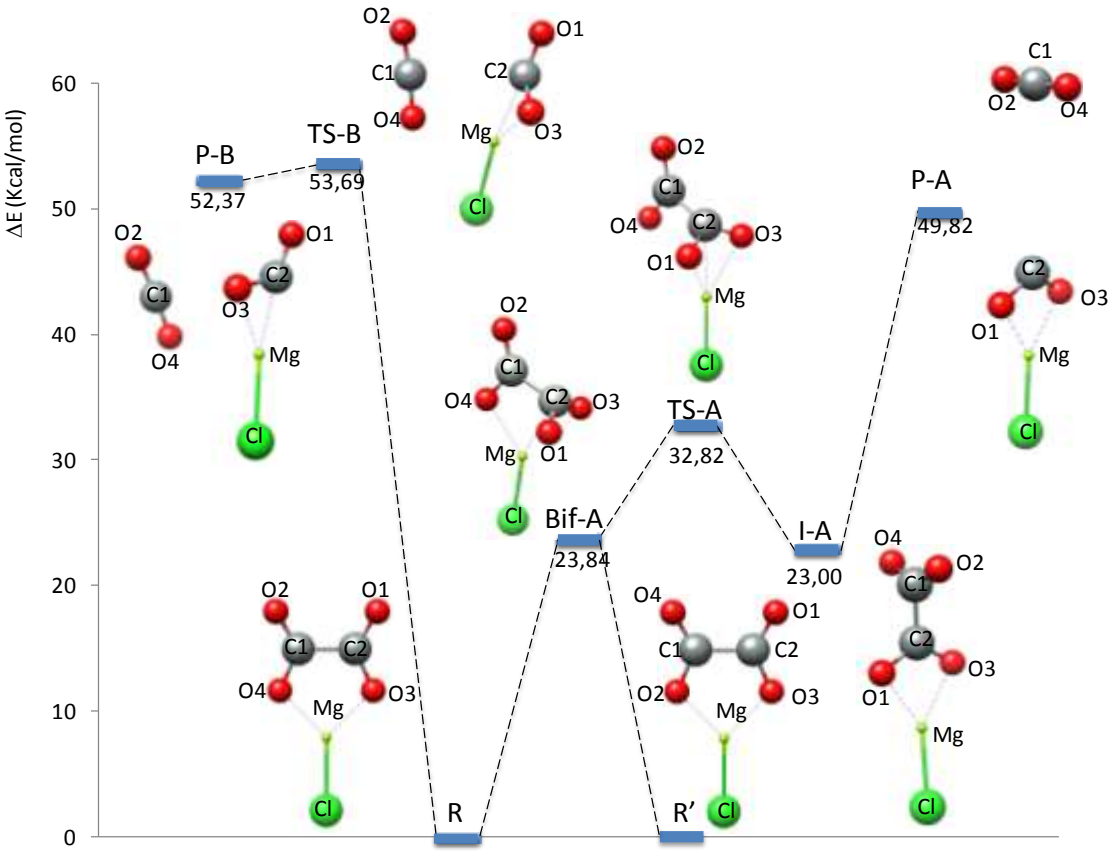


Figure 1: Potential energy profile (including the zero-point energy correction) and geometries of the stationary points for A and B mechanisms, leading to the bidentate double oxygen complex $[ClMg(\eta^2\text{-}O_2C)]^-$ (**P-A**), and bidentate carbon oxygen complex $[ClMg(\eta^2\text{-}CO_2)]^-$ (**P-B**) complex. Relative energies (in kcal mol^{-1}) to reactants (**R**).

