

[4+3] and [4+2] Mechanisms of the Diels–Alder reactions of vinylboranes: an analysis of the electron charge density distribution

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Supporting Information

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- Distances, topological properties and delocalization indexes along the IRC paths for selected TSs of the reactions under study (Fig. S1-S10). Pages S2-S11.
- Electronic population of selected atoms along the IRC paths for selected TSs of the reactions under study (Fig. S11). Pages S12 and S13.

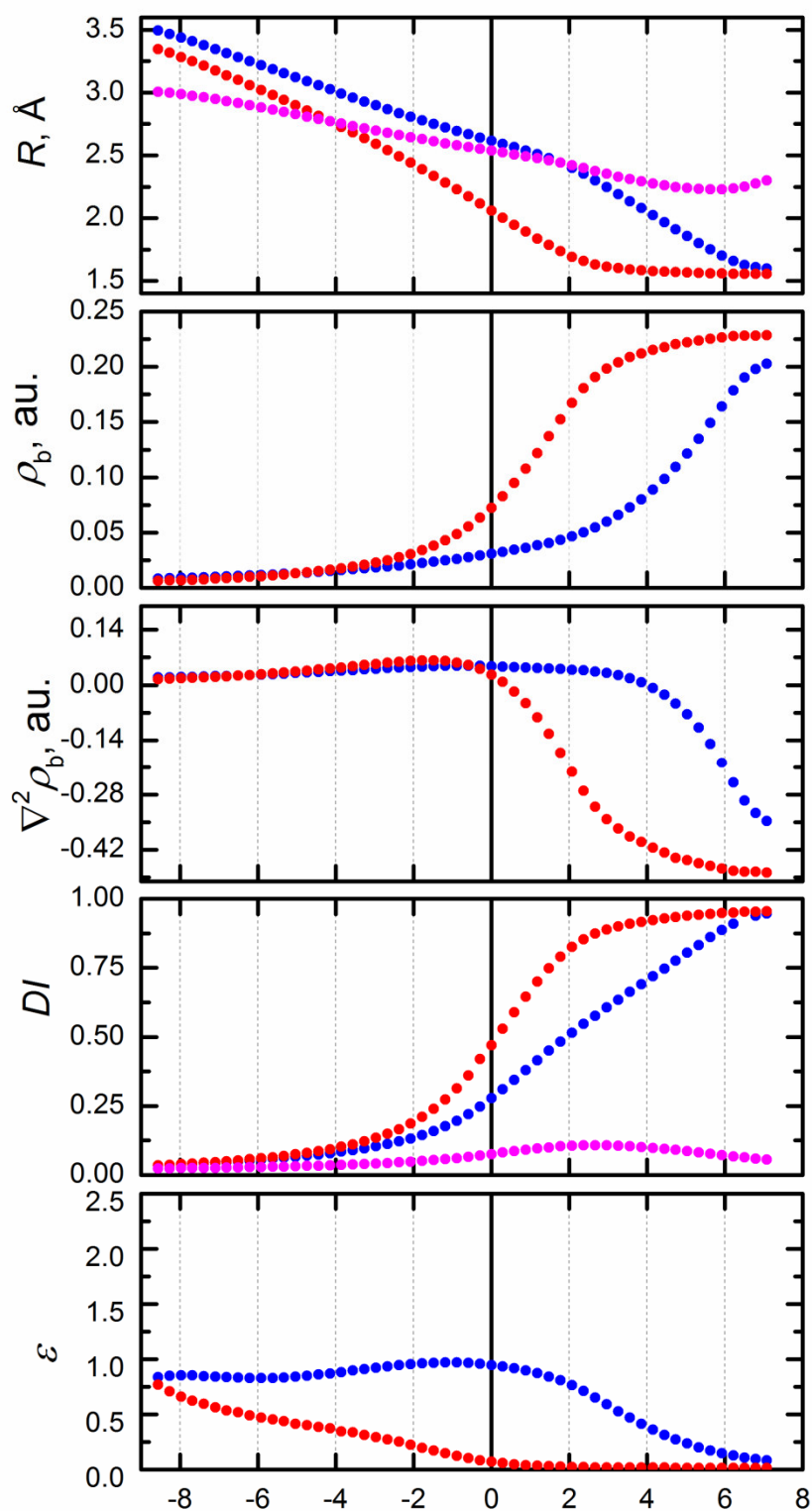


Fig. S1 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-1MX. TSs are located at $s = 0.0 \text{ amu}^{1/2} \text{ Bohr}$.

