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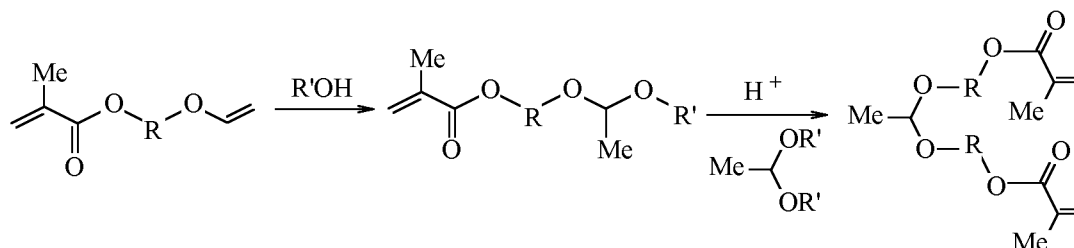
MNDO/PM3 Study Method of the Reaction Mechanism between Methane and Complexes Generated in $\text{Br}_2\cdot\text{AlBr}_3$ System

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Potential energy surface (PES) of systems AlBr_5 and $\text{AlBr}_5 + \text{CH}_4$ were investigated by MNDO/PM3 method. All the five donor-acceptor complexes $\text{Br}_2\cdot\text{AlBr}_3$ with no barrier add to methane providing multiple adducts with various localization of interactions and with different conformations. However further transformations occur only with adducts of two complexes $\text{Br}_2\cdot\text{AlBr}_3$ possessing considerable ionic character. On the reaction path resulting in CH_3Br and HBr as intermediates function bromonium type complexes $\text{CH}_3\text{BrH}^+ - \text{AlBr}_4^-$ and the intermediates on the path leading to