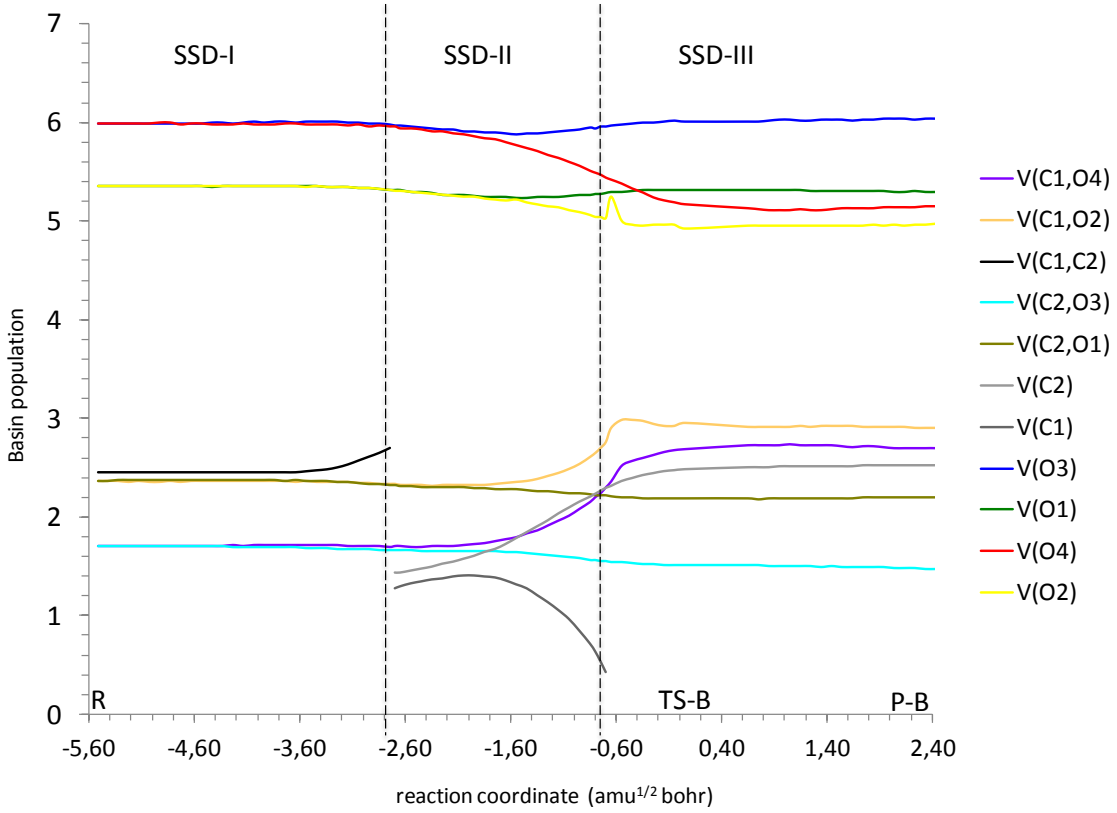


Figure 2. Evolution of the populations of some basins along the IRC pathway for the formation of **P-B** as a function of the reaction coordinate (amu^{½} bohr). Dashed lines separate the three structural stability domains (SSD). For the sake of clarity, the valence basin populations of oxygen and chlorine atoms have been unified as a unique basin population, i.e $V_{i=1,2\ldots}(X_i) = V(X_i)$.

