O-CN Bond Cleavage of Cyanates by a Transition-Metal Complex

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Abstract:

O-CN bond cleavage of cyanates (ROCN) has been achieved at room temperature in the reaction of ROCN with a methyl Fe, Mo, or W complex. A mechanistic investigation involving DFT calculations revealed that silyl migration from Mo to the CN nitrogen gave an N-silylated η2-imidato Mo complex. This intermediate analogue was isolated and characterized by X-ray analysis. Catalytic O-CN bond cleavage was achieved using Cp(CO)3MoMe under thermal conditions.

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