CH_2Br_2 and H_2 are the complexes with 3c-2e bond of H_2 quasi-molecule with the C atom of bromomethyl cation $\text{H}_2\text{C}(\text{H}-\text{H})\text{Br}^+ - \text{AlBr}_4^-$. Potential barriers on both reaction paths are about 30 kcal mol⁻¹, and the transition states (TS) are analogous to the classical 3c-2e TS (Olah scheme) with an electrophile attack on a CH bond and to the recently suggested TS with an electrophile attack on an unshared electron pair of the carbon atom in the nonclassical methane $\text{H}_2\text{C}(\text{H}-\text{H})$ respectively.

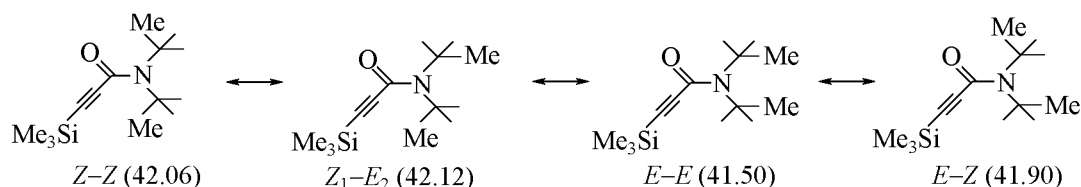
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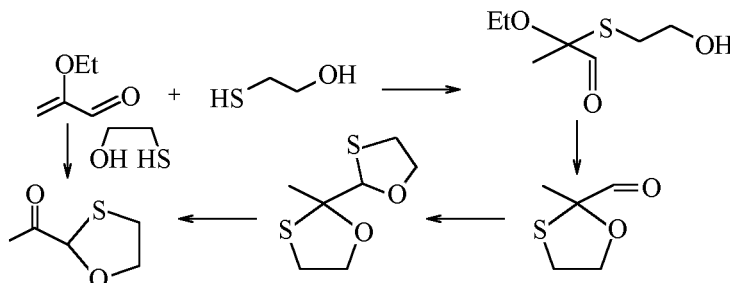
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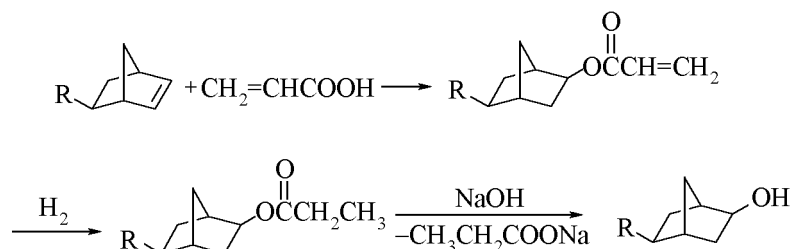
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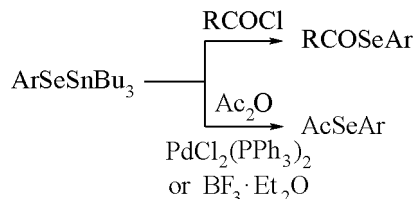
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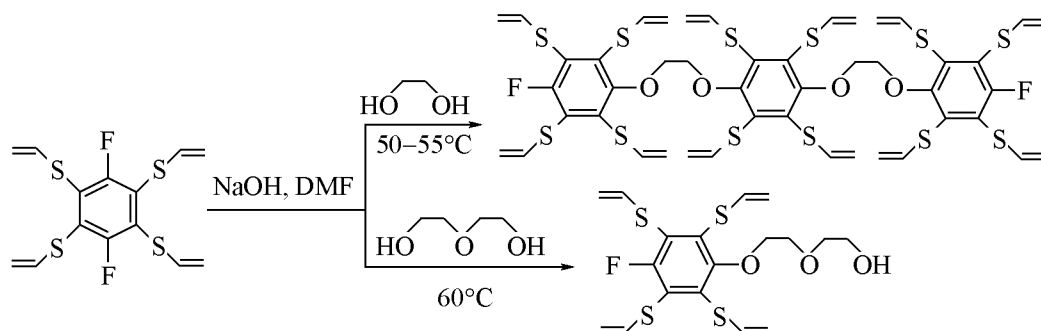