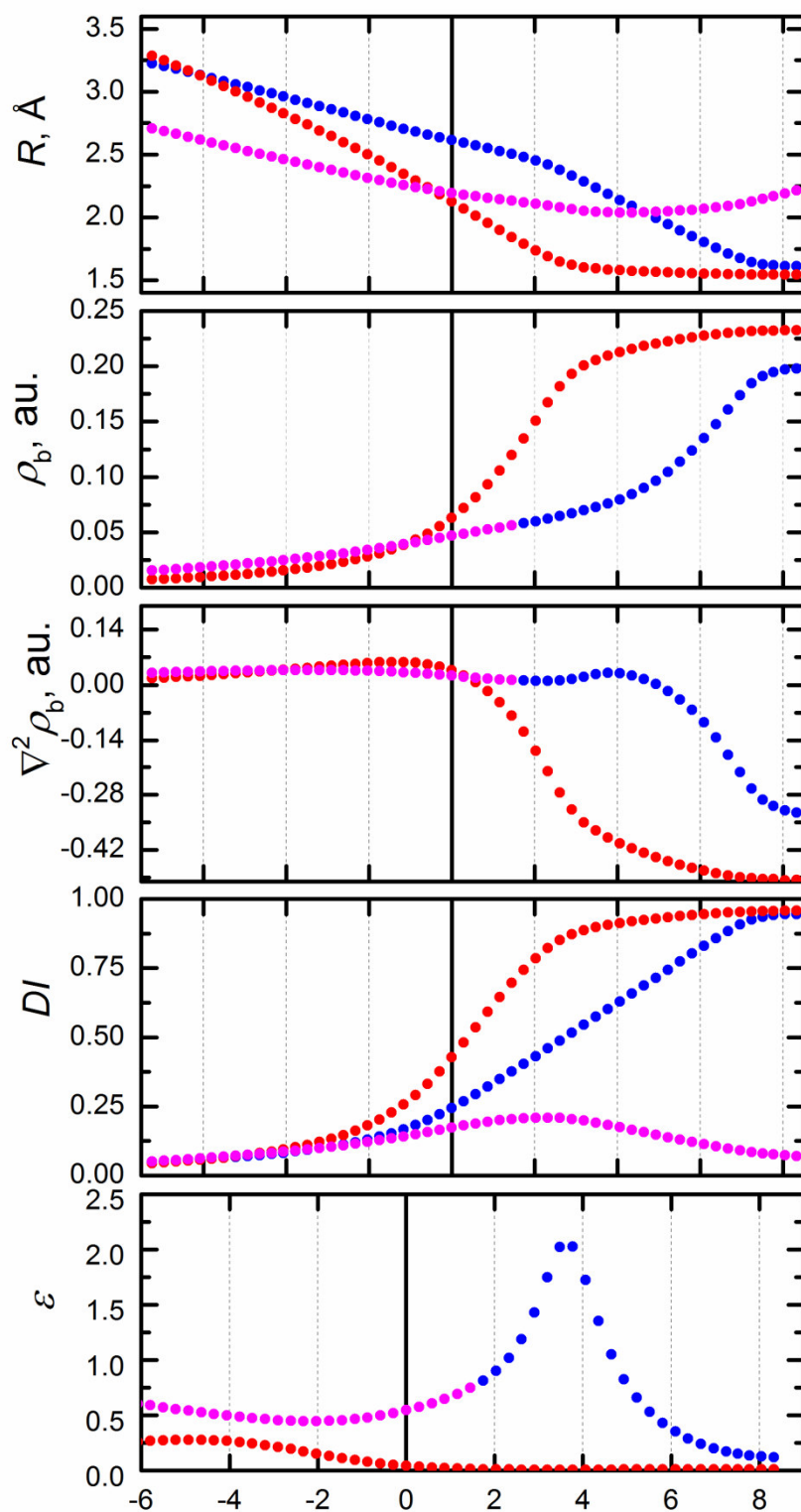


Fig. S2 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-1PN.

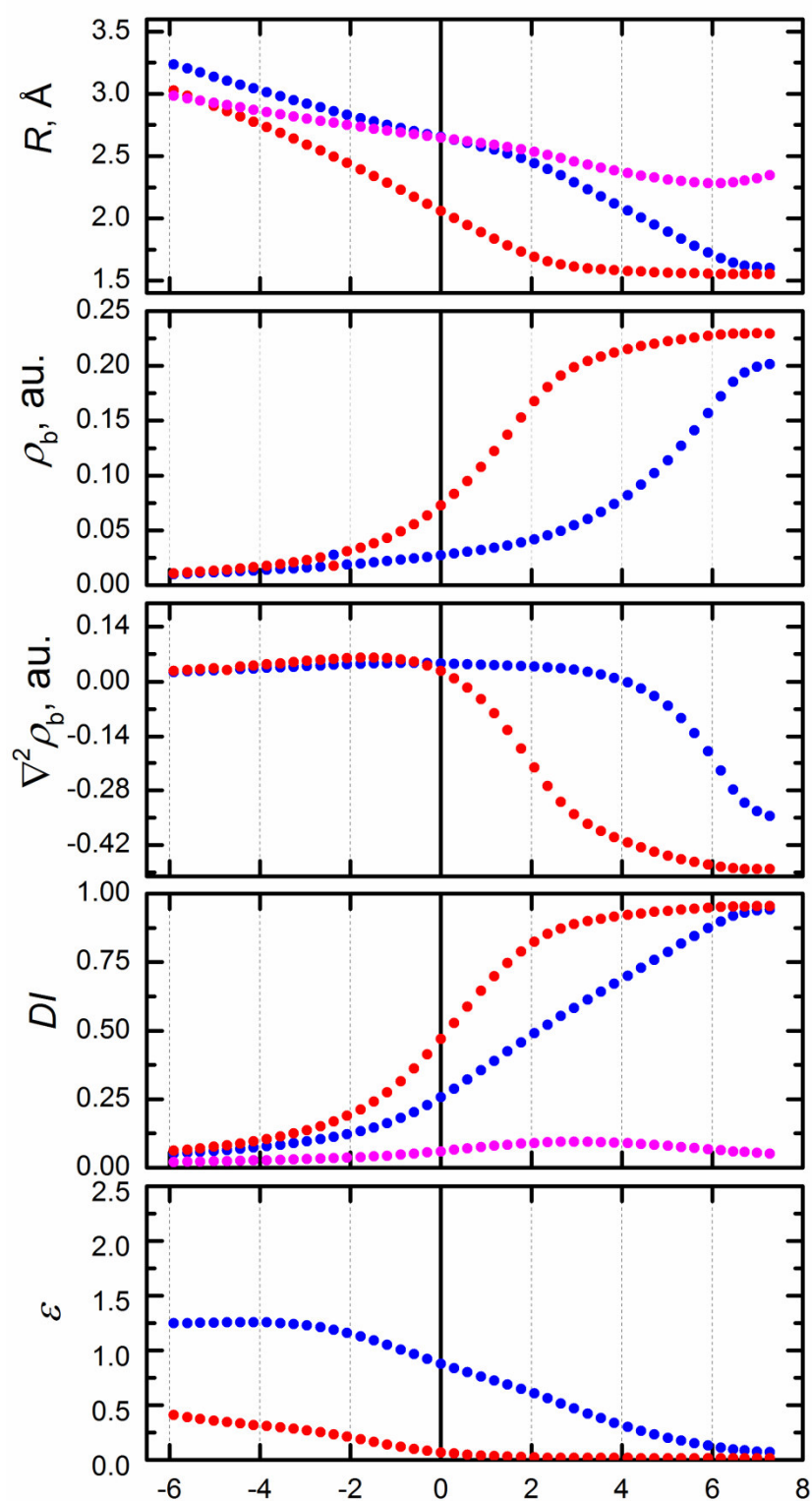


Fig. S3 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-1PX.

