This journal is © the Owner Societies 2010

Table I: Occupancy level, atomic orbital/hybrid coefficients for the $C_{11}F_{12}$ antibondng orbital

| **C11-F12 antibonding orbital in monomer** | | | |
|---|---|---|---|
| Occupancy | Bond orbital | Coefficients | Hybrids |
| 0.0801 | BD* C11- F12 | 0.8494* C 11 | s (22.89%) p 3.35(76.64%) d 0.02(0.47%) |
| | | -0.5278* F 12 | s (25.19%) p 2.97(74.74%) d 0.00(0.07%) |
| **C11-F12 antibonding orbital in the complex** | | | |
| 0.0563 | BD* C11- F12 | 0.8561* C 11 | s (22.87%) p 3.34(76.30%) d 0.04(0.83%) |
| | | -0.5168 * F 12 | s (26.75%) p 2.73(73.16%) d 0.00(0.08%) |

This journal is © the Owner Societies 2010

Figure 1:

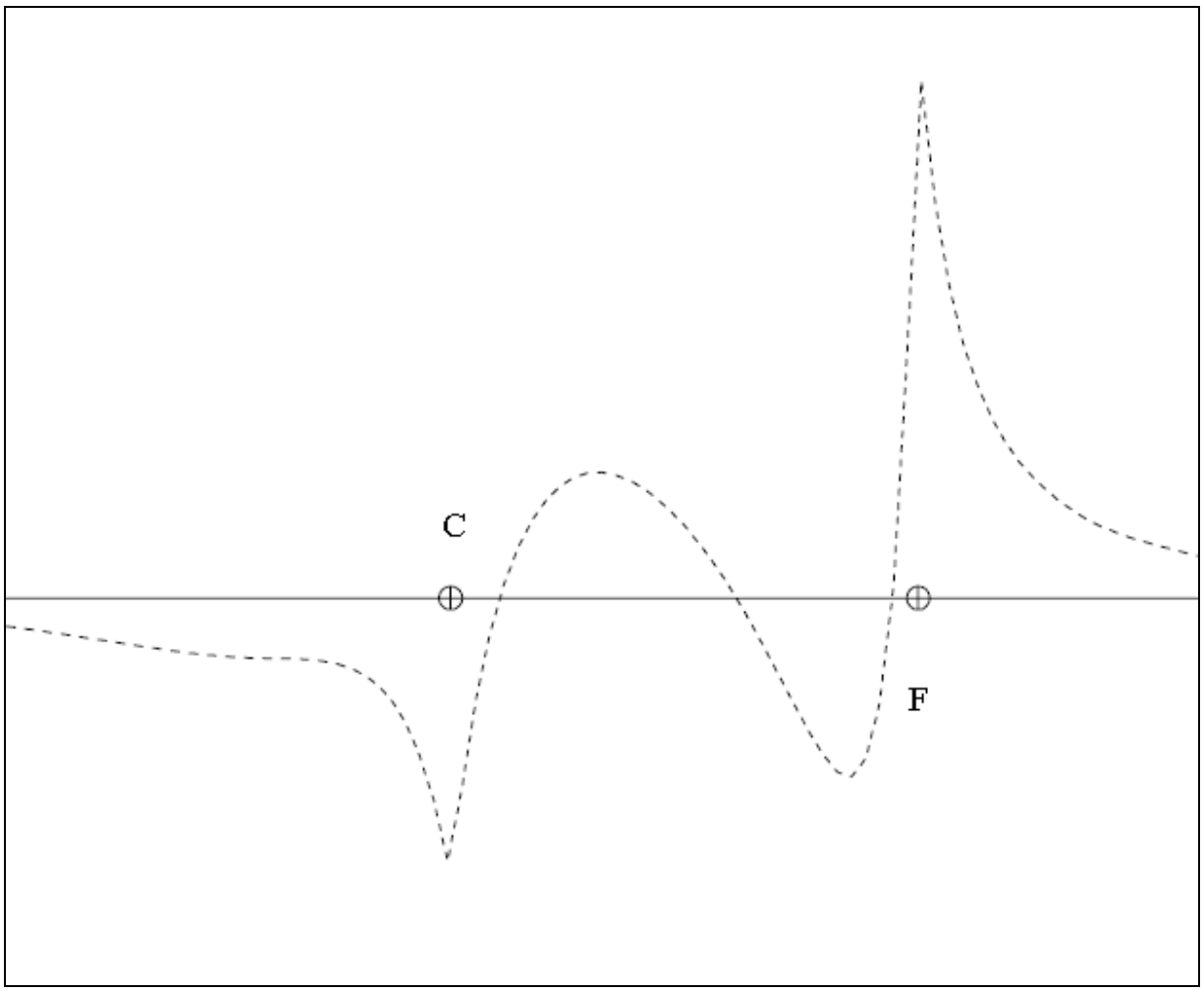


**Figure 1:** 1-D profile plot of the $\sigma^*(C_{11}F_{12})$ orbital along the C-F bond shown in Figure 7c.

The change in the sign of the wavefunction and the corresponding nodes are clearly visible showing it that it is an antibonding orbital.

