



# NORG2022

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## BOOK OF ABSTRACTS

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## PALLADIUM/PHENANTHROLINE CATALYSED SYNTHESIS OF N-HETEROCYCLES BY REDUCTION OF NITRO COMPOUNDS BY CO SURROGATES: RECENT PROGRESSES AND MECHANISTIC STUDIES

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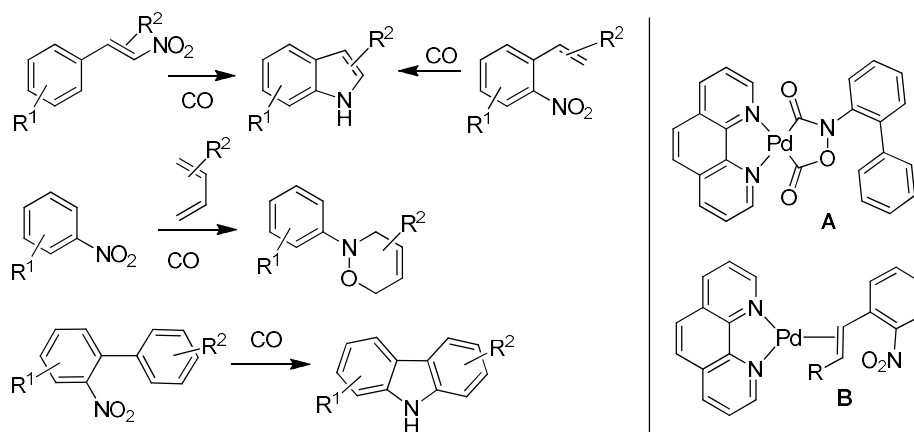
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Transition metal catalysed reductive cyclization reactions of suitably substituted nitroarenes to yield heterocycles using carbon monoxide as a reductant have been known for many years. However, their use has not become common among synthetic organic chemists due to the limitations involved in the use of pressurized CO.<sup>[1]</sup> In recent years, we have developed the use of phenyl formate as a cheap and non-toxic CO surrogate, able to liberate CO under the reaction conditions, thus allowing the same cyclization reactions to be performed in a single glass pressure tube. In particular, the synthesis of indoles from either *o*-nitrostyrenes<sup>[2-3]</sup> or  $\beta$ -nitrostyrenes,<sup>[4]</sup> oxazines from nitroarenes and conjugated dienes,<sup>[5]</sup> and carbazoles from *o*-nitrophenyls<sup>[6]</sup> were optimized (Scheme 1, left side).



**Scheme 1:** Reactions investigated and proposed catalyst resting states

However, virtually nothing is known about the mechanism of these reactions. We have thus undertaken an experimental and computational study of the reaction pathways and the results will be described. Two proposed reaction intermediates are shown in Scheme 1, right side.

[1] F. Ferretti, D. R. Ramadan, F. Ragaini, *ChemCatChem* **2019**, *11*, 4450-4488.

[2] M. A. Fouad, F. Ferretti, D. Formenti, F. Milani, F. Ragaini, *Eur. J. Org. Chem.* **2021**, 4876-4894.

[3] D. Formenti, F. Ferretti, F. Ragaini, *ChemCatChem* **2018**, *10*, 148-152.

[4] F. Ferretti, M. A. Fouad, F. Ragaini, *Catalysts* **2022**, *12*, 106.

[5] M. A. EL-Atawy, D. Formenti, F. Ferretti, F. Ragaini, *ChemCatChem* **2018**, *10*, 4707-4717.

[6] D. R. Ramadan, F. Ferretti, F. Ragaini, *J. Catal.* **2022**, *409*, 41-47.