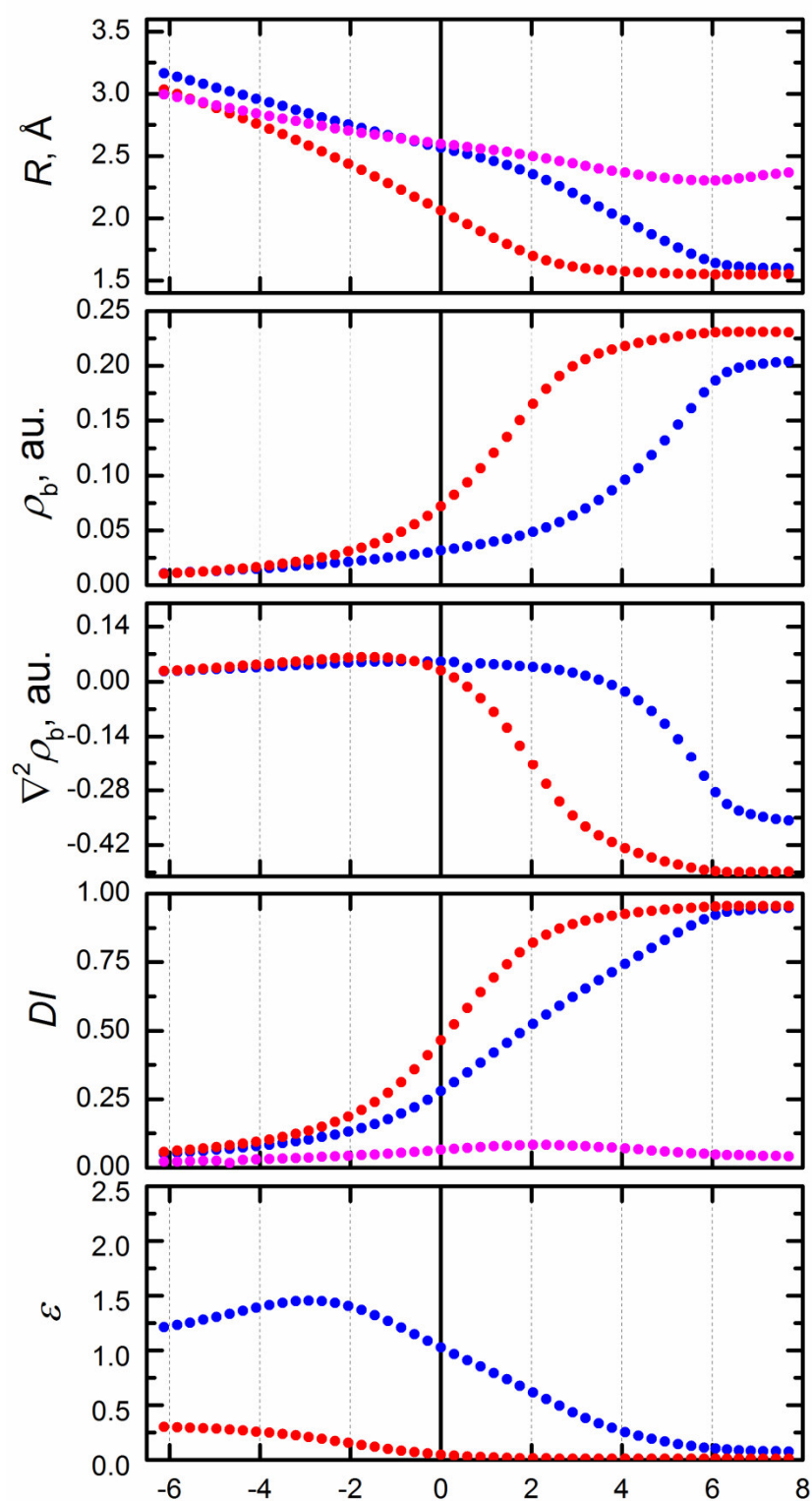


Fig. S4 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-2MN.

