The asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Source of material**

A mixture of 2-chloro-5-nitrobenzoic acid (5.0 mmol) and KOH (15.0 mmol) were added to 5.8 mL Dimethyl Formamide (DMF) in a sealed tube. The reaction was carried out at 100 °C for 14 h and monitored by thin-layer chromatography (TLC). After the reaction was completed, the mixture was diluted with saturated brine (30 mL) and extracted three times with ethyl acetate (30 mL). The organic phase was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with petroleum and ethyl acetate mixture solvent (v/v = 2/1) to obtain a white product.
Experimental details

The C-bound and O-bound H atoms were positioned geometrically and included in the riding-model approximation refinement.

Comment

N,N-Dimethylarylamine organic compounds are widely present in commercial drug structures, such as antibiotics tigecycline [5] and minocycline [6], fungicide pyrimethamine [7], antipyretic and analgesic drug aminopyrine [8], antihistamine drug diphenhydramine [9], and the narcotic analgesic drug methadone [10]. Due to their bioactive properties, the synthesis of N,N-dimethylarylamine organic compounds attracted much attention, and many similar structures were reported [11–20]. This paper reports a N,N-dimethylarylamine derivative compound.

As shown in the figure, the asymmetric unit of the crystal structure contains two molecules of the title compound, which show a different protonation state. As shown in the figure the left molecule owns a carboxy group and a dimethylamino group, whereas the right molecule is in its ylidic form with a carboxylate and an dimethyl aminium function. All bond distances and angles are consistent with the expectation and accord with the parent structure [20]. A hydrogen bond O4—H4A⋯O7 was formed between the two molecules with a bond length of 1.7020(13) Å and a bond angle of 175.36(13)°, stabilizing the crystal configuration. The intramolecular hydrogen bond between the dimethylaminium cation and one oxygen atom of the carboxylate group, stabilizes the conformation of this second molecule. The title structure represent a rare case that the ylidic amino acid is found together with its neutral analog, which must be caused by the hydrogen bonding scheme.

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