This journal is © the Owner Societies 2010

Figure 2:

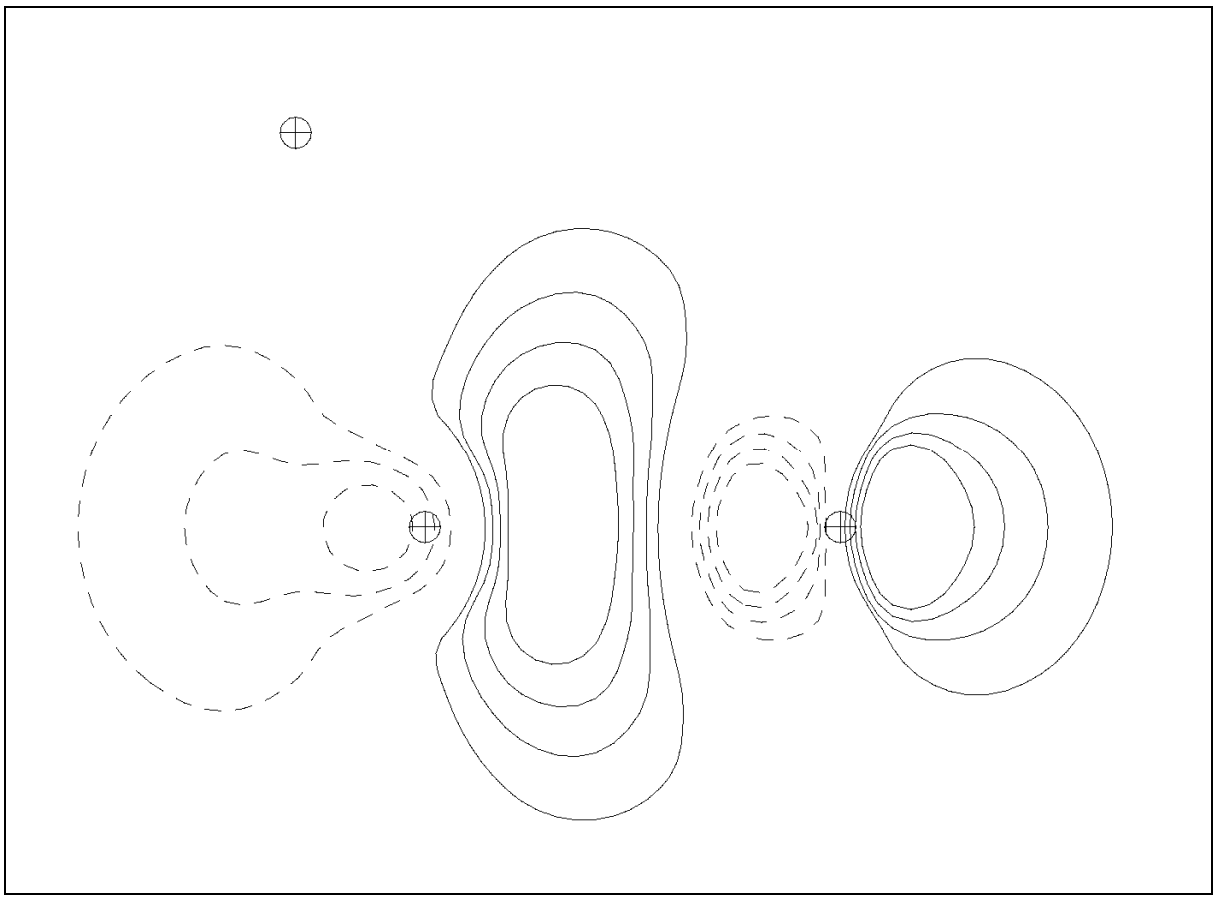

**Figure 2:** 2-D contour plot of the $\sigma^*(C_{11}F_{12})$ orbital shown in Figure 7c. Here also the change in sign of the function and the corresponding nodes characteristic of an antibonding orbital are seen clearly.