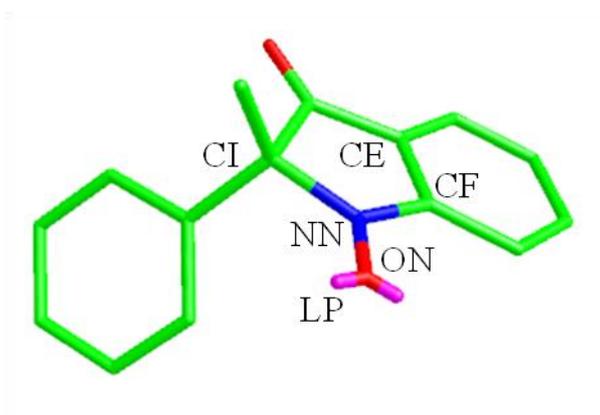


# TUTORIAL

## How to extend AMBER force field (ff99SB) to aromatic nitroxide radicals: The case of the INDCO molecule.



1,2-dihydro-2-methyl-2-phenyl-3H-indole-3-oxo-N-oxyl (INDCO)

In this tutorial the input file necessary for performing MM and MD simulations of the INDCO molecule are briefly described with the hope of helping users to extend the ff99SB AMBER force-field to the INDCO molecule.

The fitting strategy and the calculation of EPR parameters by using QM/MM/PCM integrated approaches are described in the following paper:

- 1) Interplay of stereo-electronic, environmental, and dynamical effects in determining the EPR parameters of aromatic spin-probes: INDCO as a test case. Paola Cimino, Alfonso Pedone, Emiliano Stendardo and Vincenzo Barone. Submitted to Phys. Chem. Chem. Phys.

This tutorial assumes that Amber10 package is correctly installed and the AMBERHOME environment variable defined.

### Required files:

- *frcmmod.INDCO.dat* : this file contains the new atom types, intramolecular and Van der Waals parameters added to ff99SB AMBER force field for describing the INDCO nitroxide radical.
- *INDCO09.lib*: object file format (OFF) library containing initial Cartesian coordinates, assigned atom types and restrained electrostatic potential (RESP) charges of the atoms in the INDCO nitroxide radical.
- *leap.indco.in* (optional file): input file for xleap or tleap Amber10 modules. This file contains in logical sequence, the commands to run the modules mention above. If you prefer, you can run these commands entering manually at the prompt in the modules.

From these files we have to create the input files for performing MM and MD simulations.

At the shell prompt digit the following command:

```
% tleap -s -f leap.indco.in
```

The command sequences in *leap.indco.in* are:

```
source leaprc.ff99SB                                (load ff99SB force filed)
addAtomTypes {                                     (add necessary new atom types)
  { "NN" "N" "sp2" }
  { "ON" "O" "sp2" }
  { "CI" "C" "sp3" }
  { "CE" "C" "sp2" }
  { "CF" "C" "sp2" }
}
frcmod_INDCO = loadamberparams frcmod.INDCO.dat    (load update parameters)
loadoff INDCO09.lib                                (load OFF library)
saveAmberParm IND INDCO.top INDCO.crd             (save topology and coordinates files)
quit
```

This creates the following files:

***INDCO.top***: file containing molecular topology and the necessary force field parameters.

***INDCO.crd***: file containing the atomic Cartesian coordinates

These are the input files necessary to perform geometry optimizations and molecular dynamics simulations of the INDCO nitroxide radical.

To run a Molecular mechanics optimization and Molecular dynamics simulation the following commands are used:

```
% sander -O -i INDCOmm.in -o INDCOmm.out -p INDCO.top -c INDCO.crd
-r INDCO.restart -inf INDCO.mminf
```

```
% sander -O -i INDCOmd.in -o INDCOmd.out -p INDCO.top -c
INDCObox.crd -r INDCO.restart -x INDCO_trj.mdcrd -inf INDCO.mdinf
```

The INDCOmm.in and INDCO.md.in files contain the parameters for MM optimization and MD simulations, respectively.

All these files can be found in the INDCO09.zip archive.