

# Metal-catalyzed aziridination of alkenes by organic azides: A mechanistic DFT investigation

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## Abstract

This DFT study treats thermal metal-catalyzed alkene aziridination by azides, where the catalysts are copper(II) triflate, cobalt(II) porphyrin and ruthenium(II) porphyrin. Three azides RN<sub>3</sub> (R = H, Me, Ac) react with alkene substrates in the presence of these catalysts leading to aziridine formation by a two-step catalysed mechanism. In Step I, the azide reacts with the catalyst to first form a metal nitrenoid via transition state TS1. The Ru(porph) catalyst is particularly effective for Step I. In Step II, the metal nitrenoid adds to the alkene via TS2 giving the aziridine product. Cu(trf)<sub>2</sub> is most effective as a catalyst for Step II. The facility order H > Me > Ac (with respect to the azide R group) holds for Step I, and the reverse order for Step II. Transition states TS1 and TS2 are described as “early” and “late”, respectively, in good accord with Hammond’s postulate.

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