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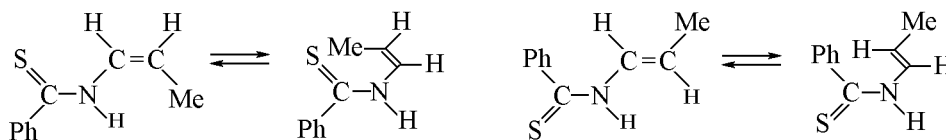
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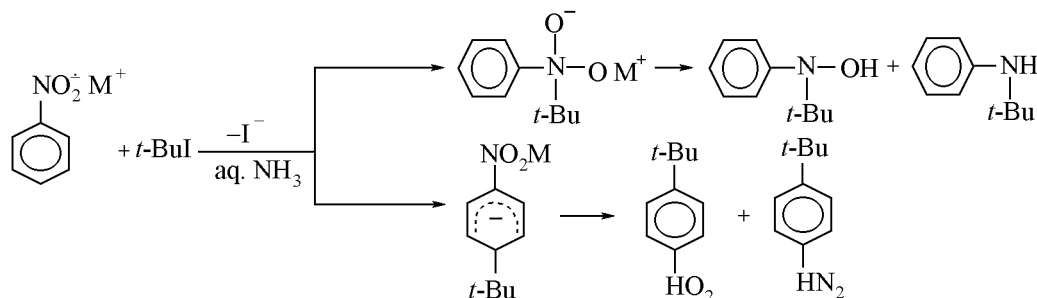
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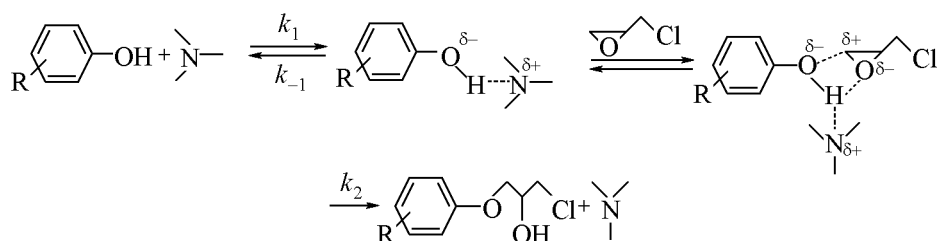
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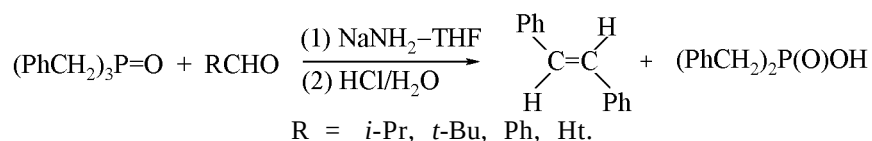
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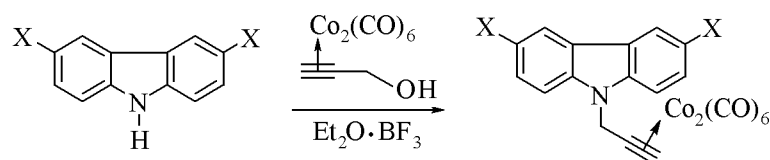
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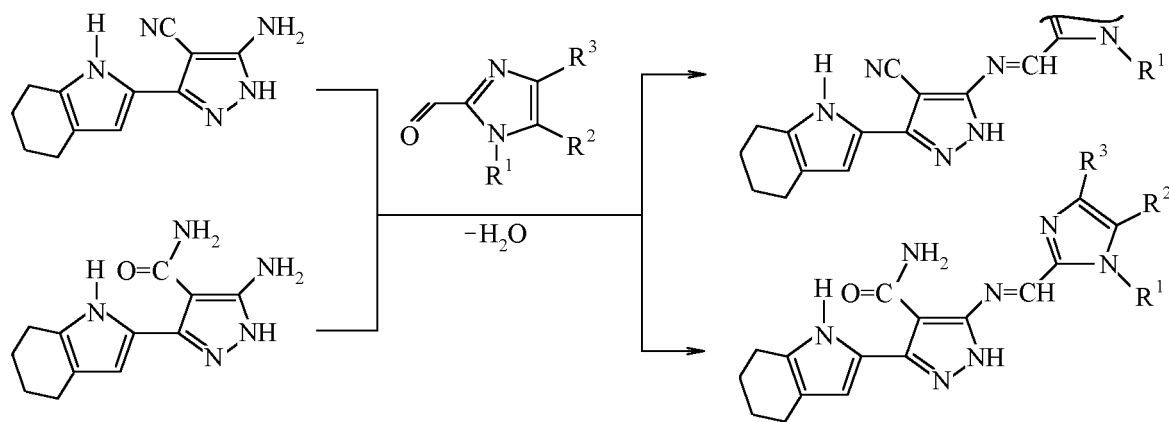
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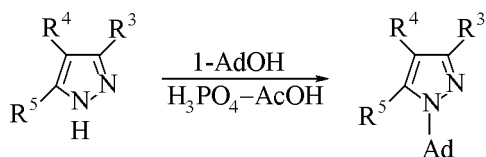
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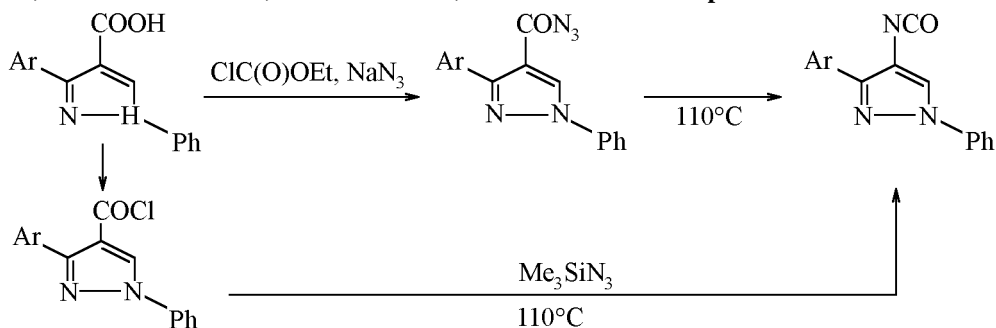
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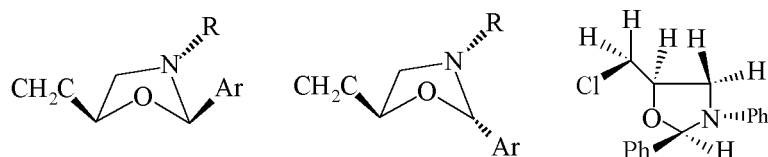
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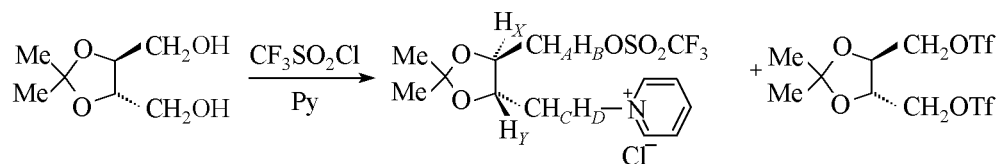
