

Fig. 3. The dynamic correlation diagram (a) and the corresponding state diagram (b) for the conversion of Dewar benzene to benzene.

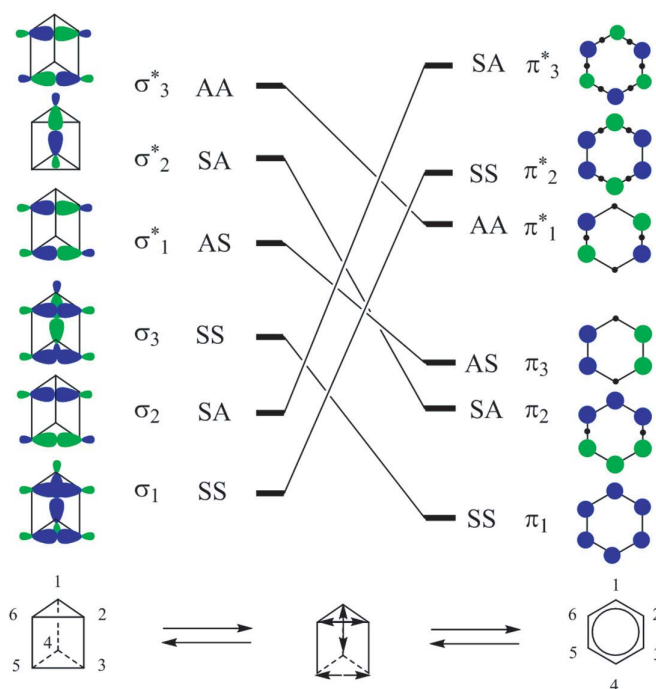


Fig. 4. The dynamic correlation diagram for the conversion of prismane to benzene.

in Figs. 3(a) and (b) (Nohira and Nohira, 2013).

The diagrams have been drawn in the same style used in the previous paper (Nohira and Nohira, 2012). The meaning of each symbol in Fig. 3 (also in Fig. 4) is as follows. σ : σ bonding orbital, σ^* : σ antibonding orbital, π : π bonding orbital, π^* : π antibonding orbital, SA: laterally symmetric and vertically antisymmetric, AS: laterally antisymmetric and vertically symmetric, SS: both laterally and vertically symmetric, AA: both laterally and vertically antisymmetric. Here, the shapes of π orbitals and the corresponding energy levels for the reactants and products are the same

ones that were used for the correlation diagram by Woodward and Hoffmann. They used the simple Hückel method to estimate the shapes and energy levels (Streitwieser, 1961; Rauk, 2001). Since this method is generally sufficient in terms of accuracy for present purposes, it has also been adopted in this study. Although we assumed that the energy level of an ordinary C–C σ bond was 1.3β in our previous paper (Nohira and Nohira, 2012), we assigned that of Dewar benzene to 1.2β , considering the effect of ring strain. From Fig. 3(b), we can easily explain the phenomenon that thermal isomerization of Dewar benzene to benzene pro-