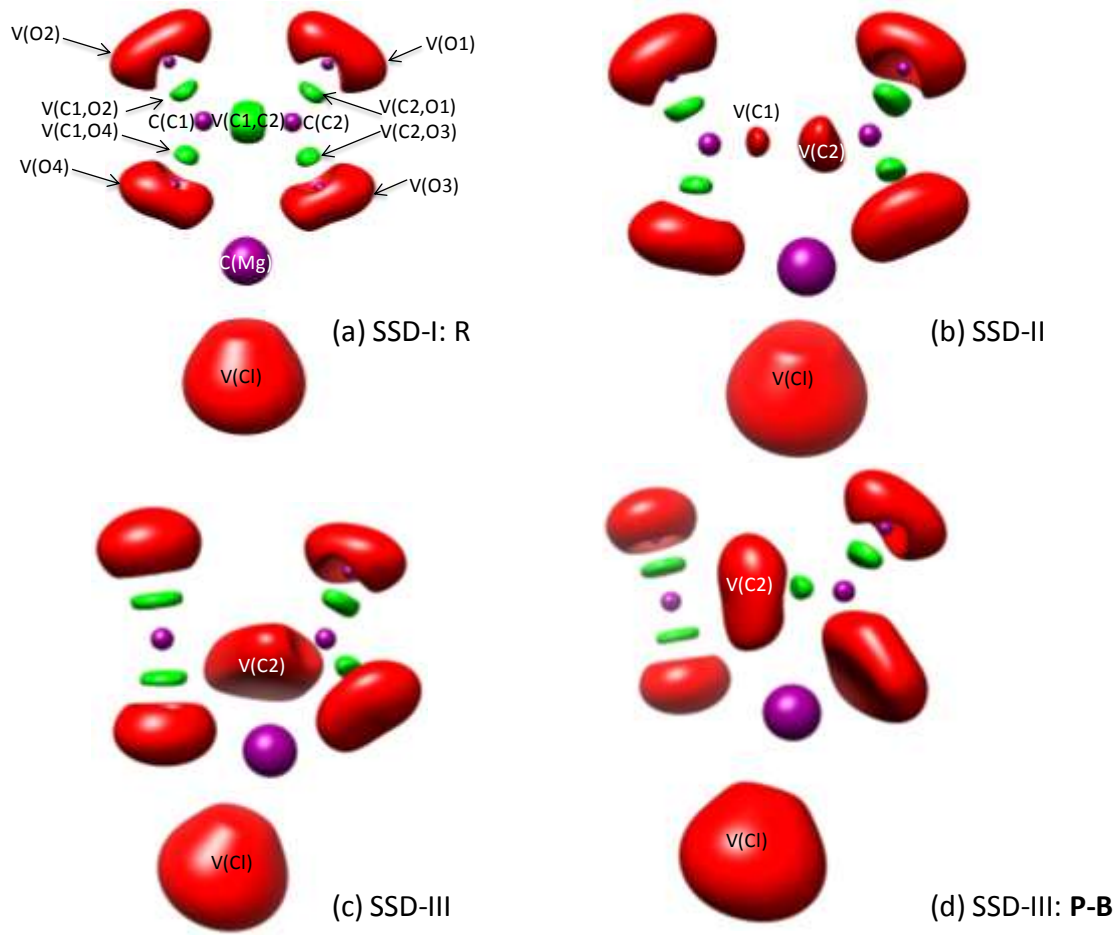


Figure 3. Snapshots of the ELF localization domains for selected points along the IRC for the formation of **P-B**. The isosurface value is η=0.814. The reaction coordinate value is: (a) s = - 5.519 $amu^{1/2}$ bohr (b) s= - 1.499 $amu^{1/2}$ bohr (c) s = -0.050 $amu^{1/2}$ bohr (d) s = 2.591 $amu^{1/2}$ bohr. The color code is as follows: green, disynaptic basins; red, monosynaptic basins; purple, core basins.