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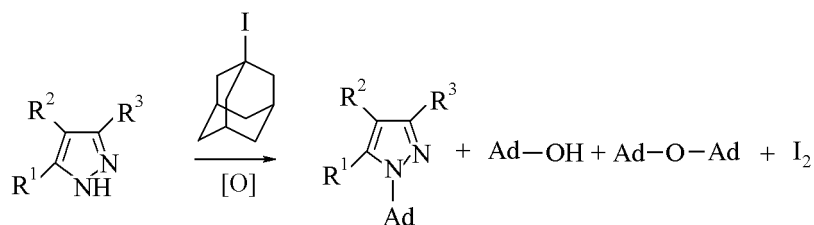
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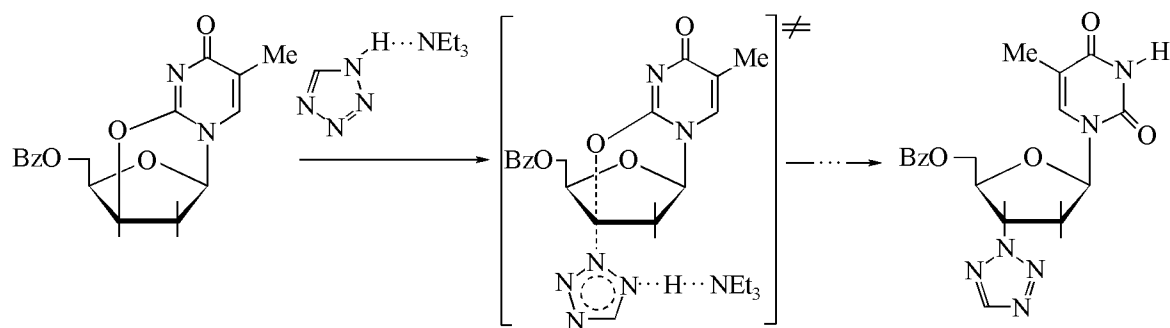
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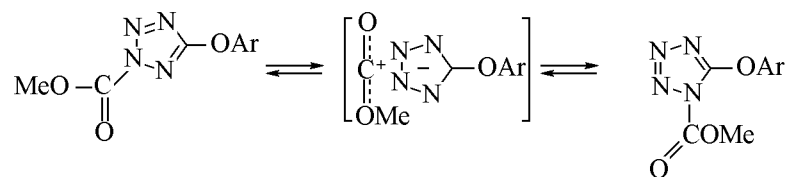


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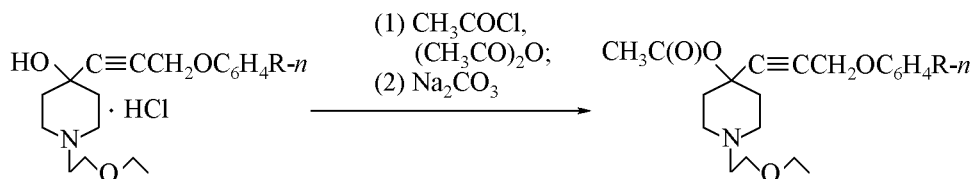
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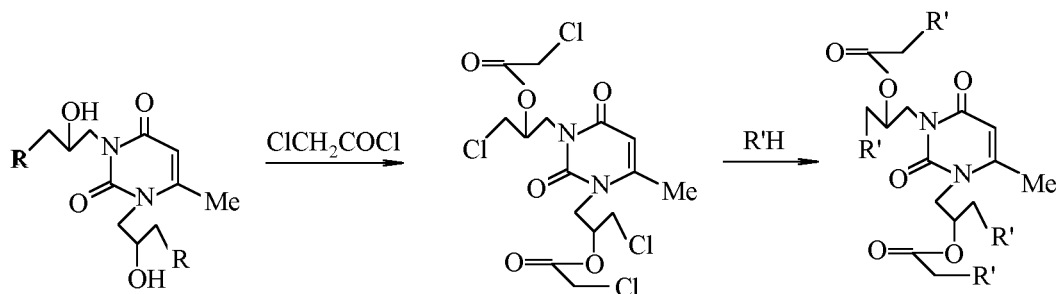




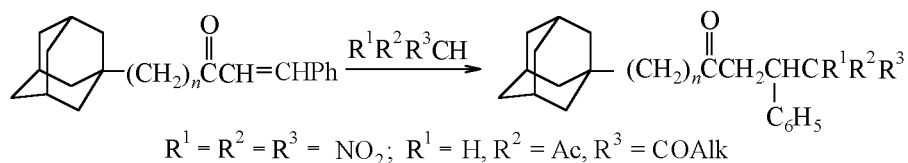
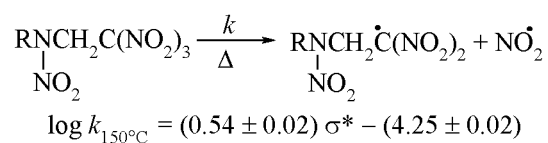
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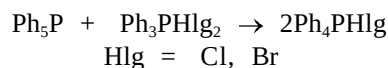
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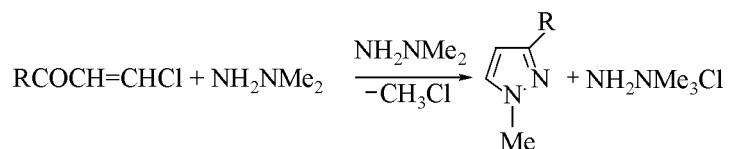
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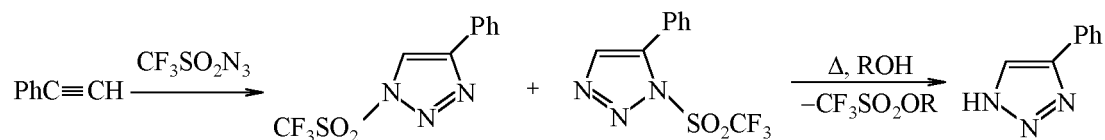
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