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Heraclenin: A Potential Optoelectronic Device Material from *Prangos pabularia*

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Heraclenin ($C_{16}H_{14}O_5$), a linear furanocoumarin, was isolated from the ethyl acetate extract of the roots of *Prangos pabularia*. The compound was characterized using x-ray diffraction (XRD), scanning electron microscopy (SEM), optical microscopy, ultraviolet (UV)–visible, and photoluminescence (PL) measurements. Structural analysis confirmed the orthorhombic structure of the system. Exploration by SEM and optical images predicted that the compound contains microcrystals with irregular morphology. From UV–visible spectroscopy, high transmission was displayed by these crystals in the entire visible range. The optical band gap (E_g) was found to be around 3.91 eV and exhibited indirect allowed transitions. Photoluminescence data showed good emission at certain wavelengths in the visible region. The observed optical properties could be due to intramolecular charge transfer (ICT) when excited by any suitable light. The present properties of the compound can be explored for use in optoelectronics and as fluorophores in biological imaging applications.

Key words: *Prangos pabularia*, heraclenin, furanocoumarin, orthorhombic, optoelectronics, wide band gap

INTRODUCTION

Currently, organic semiconductors, due to their significant physical and chemical properties, have attracted the attention of chemists, physicists, and engineers, resulting in the rapid development of organic electronics.[1–10] The promising mechanical and thermal properties of organic semiconductors also ensure their use in flexible electronics. However, the best feature of organic semiconductors is their chemical stability and solubility, which permits the incorporation of functionalities through atomic or molecular design. Organic compounds containing a polycyclic aromatic hydrocarbon skeleton, e.g., naphthalene, anthracene, perylene, fluorene, carbazole, pyrene, etc., are best known and are suitable for possible applications in organic light-emitting diodes (OLEDs).[11–14] For the last few decades, naphthalene, anthracene, perylene, fluorene, carbazole, pyrene, and their derivatives have been mostly used as efficient electron/hole-transporting materials or host emitting materials in OLED applications. The synthesis and photophysical properties of pyrene-based, multiple-conjugated, fluorescent light-emitting materials have been disclosed in recent literature.[11] Several pyrenes have been successfully used as efficient hole/electron-transporting materials or host emitters or emitters in OLEDs.[1] Most of the pyrene-based, cruciform-shaped π-conjugated and blue light-emitting architectures can be prepared with an emphasis on synthetic design that promises their potential application in OLEDs.[1,11]

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