

The Role of TEOA in Photocatalytic Conversion of CO₂ to CO by Re Complex: A DFT Study

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Triethanolamine (TEOA) has been used for photocatalytic reduction of CO₂ as a sacrificial electron donor and the experimental investigations have shown that the TEOA increases catalytic efficiency. One of the representative homogeneous photocatalysts for CO₂ reduction is *fac*-[Re(bpy)(CO)₃Br], where the Re complex works as both photosensitizer and catalyst. The photocatalytic CO₂ reduction by the Re complex in dimethylformamide (DMF)/TEOA mixed solvent was first reported by Lehn and co-workers.¹ Following this study, Ishitani and co-workers recently revisited CO₂ reduction by *fac*-[Re(bpy)(CO)₃Br].^{2,3} They reported that monoalkyl carbonate complex, *fac*-[Re(bpy)(CO)₃(R₂N-CH₂CH₂O-COO)] was formed under dark condition in this photocatalytic system. They also reported that the monoalkyl carbonate complex was also formed when Ru-Re bimetallic complex was used as photocatalyst. They found that the linear relationship between the initial rate of CO formation and concentration of monoalkyl complex in the Ru-Re system, and suggested that the monoalkyl carbonate complex is the active species of the CO formation.^{4,5} However, the details of catalytic process for CO₂ reduction has not been revealed. This DFT investigation was conducted to elucidate the reaction mechanism and the role of TEOA.

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