

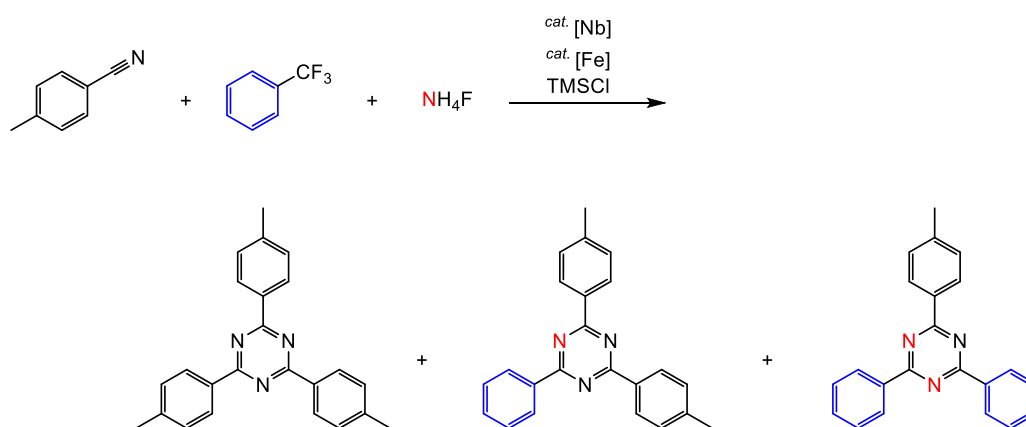
Synthesis of 1,3,5-triazine using Nb/Fe catalyzed cross-cycloaddition with nitrile and trifluorotoluene

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1,3,5-triazine derivatives are a class of nitrogen containing six-membered heterocycles and have much attention for the sake of their characteristic activity in pharmaceuticals and electronic devices.¹ As a conventional synthesis method of 1,3,5-triazine, cyclotrimerization of nitrile catalyzed by Lewis acid was reported.² However, this reaction requires harsh reaction conditions and has limited substrate scope. Recently, synthesis of 1,3,5-triazine using cyclization of aldehyde with ammonium iodide as nitrogen source was reported.³ This reaction is an efficient synthesis because of its high atom economy, but in synthesis of unsymmetrical 1,3,5-triazine derivative, this reaction has low chemoselectivity. Our group has reported the synthesis of various heterocyclic compounds using niobium catalyzed cycloaddition reaction.⁴ In the synthesis of pyrimidine, high Lewis acid and azaphilicity of niobium promoted the cycloaddition reaction.^{4b}

Here, we synthesized 1,3,5-triazine using niobium and iron catalyzed cycloaddition reaction with nitrile and trifluorotoluene derivatives. Ammonium fluoride serves as a nitrogen source. In this work, triazines with various substituents were obtained and the addition of trimethyl silyl chloride made further improvement on yield. The details of reaction conditions and substrate scope are reported.



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