Borazine

Borazine ($B_3N_3H_6$) has been chosen because this molecule possesses a hexagonal structure comparable to the one of benzene, but with a complete different set of atoms, providing a similar but different DF stereographic environment.

Figure 4a presents a map obtained with the sphere center at the hexagon center and with three radii, from left to right: *R=4.2, R=4.6* and *R=4.*8. These radii have been chosen different than in the benzene case to obtain an alternative view of a hexagonal molecular structure. In this case, the surface of the sphere is placed outside of the hexagonal B and N skeleton, with the surface nearby to the H atoms. The peaks identify the B-H and N-H bond densities. Higher peaks correspond to N-H bonds, while the small ones to the B-H.

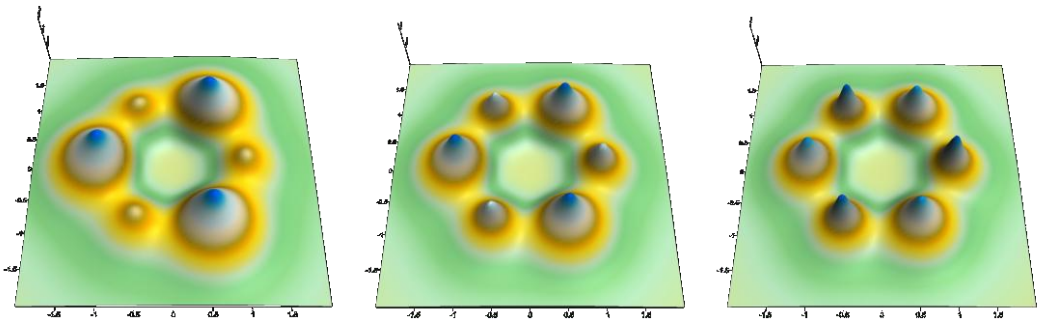

Figure 4a. Borazine ($B_3N_3H_6$) DF stereographic projection using a sphere centered at the hexagon molecular center and three radii *R=4.2, R=4.6* and *R=4.*8, the resulting maps can be observed from the pictures from left to right.

Figure 4b corresponds again to borazine, but the stereographic sphere is now centered at a chosen reference boron atom. From left to right pictures the sphere radius corresponds to the values: *R=3.8, R=4.0* and *R=4.1*. Here, the two peaks in the leftmost stereographic projection are attached to H densities. From left to right the initial H density values decrease, while the densities attached to the two nearby boron atoms become increasingly revealed. The N density is located at the central position of the curved shape density range.

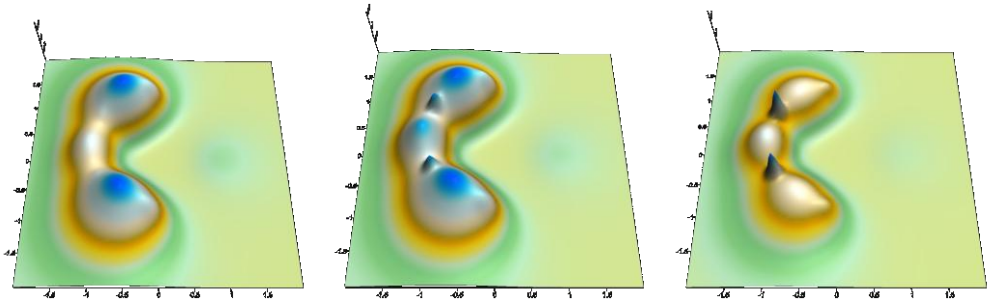

Figure 4b. Borazine ($B_3N_3H_6$) DF stereographic projection using a sphere centered at a boron atom by means of choosing three different radii *R=4.2*, *R=4.6* and *R=4.*8, the resulting maps can be observed from the pictures from left to right.