

 11025.24812 495.5426500 249.1868198

F 803

 2.541463198 -8.579011978 -8.504126679

 2.584513367 0.9021714953 -2.157459181

 -4234.448260 -3192.259552 -3088.257816

F 804

 1.426932122 -10.21521420 -9.465310657

 -2.483071868 -1.773611717 -1.542826234

 628.9992725 -975.5098395 4235.145480

F 805

 1.412995911 -9.955024391 -7.252180188

 -4.830183814 2.271401860 3.456326522

 -1134.771621 -1979.767577 -603.6420897

s 806

 3.869166231 6.587641453 -7.959381685

 -1.945239139 2.947309292 -1.466729940

 -49.02396360 11238.54909 716.2651059

o= 807

 3.514627311 6.024478709 -9.238799735

 9.807546688 0.3025041966 1.617737569

 -5797.080520 2182.146484 -1675.187440

o= 808

 3.398598015 5.769947751 -6.850231829

 -1.863599925 -8.744815827 8.052734530

 3099.659287 -5186.343708 4937.321218

c3 809

 5.726702125 6.701953626 -7.927910971

 -8.766663336 9.093035770 3.418616743

 11434.95627 -452.5300396 -14615.62256

F 810

 6.252673216 6.251280143 -9.135980357

 -8.954807806 3.933735233 0.8958800086

 -2802.189241 -2329.327004 6786.856514

F 811

 6.335858987 5.893062479 -6.983454987

 5.235728290 0.9267119355 3.662995633

 -629.8443873 -1387.977332 2683.883459

F 812

 6.355664203 7.898151399 -7.837181079

 7.584469872 0.8822965660E-01 6.125317535

 -1790.380974 4913.235345 3678.440084

n 813

 10.89694895 8.784818734 11.11505713

 9.390385543 -2.335336744 -1.837141251

 -1222.231233 -10147.42029 3202.721088

s 814

 10.18074127 7.688099377 10.27705084

 -2.525080413 -0.8947988204 1.191037564

 38991.04388 127.1214137 -721.2289913

o= 815

 11.14282851 7.218934300 9.231921089

 -6.053142819 9.684376064 -6.522256199

 -8418.427696 255.6756442 6230.223351

o= 816

 9.091940835 8.268779848 9.743216557

 3.210039704 -8.466540458 2.187800433

 -27697.48994 1890.633390 -7870.383836

c3 817

 9.825533505 6.362132899 11.54384222

 1.884094562 4.450811928 -1.735490738

 8254.741073 -6807.175645 -5066.078226

F 818

 10.85208137 5.438849269 11.65400403

 -0.4685336015 -0.1741993350 -0.4896900688

 -3189.213930 2282.869730 -3254.055609

F 819

 8.719948456 5.638985392 11.29454756

 -0.6881646404 5.469615036 2.539001172

 -4920.284475 -3348.326391 -3473.069804

F 820

 9.669360384 6.779522203 12.80028101

 -7.384742407 2.348829645 -4.516412311

 -2510.611219 8214.636555 7449.009350

s 821

 11.04961745 10.22463333 10.64664379

 0.8696362515 -1.376455665 -3.968806733

 4521.701772 13183.39234 -5007.646221

o= 822

 11.25302764 -10.03036582 9.215633995

 -1.245125053 5.434890849 -3.205999081

 -1824.874989 -8855.911863 -3303.419847

o= 823

 -10.53614171 -9.637105535 11.37113038

 1.532292365 -2.021256025 1.904443576

 -3508.289908 -97.42818273 521.0601272

c3 824

 9.441564730 -9.421075235 11.10734032

 -0.6409271116E-01 3.284505764 6.729569766

 4587.180394 -392.6159047 214.2952501

F 825

 9.691872368 -8.089327673 11.41283375

 2.671728269 3.803108529 2.943379110

 -7627.732708 -3751.536233 -3423.910669

F 826

 8.963823336 -9.984602122 12.22888461

 2.736176886 0.7272694630 2.433063727

 -5287.533133 -378.5032294 6174.369252

F 827

 8.378709989 -9.466424487 10.18454386

 4.240752613 5.016210896 -4.555295952

 9723.380672 5079.844727 5262.704704

VACF Python program

#updated velocity autocorrelation function calculation

#only calculate the mass-weighted VACF

#aaron byrne

import sys

import numpy as np

from scipy.fftpack import fft

import matplotlib.pyplot as plt

file\_name\_1 = sys.argv[1]

file\_name\_2 = file\_name\_1

print 'Analyzing autocorrelation for %s' %(file\_name\_1)

if 'PBE' in file\_name\_1:

 repres = 'PBE'

