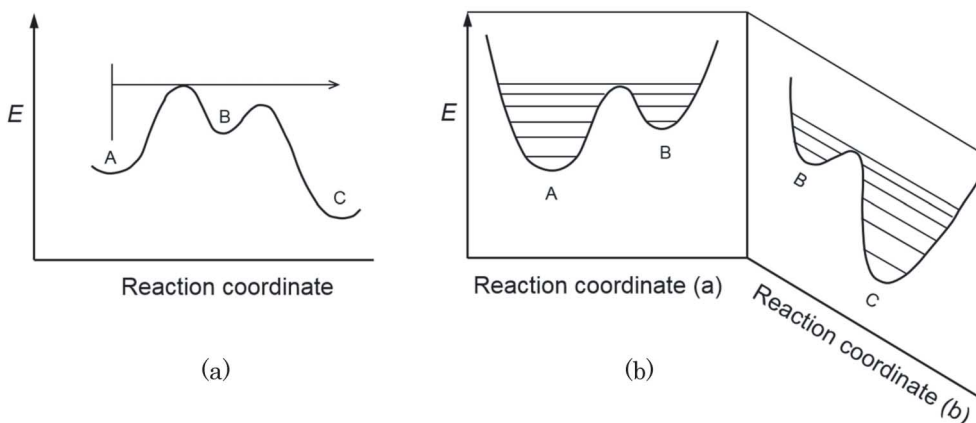Fig. 5. The energy surface for an elementary reaction.

Fig. 6. Exemplified energy profiles for a two-step reaction: (a) commonly used figure; (b) proposed one showing clearly the situation consists of two elementary reactions.

ceeds via the formation of an excited state of benzene, accompanied by chemiluminescence.

4.3 Prismane-benzene

Woodward and Hoffmann have indicated a reasonable relation between the orbitals of reactant and product for the conversion of prismane to benzene (Woodward and Hoffmann, 1969). In their figure, however, the orbitals have not been drawn in the order of energy level, because the crossing of the correlation lines, which have the same symmetry, cannot be avoided. As the result, they have not provided a complete correlation diagram.

If we are not restrained by the non-crossing rule, then we can complete the diagram for this conversion as shown in Fig. 4. This figure clearly shows that the σ_1 and σ_2 bonding orbitals of prismane are linked to the π_2^* and π_3^* antibonding orbitals of benzene. Thus, this reaction is forbidden in the ground state.

5. The Validity of the Schrödinger Equation for the Midway State of Elementary Chemical Reactions

As mentioned earlier, we have defined an elementary reaction as a one-step reaction that does not have any stable intermediates. This means that the electronic structure of the intermediate state is continuously changing over time, and that there is no steady state. As stated in Section 3, a typical elementary chemical reaction proceeds in time

intervals of $10^{-14}-10^{-13}$ s.

Figure 5 shows a schematic of the potential energy surface for an elementary reaction. The horizontal axis is the reaction coordinate, r, and the vertical axis is the energy level of the electronic system of the molecule, E. We assume that the stable state of molecule A changes to another stable state of molecule B. M and N denote the centers for the position coordinates of A and B, respectively.

The moment of elementary reaction from A to B is the point at which the reaction coordinate changes from M to N. In conventional discussions of a potential surface diagram, time, t, is not considered. For elementary reactions, however, t should be considered, because the state changes with time, i.e. r is a function of t:

$$r = f(t). \tag{1}$$

Meanwhile, there is an inherent uncertainty in the energy levels of the midway states of chemical reactions according to the Heisenberg uncertainty principle (Heisenberg, 1927):

$$\Delta E \times \Delta t \geq h/2\pi = \hbar \tag{2}$$

where, h is the Planck constant and $\hbar$ is the reduced Planck constant. This principle clearly states that "a state that only exists for a short time cannot have a definite energy".

We have previously pointed out that the midway state of a chemical reaction cannot be accurately described within the