STRUCTURE OF 2-CHLORO-3-PHENYLBENZOIC ACID

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UDC 543.442:547.022.1:547.62:547.624:544.437.3:544.47

The carbonylation reaction of 2,3-dichlorobiphenyl proceeds with a substitution of the chlorine atom in position 3 and results in the formation of 2-chloro-3-phenylbenzoic acid. The structure of this acid is revealed by single crystal XRD. It is determined by steric interactions of substituents in positions 2,4,2′, and 6′, a stable carboxyl supramolecular synthon, and weak interactions with the participation of the carbonyl oxygen atom and the chlorine atom.

Keywords: polychlorobiphenyls, carbonylation, aromatic carbonic acids, synthesis, crystal structure.