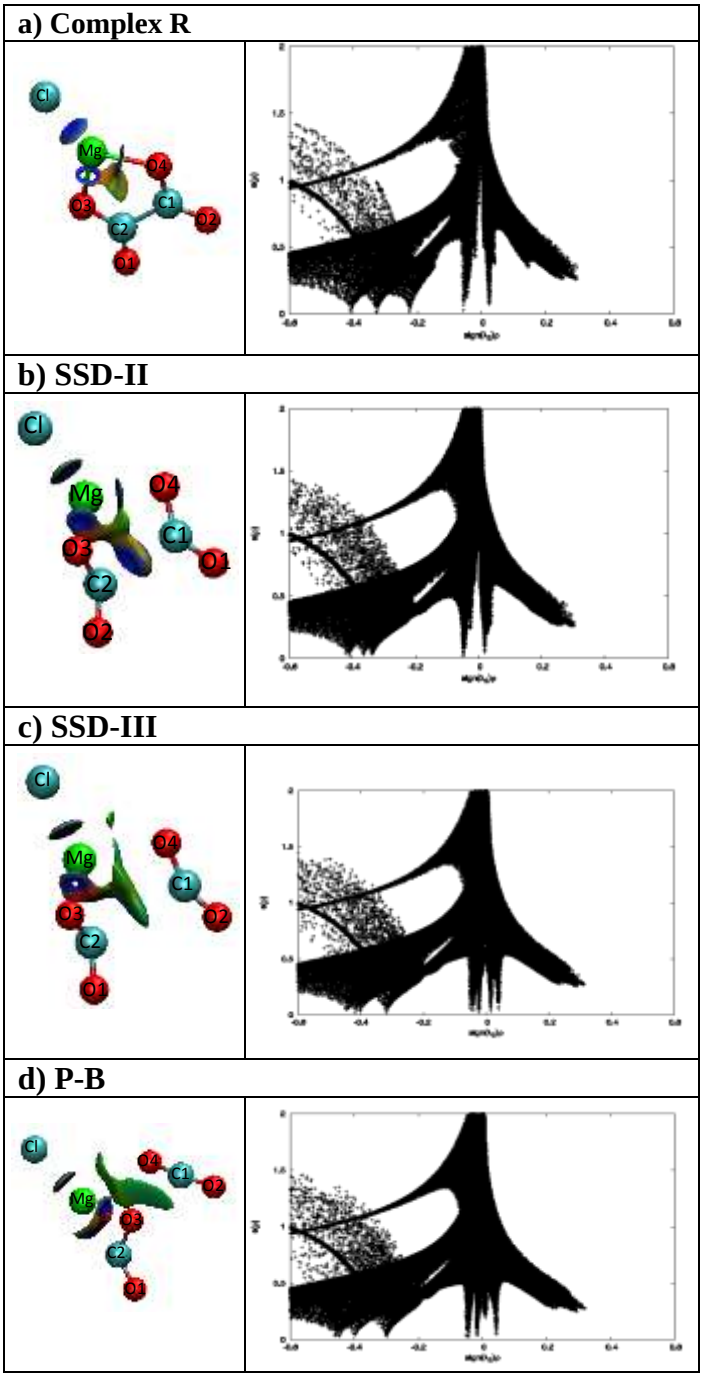
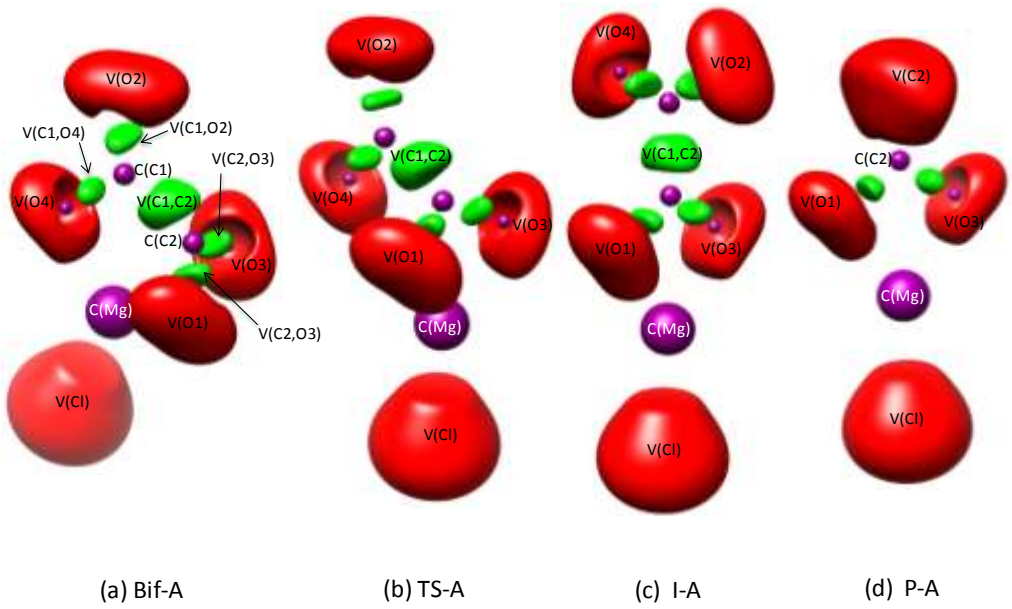


Figure 4. Plots of the reduced density gradient versus the electron density multiplied by the sing of the second Hessian eigenvalue $\rho(r)(\lambda_2)$ and the respective reduced gradient isosurfaces.



(a) Bif-A (b) TS-A (c) I-A (d) P-A

Figure 5. Snapshots of the ELF localization domain (η=0.814 isosurface) for Bif-A, TS-A, I-A and P-A. The color code is as follows: green, disynaptic basins; red, monosynaptic basins; purple, core basins.