Benzene

Figures 3a provide the DF for the benzene molecule obtained from a sphere center located at the center of the hexagonal carbon structure and with three different radius R=1.5, R=1.8 and R=2.0. While figures 3b, depict the stereographic projection of the benzene DF from a sphere surface centered at a carbon atom at varied radius R=1.4, R=1.8 and R=2.0. The resulting pictures show how the sphere radius and the center around a molecule can give pictures indicating the nature of the atomic sites and the density distribution around the molecular bonds. For instance, the leftmost surface in figure 3a corresponds to consider a projection sphere located inside the hexagonal ring. In such sphere surface it is projected the density attached to the carbon C₆ hexagon. Then, a sort of circular torus is obtained. Taken from left to right, in the other two following projection surfaces in figure 3a, the density stereographic projections reveal the position of the heavy atoms in a better form as the spherical radius increases and the hexagon becomes nearest to the sphere surface.

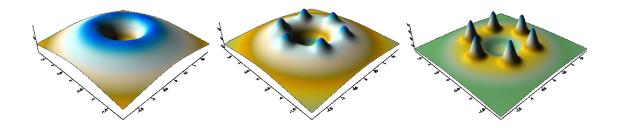


Figure 3a. Stereographic projection of the benzene DF on the surface of a sphere centered at the molecular hexagon center and radius from left to right: R=1.5, R=1.8 and R=2.0.

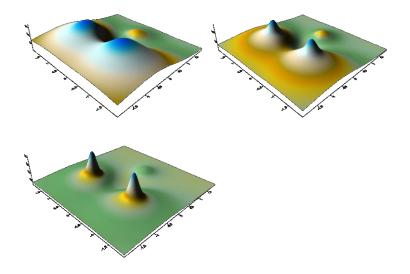


Figure 3b. Stereographic projection of the benzene DF on the surface of a sphere centered at a reference carbon atom, with increasing sphere radius from left to right: R=1.4, R=1.8 and R=2.0.

In figure 3b, the two twin peaks correspond to the density due to the two C-C bonds associated to a reference C atom bonded to two nearest C atoms. The reference C atom is now placed at the projection sphere center and thus into the stereographic plane origin, which as depicted in figure 2, it is chosen as the plane center. When the sphere radius R increases (from left to right) the position of the nearby carbon atoms is increasingly revealed by increasing density peaks. The third small peak, which can be seen in the three figure 3b projections, corresponds to the reference C atom C-H bond density.