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# Spectroscopic studies on the interaction of cilostazole with iodine and 2,3-dichloro-5,6-dicyanobenzoquinone

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ABSTRACT

The electron accepting properties of the 2,3-dichloro-5,6-dicyanobenzoquinone and iodine and electron donating properties of the drug cilostazole have been studied using the UV–vis, FT-IR, GC–MS and Far-IR techniques. The interaction of cilostazole drug with iodine and 2,3-dichloro-5,6-dicyanobenzoquinone resulted via the initial formation of charge-transfer complex as an intermediate. The rate of formation of the product have been measured and discussed as a function of solvent and temperature. The complexes have been found by Job's method of continuous variation revealed that the stoichiometry of the complexes in both the cases was 1:1. The enthalpies and entropies of formation of the complexes have been obtained by determining their rate constant at three different temperature. The ionization potential of the donor was determined using the charge-transfer absorption bands of the complexes and the same was found comparable with that computed using MOPAC PM3 method.



## 1. Introduction

Over the years scientists have paid much attention on the spectral studies of charge-transfer (CT) complexes of 2,3-dichloro-5,6-dicyanobenzoquinone (DDQ) and iodine with variety of donors [1–12]. Quinones are biologically significant molecules and are common constituent of many biologically relevant molecules. The reversible oxidation–reduction reactions of quinones play a key role in several biological processes [13,14]. Further, quinones are one of the well-known electron acceptors and the studies of their CT-interaction stem from their possible role in biological reactions [15,16]. Likewise iodine is also a biologically significant molecule [17–19]. Thus, the mechanism of interaction of these biologically important acceptors with drugs, in general, is a research topic of significant interest and hence the present study.

Chemically cilostazole is 6-(4-(1-cyclohexyl-1H-tetrazol-5-yl)butoxy)-3,4-dihydroquinolin-2(1H)-one. It is used to reduce the symptoms of intermittent claudication and helps people walk a longer distance. Hence, in continuation of our earlier works on the spectroscopic studies on the interaction of drug molecules with these acceptors [20–23], the present work report the CT interaction of cilostazole (CLZ) with DDQ and iodine. The spectral, kinetic and thermodynamic characteristics of the interaction between the donor drug and the acceptors were investigated and discussed.

## 2. Experimental

### 2.1. Material and methodology

The electron acceptors DDQ (minimum assay 98%) and iodine (minimum assay 99.9%) were obtained from Aldrich, India. Commercially available spectroscopy grade chloroform, dichloromethane, 1,2-dichloroethane, *tert*-butyl alcohol, *iso*-butyl alcohol, *iso*-propyl alcohol, methanol, acetonitrile and DMSO (all Merck, India, minimum assay > 99%) were used without further purification. The selection of the solvents is based on the solubility of the components and so as to have a wide range of relative permittivity of the medium. The electron donor CLZ was obtained as gift sample from a locally available pharmaceutical company and was used after confirming the purity. The purity of CLZ was checked by its m.p. (experimental 157–158 °C; theoretical 157–160 °C) and also by comparing its FT-IR spectrum with that of the authentic sample. The structure of the donor is shown below (Scheme 1).

Solutions for the spectroscopic measurements were prepared by dissolving accurately weighed amounts of donor (D) and acceptor (A) in the appropriate volume of solvent just before running the spectra. The electronic absorption spectra were recorded on a Shimadzu (UV 240, Graphicord) double beam spectrophotometer using 1 cm matched quartz cells. The temperature of the cell holder was controlled with a water flow (±0.2 °C). The FT-IR spectra were recorded in a JASCO FT-IR 460 Plus spectrometer. The GC–MS spectra of the reaction product were obtained from Central Salt and Marine Research Institute, Bhavanagar, India. The molecular orbital package, MOPAC 2000 version 1.11 (PM3 method) was used for the

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