 T = 8501

 max\_lag\_time = 7500

elif 'BLYP' in file\_name\_1:

 repres = 'BLYP'

 T = 8501

 max\_lag\_time = 7500

elif 'mull' in file\_name\_1:

 repres = 'mull'

 T = 15000

 max\_lag\_time = 12500

elif 'EHT' in file\_name\_1:

 repres = 'EHT'

 T = 15000

 max\_lag\_time = 12500

elif 'lopes' in file\_name\_1:

 repres = 'lopes'

 T = 15000

 max\_lag\_time = 12500

elif 'hirsh' in file\_name\_1:

 repres = 'hirsh'

 T = 15000

 max\_lag\_time = 12500

else:

 print 'error'

 exit()

header = 2 #number of header lines in file

step = 1 #1fs

f = file\_name\_1.split('/')

f1 = f[-1]

f2 = f1.split('.')

f3 = f2[0]

f4 = f3 + '.vacf'

f5 = f[2]

file\_name\_out = './' + f5 + '/' + f4

#\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

xyz1 = open(file\_name\_1,"r")

line = xyz1.readline() #1st line of xyz file containing number of atoms (always 1)

line = xyz1.readline() #2nd line of xyz file containing time information

data1=[]

for i in range(0,T): #different times

 line = xyz1.readline()

 atom, velx , vely, velz = line.split()

 data1.append([i,atom,float(velx), float(vely), float(velz)]) #i is time index

 for k in range(0,header): #headers of next timestep

 line = xyz1.readline()

xyz1.close()

#print atom

#should always be the same for each file

#\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

#\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

xyz2 = open(file\_name\_2,"r")

line = xyz2.readline() #1st line of xyz file containing number of atoms (always 1)

line = xyz2.readline() #2nd line of xyz file containing time information

data2=[]

for i in range(0,T): #different times

 line = xyz2.readline()

 atom, velx , vely, velz = line.split()

 data2.append([i,atom,float(velx), float(vely), float(velz)]) #i is time index

 for k in range(0,header): #headers of next timestep

 line = xyz2.readline()

xyz2.close()

#\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

n\_t0 = T - max\_lag\_time #number of different starting points (T=8500)

massDict = {'O':16.0,'H':1.008,'C':12.01,'N':14.01,'Ru':101.07,'S':32.06}

mass = massDict[atom] #get mass of atom

G = [] #normalised and averaged over three components correlation vector

for d in range(0,max\_lag\_time): # different values of lag time

 Cx = 0

 Cy = 0

 Cz = 0

 for t0 in range(0,n\_t0): #different starting points t0

 Cx = Cx + float(data1[t0][2])\*float(data2[t0+d][2]) #/(float(data1[t0][2])\*float(data2[t0][2])) # sum( vx(t0)\*vx(t0+d) )

 Cy = Cy + float(data1[t0][3])\*float(data2[t0+d][3])

 Cz = Cz + float(data1[t0][4])\*float(data2[t0+d][4])

 #average over different starting times

 Cx = Cx/n\_t0

 Cy = Cy/n\_t0

 Cz = Cz/n\_t0

 if d == 0: #no lag : <A(0)B(0)>

 normx = Cx

 normy = Cy

 normz = Cz

 Cx = Cx/normx

 Cy = Cy/normy

 Cz = Cz/normz

 C = (Cx + Cy + Cz )/3.0 #3components averaged s.t. autocorrellation between -1 and +1

 G.append(C)

#cross correlation can of course be outside the +1 <--> -1 range and should be normalised by dividing by the max correlation

G = G/np.amax(np.absolute(G))

#G can be normalised without affecting whether F is normalised or not?

#F = dct(G)

#fourier transform

N = G.size

time = [i for i in range(0,N)]

#f\_signal = fft(G)

#f\_signal = abs(f\_signal)\*\*2

##normalize or not

#f\_signal = f\_signal/np.amax(f\_signal)

#freq = np.fft.fftfreq(N, d=step)

#freq = freq\*1000.0 #convert from fs^-1 to ps^-1

#freq = freq\*33.356 #convert to wavenumbers

##\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

#OUTPUT

cfile = open(file\_name\_out,"w")

#write output file

for i in range(0,max\_lag\_time):

 g1 = G[i]\*mass

 t = time[i]

 g2 = G[i]

 out = "%16.9f%20.9f%20.9f\n" %(g1,t,g2)

 cfile.write(out)

cfile.close()