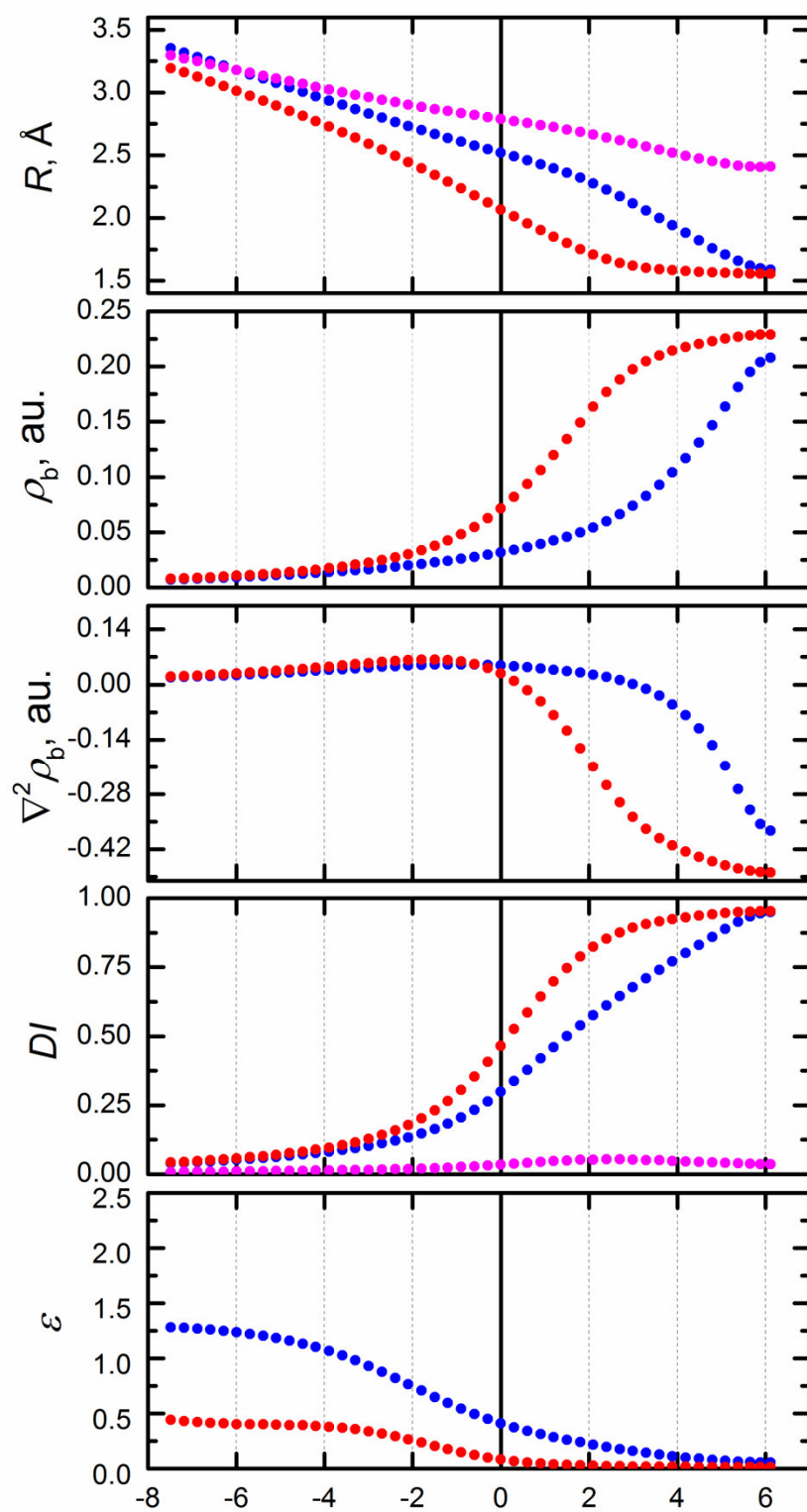


Fig. S5 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-2MX.

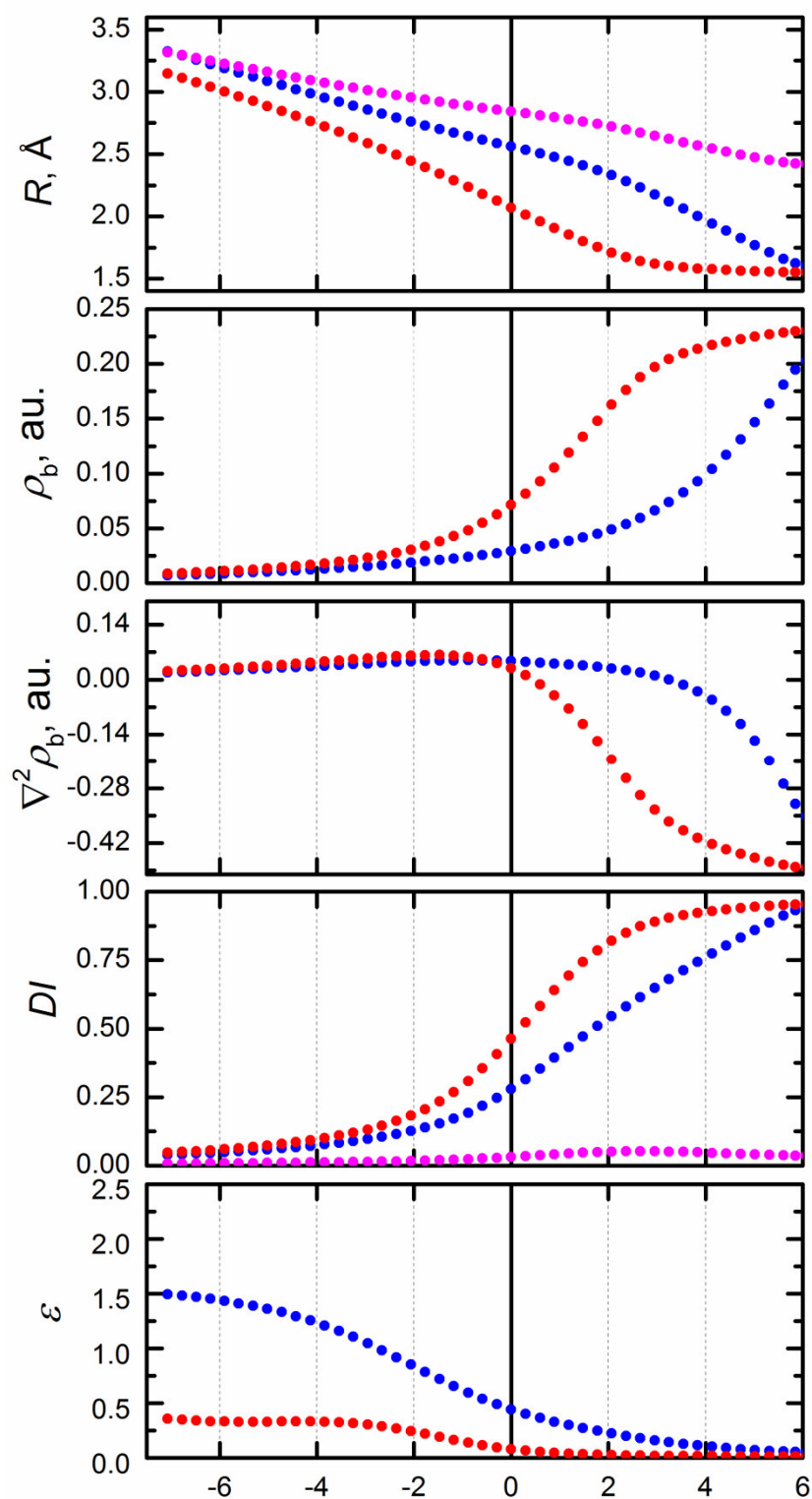


Fig. S6 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-2PX.

