

```

1  -- vismol2-1.hs
2
3  import Data.IORef
4  import Graphics.UI.GLUT
5  import Graphics.Rendering.OpenGL.GLU.Quadrics
6  import Data.List (isPrefixOf)
7
8  main :: IO ()
9  main = do
10     m <- getMolecule "yperite.mol2"
11     visualize $ moveMolecule m 5.0 5.0 5.0 -- to test out the centering
12
13  getMolecule :: FilePath -> IO Molecule
14  getMolecule filePath = do
15     theText <- readFile filePath
16     return (getRecords (lines theText) OtherRecord [] [])
17
18  data Molecule = Molecule [Atom] [Bond] deriving (Show)
19  data Atom = Atom Int Float Float Float String deriving (Show) -- i x y z type
20  data Bond = Bond Int Int String deriving (Show) -- i j type
21
22  data RecordType = AtomRecord | BondRecord | OtherRecord
23
24  getRecords :: [String] -> RecordType -> [Atom] -> [Bond] -> Molecule
25  getRecords ("<TRIPOS>ATOM":ls) _ atoms bonds = getRecords ls AtomRecord atoms bonds
26  getRecords ("<TRIPOS>BOND":ls) _ atoms bonds = getRecords ls BondRecord atoms bonds
27  getRecords ((' ':_):ls) _ atoms bonds = getRecords ls OtherRecord atoms bonds
28  getRecords (_:ls) OtherRecord atoms bonds = getRecords ls OtherRecord atoms bonds
29  getRecords (l:ls) AtomRecord atoms bonds =
30     getRecords ls AtomRecord (atom:atoms) bonds where
31         atom = Atom i x y z t where
32             fields = words l
33             i = read $ fields !! 0
34             x = read $ fields !! 2
35             y = read $ fields !! 3
36             z = read $ fields !! 4
37             t = fields !! 5
38  getRecords (l:ls) BondRecord atoms bonds =
39     getRecords ls BondRecord atoms (bond:bonds) where
40         bond = Bond i j t where
41             fields = words l
42             i = read $ fields !! 1
43             j = read $ fields !! 2
44             t = fields !! 3
45  getRecords [] _ atoms bonds = Molecule atoms bonds
46
47  moveMolecule :: Molecule -> Float -> Float -> Float -> Molecule
48  moveMolecule m@(Molecule atoms bonds) dx dy dz =
49     Molecule ( map (\a -> moveAtom a dx dy dz) atoms ) bonds
50
51  moveAtom :: Atom -> Float -> Float -> Float -> Atom
52  moveAtom a@(Atom i x y z t) dx dy dz =
53     Atom i (x+dx) (y+dy) (z+dz) t
54
55  data Axis = Ox | Oy | Oz
56
57  rotateMolecule :: Molecule -> Axis -> Float -> Molecule
58  rotateMolecule m@(Molecule atoms bonds) aroundAxis angle =
59     Molecule ( map (\a -> rotateAtom a aroundAxis angle) atoms ) bonds
60
61  rotateAtom :: Atom -> Axis -> Float -> Atom
62  rotateAtom a@(Atom i x y z t) Ox angle =
63     Atom i x y' z' t where
64         y' = y * (cos angle) + z * (sin angle)
65         z' = -y * (sin angle) + z * (cos angle)
66  rotateAtom a@(Atom i x y z t) Oy angle =
67     Atom i x' y z' t where
68         x' = x * (cos angle) - z * (sin angle)
69         z' = z * (sin angle) + x * (cos angle)
70  rotateAtom a@(Atom i x y z t) Oz angle =
71     Atom i x' y' z t where
72         x' = x * (cos angle) - y * (sin angle)
73         y' = x * (sin angle) + y * (cos angle)
74

