INTRODUCTION

Imidazole is nitrogen containing heterocyclic ring which possesses biological, pharmaceutical and unique optical properties. Thus, imidazole compounds have been an interesting source for researchers for more than a century [1, 2]. Heterocyclic imidazole derivatives plays very important role in chemistry as mediators for synthetic reactions, primarily for preparing functionalized materials [2]. In addition, they are widely used in many fields, such as P38 MAP kinase [3], antivascular disrupting, antitumour activator [4], ionic liquids [5], anion sensors [2], as well as electrical and optical materials [6–8].

Imidazole derivatives show unique chemical and physical properties because they contain imidazole heterocycle which has better thermal stability, and benzene rings can increase the degree of conjugation of the organic molecule. Imidazole derivatives has also significant analytical applications by utilizing their fluorescence and chemiluminescence properties [9]. An important property that makes imidazole derivatives more attractive as a chelator is the appreciable change in its fluorescence upon metal binding. As a result, luminescent, materials of imidazole derivative have emerged as the attractive blue-emitting materials. Therefore, imidazole derivatives have been used to construct highly sensitive fluorescent chemisensors for sensing and imaging of metal ions and its chelates in particular those with \( \text{Ir}^{3+} \) are major components for organic light emitting diodes [9, 10] and are promising candidates for fluorescent chemisensors for metal ions. Recently the research by Huang and Zhao [11] was aimed at the production of imidazole derivatives for luminophores, but such materials are oligomers which restricted the application.

Organic luminescent materials have recently received much attention due to their potential applications in organic lightemitting diodes [12], ceramics [13], fluorescent biological labels [14], photovoltaic cells [15], and optical sensors [16]. A great number of luminescent organic materials have been synthesized and investigated, for example, recently the better blue lightemitting materials were achieved for the pyrazoloquinolinium chromophore, where the quantum efficiency was about 1.7 [17, 18]. However, organic luminescent materials still have stability problems and the correlation between structure and fluorescence efficiency remains a big challenge in this area.

FT-IR, FT-Raman and FT-NMR spectra of 4-(4-Chlorophenyl)-1H-imidazole (4-ClPI) molecule along with the theoretical prediction using DFT method.

**SPECTROSCOPY OF ATOMS AND MOLECULES**

**DFT Simulations, FT-IR, FT-Raman, and FT-NMR Spectra of 4-(4-Chlorophenyl)-1H-imidazole Molecules**

Y. Erdogdu, M. T. Gulluoglu, S. Yurdakul, and Ö. Dereli

*aDepartment of Physics, Ahi Evran University, 40040 Kirsehir, Turkey
bDepartment of Physics, Gazi University, 06500 Ankara, Turkey
cA. Keleçoğlu Education Faculty, Department of Physics, Selcuk University, 42090 Konya, Turkey

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Abstract—The FT-IR, FT-Raman and FT-NMR spectra of the compound 4-(4-Chlorophenyl)-1H-imidazole (4-ClPI) was recorded and analyzed. Density functional method has been used to compute optimized geometry, vibrational wavenumbers and NMR spectra of the 4-ClPI. Only one tautomeric form was found most stable by using B3LYP functional with the 6-311++G(d,p) as basis sets. The detailed interpretation of the vibrational spectra was carried out with the aid of total energy distribution (TED) following the scaled quantum mechanical force field methodology.

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**EXPERIMENTAL**

The FT-IR spectrum of this molecule recorded in the region 4000–400 cm\(^{-1}\) on IFS 66V spectrophotometer using KBr pellet technique is shown in Fig. 1. The FT-Raman spectrum of 4-ClPI recorded using 1064 nm line of Nd : YAG laser as excitation wavelength in the region 50–3500 cm\(^{-1}\) on a Thermo Electron Corporation model Nexus 670 spectrophotometer equipped with FT-Raman module accessory are shown in Fig. 2. The \(^1\)H and \(^{13}\)C NMR spectra are taken in chloroform solutions and all signals are refer-
enced to TMS on a BRUKER DPX-400 FT-NMR Spectrometer. All NMR spectra are measured at room temperature.

**COMPUTATIONAL DETAILS**

Gaussian 09 quantum chemical software was used in all calculations [20]. The optimized structural parameters and vibrational wavenumbers for the 4-ClPI molecule were calculated by using B3LYP functional with 6-311G+(d,p) as basis set. The vibrational modes were assigned on the basis of TED analysis using SQM program [21]. Normal coordinate analysis of the title molecules has been carried out to obtain a more complete description of the molecular motions involved in the fundamentals. The calculated harmonic vibrational wavenumbers were scaled down uniformly by a factor of 0.967 (for wave numbers under 1800 cm$^{-1}$) and 0.955 (for those over 1800 cm$^{-1}$) for B3LYP/6-311++G(d,p) level of theory, which accounts for systematic errors caused by basis set incompleteness, neglect of electron correlation and vibrational anharmonicity [22–24].