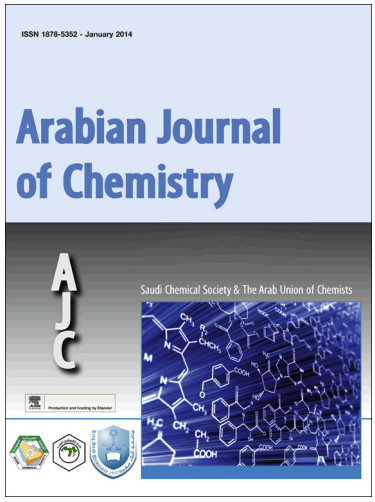


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# Comparative spectroscopic and electrochemical study of N-1 or N-2-alkylated 4-nitro and 7-nitroindazoles

Gabriele Micheletti, [a] Assoman Kouakou, [b] Carla Boga, [a] Paola Franchi, [c] Matteo Calvaresi, [c] Lorella Guadagnini, [a] Marco Lucarini, [c] El Mostapha Rakib, [b] Domenico Spinelli, [c,*] Domenica Tonelli, [a] Issam Forsal [b]

[a]*Department of Industrial Chemistry 'Toso Montanari' Alma Mater Studiorum – University of Bologna, Viale del Risorgimento 4, 40136 Bologna, Italy;* [b]*Laboratoire de Chimie Organique et Analytiques, Faculté des Sciences et Techniques, Université Sultan Moulay Slimane, B.P. 523, Béni-Mellal, Morocco.* [c]*Department of Chemistry 'G. Ciamician' Alma Mater Studiorum – University of Bologna, Via Selmi 2, 40126 Bologna, Italy.*

**Correspondig author:domenico.spinelli@unibo.it*

**Abstract:** Our research groups are by long time involved in the study of the reactivity and the pharmacological activity of nitrogen-containing heterocyclic compounds: in this line we have now examined the behaviour of some substituted 4- and 7-nitroindazoles. Considering the fact that nitroreduction processes are often essential steps for the biological activity of nitro compounds and remembering that some nitroindazoles show interesting biological activities, we have collected nuclear magnetic resonance, electron spin resonance, and cyclic voltammetry data and carried out density functional theory computations on the above compounds thus obtaining an accurate picture of electronic distribution and reduction processes of the examined substrates as a function of their chemical structure. Looking also to our previous results obtained examining the behaviour of 5- and 6-nitroindazoles, we have confirmed the different general behaviour of 1- and 2-alkyl substituted nitroindazoles strictly related to the known different electronic distribution in these two classes of compounds. Interestingly, cyclic voltammetry data have confirmed the ability of N-1–H nitroindazoles to give rise to the formation of dimers, already observed by us studying 5- and 6-nitroindazoles.

**Keywords:** Nitroindazoles, electron spin resonance measurements, NMR spectroscopy, cyclic voltammetry, density functional theory computations, radical anions.

**List of abbreviations:** nuclear magnetic resonance (NMR); electron spin resonance (ESR); cyclic voltammetry (CV); density functional theory (DFT); quantum mechanics (QM).

## INTRODUCTION