```

```

75 visualize m@(Molecule atoms bonds) = do
76   -- initialization and window
77   getArgsAndInitialize
78   initialDisplayMode $= [ DoubleBuffered, RGBMode, WithDepthBuffer ]
79   initialWindowSize $= Size 300 300
80   initialWindowPosition $= Position (-1) (-1)
81   createWindow "Zzzz!.."
82   -- unchanging attributes of the scene
83   clearColor $= Color4 0 0 0 1
84   shadeModel $= Smooth
85   materialAmbient Front $= Color4 1 1 1 1
86   lighting $= Enabled
87   position (Light 0) $= Vertex4 (-1) 1 1 0
88   light (Light 0) $= Enabled
89   depthFunc $= Just Less
90   materialDiffuse Front $= Color4 1 1 1 1
91   -- callbacks
92   displayCallback $= (display $ moveMolecule m (-cx) (-cy) (-cz))
93   reshapeCallback $= Just (reshape sz)
94   -- keyboardMouseCallback $= (Just keyboardMouse)
95   mainLoop
96   where
97     maxx = maximum $ map (\a@(Atom _ x _ _) -> x) atoms
98     maxy = maximum $ map (\a@(Atom _ _ y _) -> y) atoms
99     maxz = maximum $ map (\a@(Atom _ _ _ z) -> z) atoms
100    minx = minimum $ map (\a@(Atom _ x _ _) -> x) atoms
101    miny = minimum $ map (\a@(Atom _ _ y _) -> y) atoms
102    minz = minimum $ map (\a@(Atom _ _ _ z) -> z) atoms
103    sz = realToFrac $ 1.05 * maximum [maxx-minx, maxy-miny, maxz-minz]
104    cx = (sum $ map (\a@(Atom _ x _ _) -> x) atoms) / (fromIntegral $ length atoms)
105    cy = (sum $ map (\a@(Atom _ _ y _) -> y) atoms) / (fromIntegral $ length atoms)
106    cz = (sum $ map (\a@(Atom _ _ _ z) -> z) atoms) / (fromIntegral $ length atoms)
107
108 display m@(Molecule atoms bonds) = do
109   print "-- display"
110   clear [ ColorBuffer, DepthBuffer ]
111   renderAtoms atoms
112   renderBonds atoms bonds
113   swapBuffers
114
115 renderAtoms (a@(Atom _ x y z t):atoms) = do
116   materialDiffuse Front $= atomColor4 t
117   translate $ Vector3 x y z
118   renderObject Solid $ Sphere' (radiusOfAtom t) 32 32
119   translate $ Vector3 (-x) (-y) (-z)
120   renderAtoms atoms
121 renderAtoms [] = do return () -- do nothing
122
123 atomColor4 atomType
124 | atomType == "H" = Color4 1 1 1 1 -- white
125 | atomType == "F" = Color4 0 1 0 1 -- green
126 | atomType == "Cl" = Color4 0 1 0 1 -- green
127 | atomType == "Br" = Color4 0 1 0 1 -- green
128 | atomType == "I" = Color4 0 1 0 1 -- green
129 | isPrefixOf "C." atomType = Color4 0 1 1 1 -- cyan instead of gray
130 | isPrefixOf "N." atomType = Color4 0 0 1 1 -- blue
131 | isPrefixOf "O." atomType = Color4 1 0 0 1 -- red
132 | isPrefixOf "S." atomType = Color4 1 1 0 1 -- yellow
133 | isPrefixOf "P." atomType = Color4 1 0 1 1 -- magenta
134 | otherwise = Color4 1 0 1 1 -- magenta
135
136 radiusOfAtom atomType
137 | atomType == "H" = 0.38
138 | otherwise = 0.62
139
140 renderBonds atoms (b@(Bond i j _):bonds) = do
141   materialDiffuse Front $= Color4 1 1 1 1
142   --translate $ Vector3 x y z
143   renderQuadric style $ Cylinder 1.0 0.24 1.0 32 1 -- not from GLUT
144   --translate $ Vector3 (-x) (-y) (-z)
145   renderBonds atoms bonds
146   where
147     style = QuadricStyle (Just Smooth) NoTextureCoordinates Outside FillStyle

```

```

149 renderBonds _ [] = do return () -- do nothing
150
151 reshape sz size@(Size width height) = do
152     print "--reshape"
153     print width
154     print height
155     --
156     viewport $= (Position 0 0, size)
157     matrixMode $= Projection
158     loadIdentity
159     if width <= height
160     then ortho (-sz) sz (-sz * h/w) (sz * h/w) (-sz) sz
161     else ortho (-sz * w/h) (sz * w/h) (-sz) sz (-sz) sz
162     matrixMode $= Modelview 0
163     loadIdentity
164     where
165         w = fromIntegral width
166         h = fromIntegral height
167
168 -- keyboardMouse _ _ (Char '\27') Down _ _ = exitWith ExitSuccess -- exit on ESC

```