

Experimental and density functional theory investigation of imine formation using microwave irradiation

ABSTRACT

Four starting materials comprising of N-(4,6-dimethylpyridin-2-yl)-4-formylbenzamide 1, 4-amino-N-(4,6-dimethylpyridin-2-yl)benzamide 2, 4-amino-2-methylbenzoic acid 3 and 4-formylbenzoic acid 4 react in a pairwise manner through the condensation reaction to give four imine derivatives, Imine 5, 6, 7 and 8. A simple method has been developed for the synthesis of these imine derivatives under microwave irradiation. In addition, these compounds were synthesised also by conventional heating procedures for comparison. All the compounds synthesised were characterised by melting point, infrared, mass spectrometry, ¹H and ¹³C NMR spectroscopy. Comparison between conventional and microwave irradiation was done by comparing total reaction time and percentage yield. The results suggest that microwave-irradiation lead to higher yields within very short reaction times. Compounds 1 and 2 crystallised in the orthorhombic (P212121 space group) and monoclinic (P21/c space group) crystal systems, respectively. The nature of minimal replicator of imine 6 via autocatalytic reaction was calculated using density functional theory (DFT) with the combination of hybrid functional B3LYP and 6-311G(d,p) basis set. The reaction pathway facilitated with the addition of imine 6 or imine 5 equipped with complementary recognition sites of two carboxylic acids and two 4,6 dimethylamidopyridines were predicted to be thermodynamically favourable.

Keyword: Imine; Condensation; Conventional heating; Microwave irradiation; Density functional theory