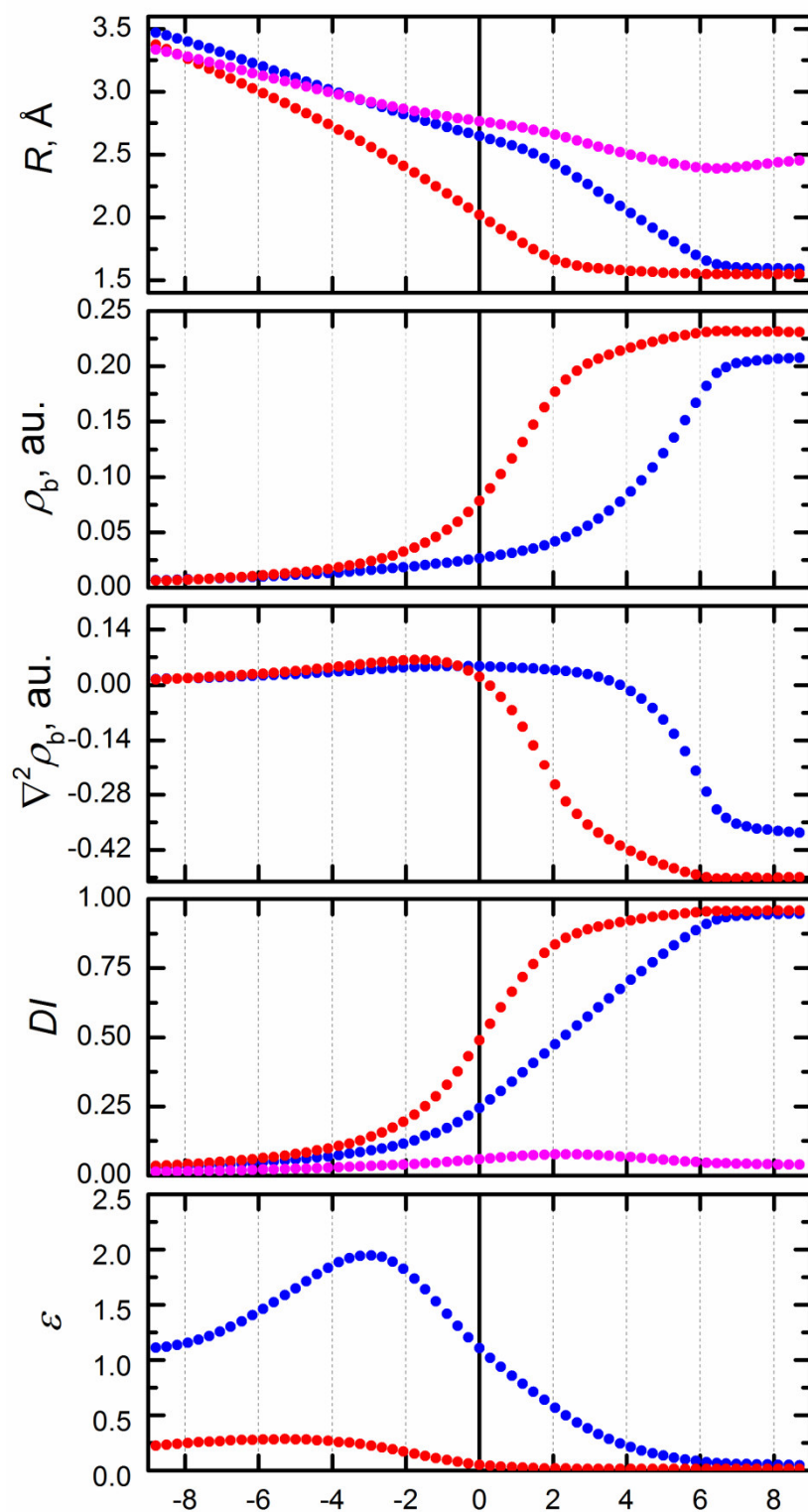


Fig. S7 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-3MN.

