Área: FIS

A novel route to capture CO_2 using the superbase DBU and ionic liquids

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Highlights

The adduct between CO_2 and the superbase DBU has remained elusive so far. Herein we report its first unambiguous detection, which occurs in ionic liquid medium.

Abstract

The absorption of CO_2 by solutions of 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) in the ionic liquids (ILs) 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [Emim][TFSI], and butyltrimethylammonium bis(trifluoromethylsulfonyl) imide, [Btma][TFSI], was investigated via ^{13}C Nuclear Magnetic Resonance (NMR) and infrared spectroscopy (IR), and supported by theoretical calculations. It was observed that the reactivity of DBU towards CO_2 is influenced by the presence of water. In dry medium, the absorption of CO_2 by a DBU solution in [Emim][TFSI] yields the expected carboxylate, generated by CO_2 bonding to the deprotonated IL cation, whereas in [Btma][TFSI], there is no reaction at all. However, in the presence of water, the absorption of CO_2 proceeds differently, yielding a product with an unknown peak at 160.4 ppm in the ^{13}C NMR spectrum. Experiments with isotopically labelled $^{13}CO_2$ indicated that the formation of this distinct product is favored over the formation of (bi)carbonate (Figure 1). Then, IR spectroscopy analysis could identify it as the adduct DBU-CO_2. We can conclude that water plays a critical role in stabilizing the adduct as observed experimentally and assessed theoretically. Also, the ionic liquid is crucial to the formation of the adduct, which is still under investigation.

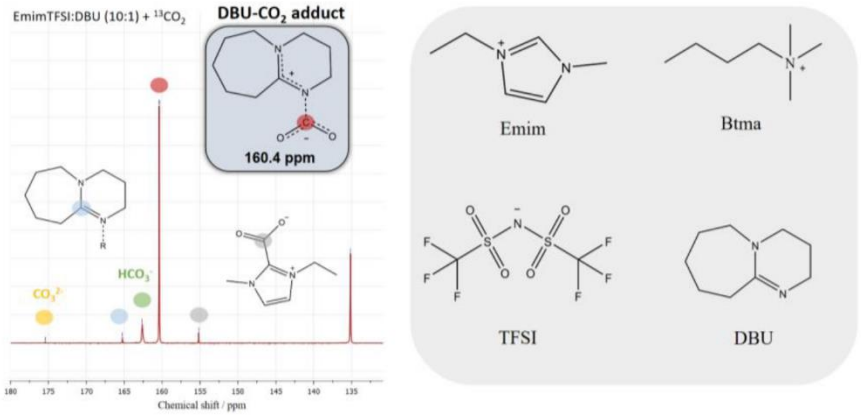

Figure 1. ^{13}C NMR spectrum of a DBU solution in EmimTFSI with $^{13}CO_2$. The assignments and chemical structures of ions and DBU are shown.

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