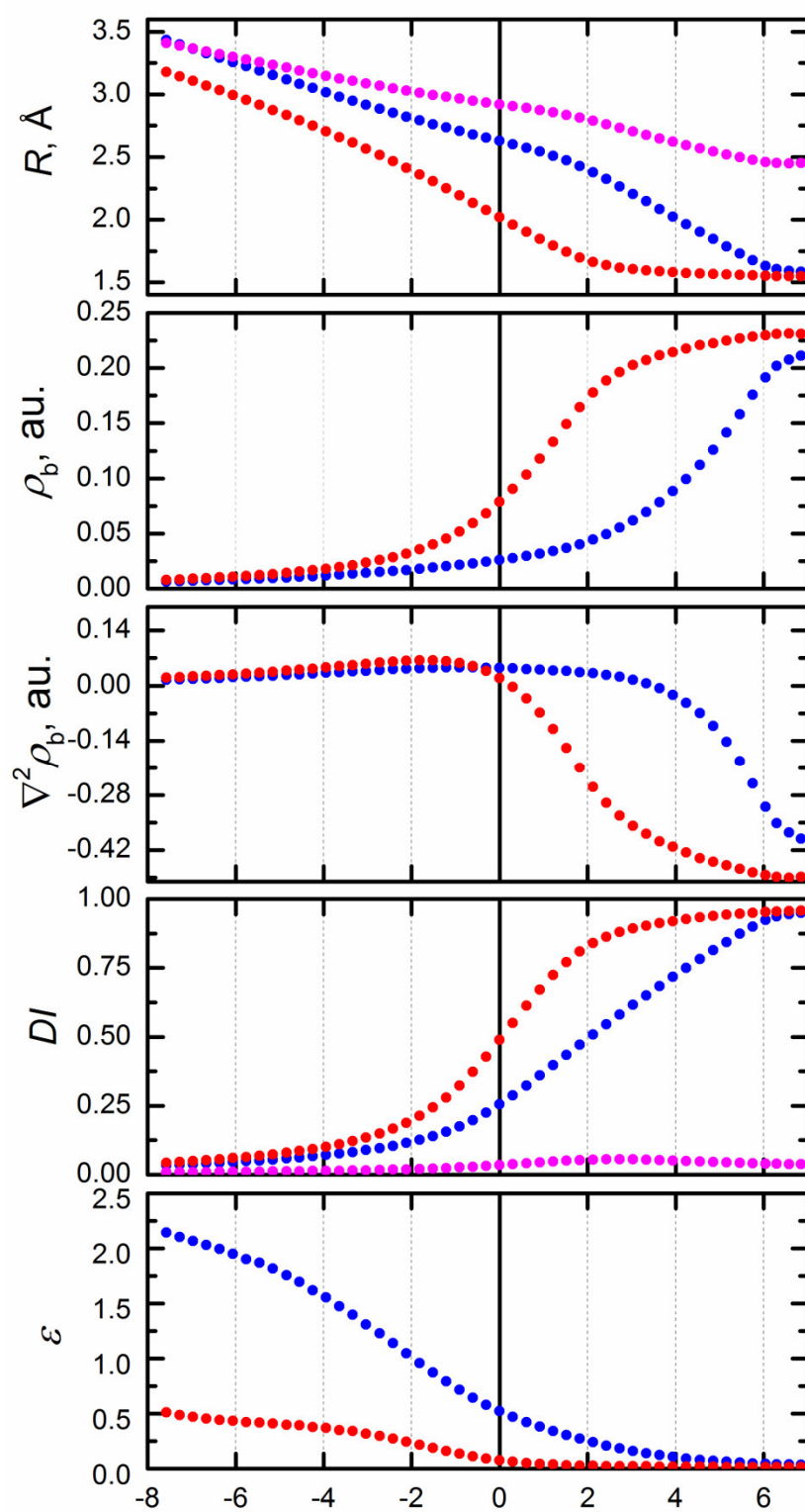


Fig. S8 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-3MX.

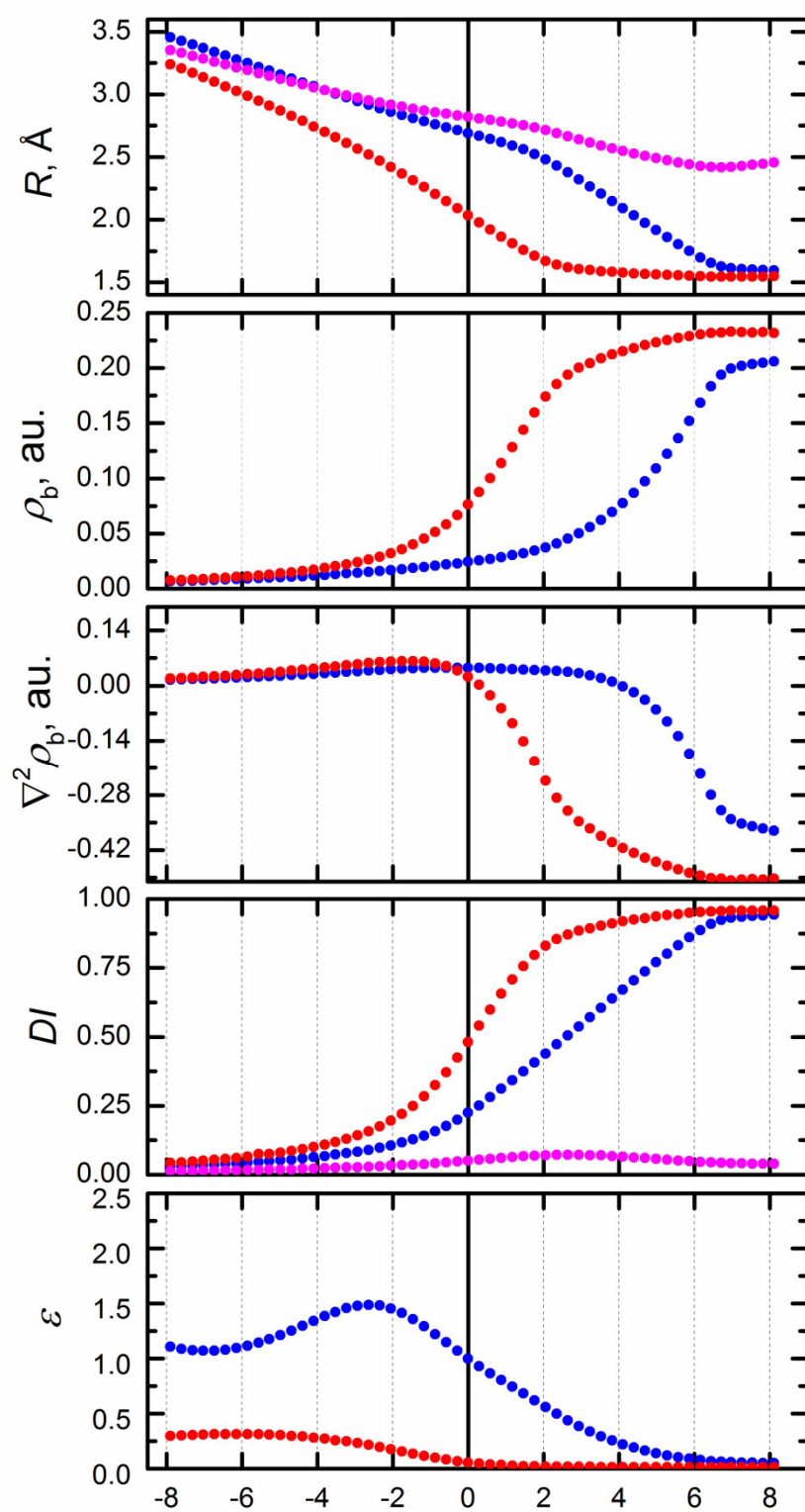


Fig. S9 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-3PN.

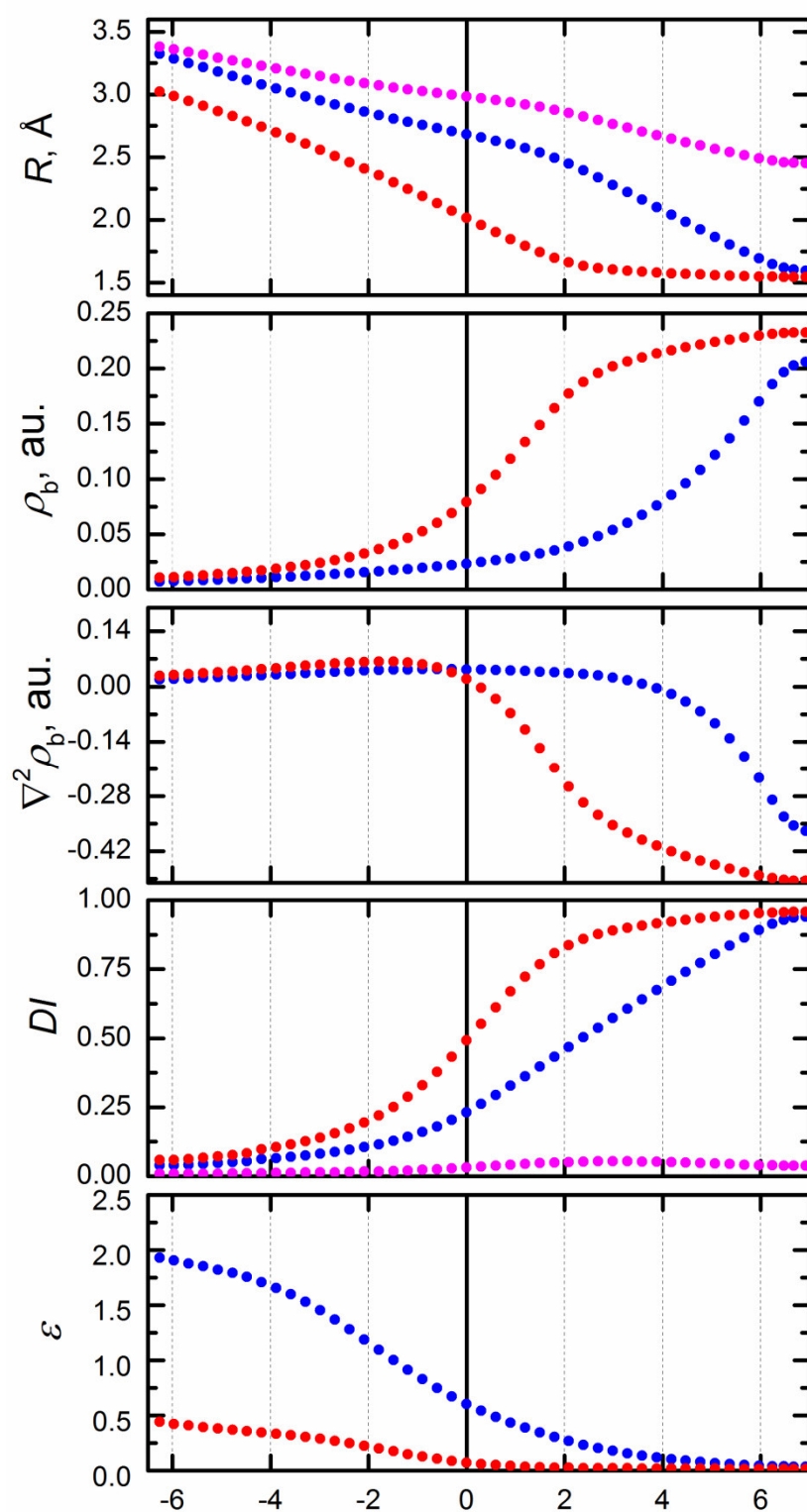


Fig. S10 Distances, topological properties and delocalization indexes along the IRC path corresponding to TS-3PX.

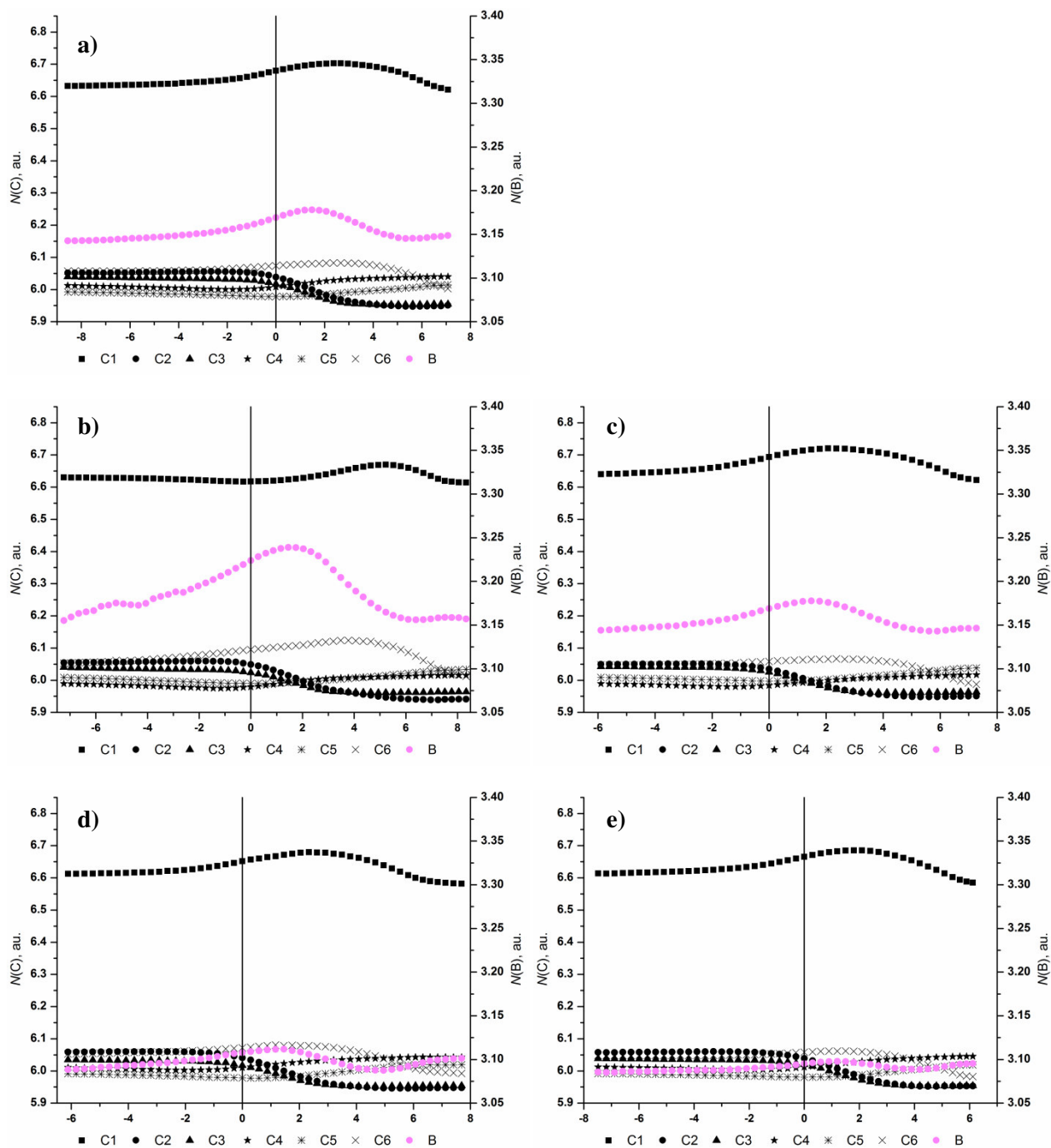


Fig. S11 Part a Electronic population of selected atoms (in e) along the IRC path corresponding to a) TS-1MX, b) TS-1PN, c) TS-1PX, d) TS-2MN, e) TS-2MX, f) TS-2PX, g) TS-3MN, h) TS-3MX, i) TS-3PN and j) TS-3PX. The TSs are located at the value $s = 0.0$ of the reaction coordinate

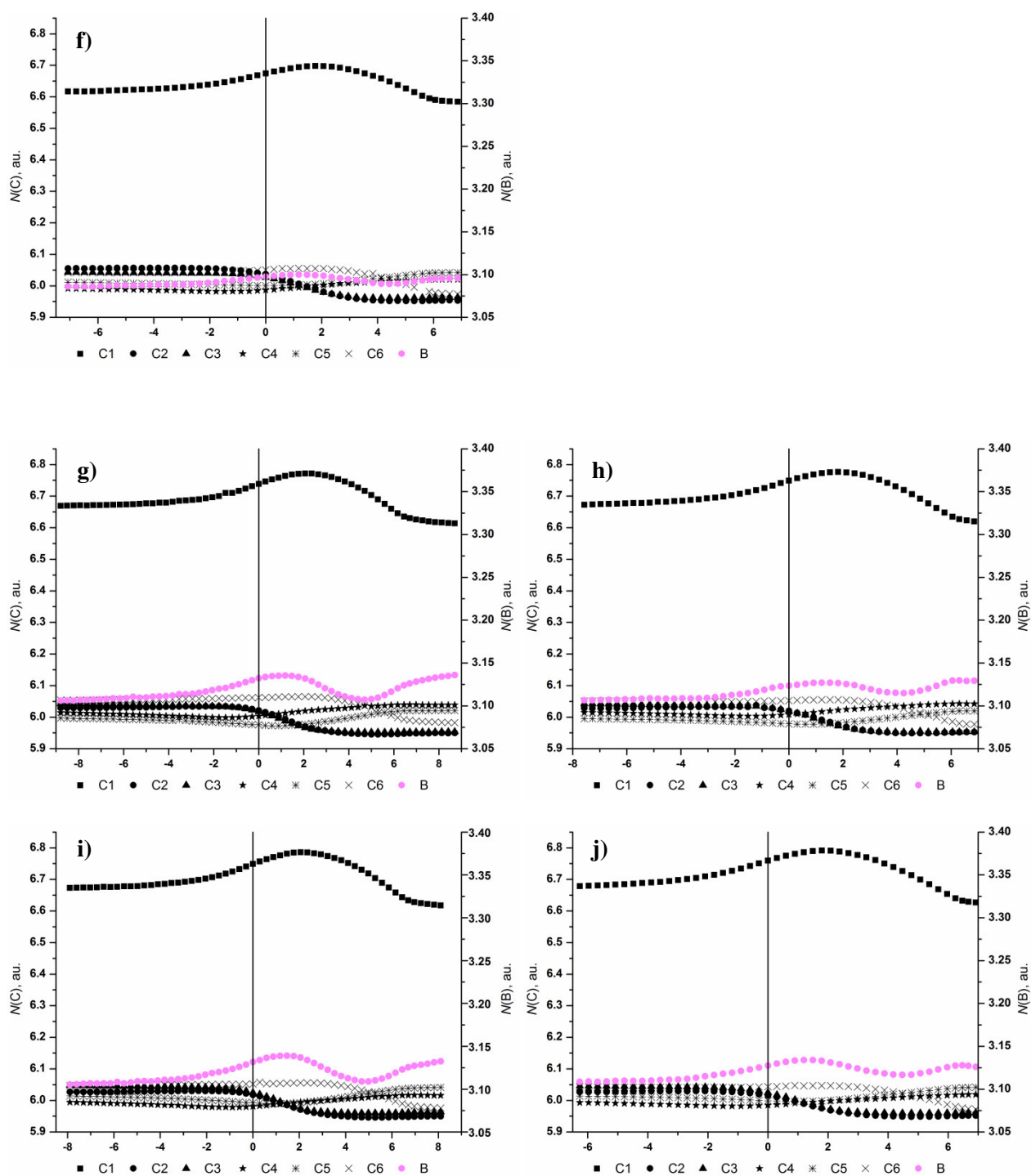


Fig. S11 Part b Electronic population of selected atoms (in e) along the IRC path corresponding to a) TS-1MX, b) TS-1PN, c) TS-1PX, d) TS-2MN, e) TS-2MX, f) TS-2PX, g) TS-3MN, h) TS-3MX, i) TS-3PN and j) TS-3PX. The TSs are located at the value $s = 0.0$ of the reaction coordinate