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## Experimental studies and *in silico* approaches in evaluating the effect of solvent on the <sup>77</sup>Se NMR chemical shift profile of diphenyl diselenides

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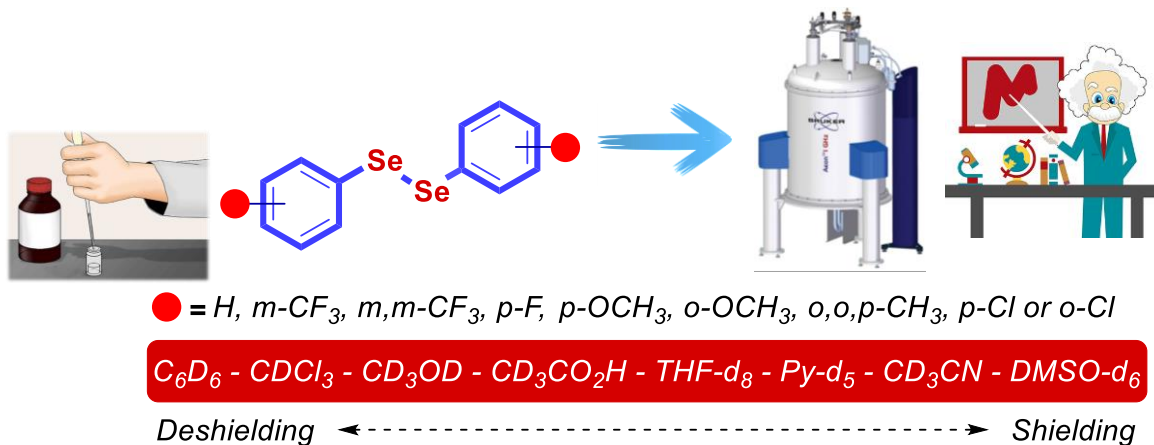
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### ABSTRACT

Nowadays, the chemical<sup>1a-c</sup> and pharmacological<sup>2a-d</sup> relevance of organoselenium compounds makes it imperative to know the behavior of the <sup>77</sup>Se nucleus in NMR analyzes under different experimental conditions, especially of the compounds used to provide the reference signal in the spectra. Diphenyl diselenide has been widely used as an internal reference standard due to its stability and ease of handling.<sup>3a,b</sup> However studies on the effect of experimental conditions on chemical shift in <sup>77</sup>Se NMR analyzes are scarce.

Therefore, we have prepared some common diphenyl diselenides and we evaluated the effect of solvent on the <sup>77</sup>Se NMR chemical shifts. Thus, <sup>77</sup>Se NMR spectra of diphenyl diselenides containing electron-withdrawing (EWG) or electron-donating (EDG) groups were recorded in eight different deuterated solvents with distinct polarities. The effects of temperature and concentration were also assessed and were found to play a minor role in the precise value of <sup>77</sup>Se chemical shifts. Finally, a computational study was performed to rationalize the <sup>77</sup>Se NMR chemical shifts behavior and to highlight the limits of standard approaches (Scheme 1)<sup>4</sup>.



Scheme 1. Graphical abstract of this work

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### REFERENCES

- References:** 1. a) Singh, F. V.; Wirth, T. *Catal. Sci. Technol.*, **2019**, v. 9, p. 1073-1091. b) Thurow, S.; Abenante, L.; Anghinoni, J. M.; Lenardão, E. J. *Curr. Org. Synth.*, **2022**, v. 19, p. 331-365. c) Goulart, H. A.; Araujo, D. R.; Barcellos, A. M.; Jacob, R. G.; Lenardão, E. J.; Perin, G. *Eur. J. Org. Chem.*, **2022**, v. 2022, p. e202201027.
2. a) Lopes, E. F.; Penteado, F.; Thurow, S.; Pinz, M.; Reis, A. S.; Wilhelm, E. A.; Luchese, C.; Barcellos, T.; Dalberto, B.; Alves, D.; Silva, M. S.; Lenardão, E. J. *J. Org. Chem.*, **2019**, v. 84, p. 12452-12462. b) Mailahn, D. H.; Iarocz, L. E. B.; Nobre, P. C.; Perin, G.; Sinott, A.; Pesarico, A. P.; Birmann, P. T.; Savegnago, L.; Silva, M. S. *Eur. J. Med. Chem.*, **2021**, v. 213, p. 113052. c) Anghinoni, J. M.; Birmann, P. T.; Rocha, M. J.; Gomes, C. S.; Davies, M. J.; Brüning, C. A.; Savegnago, L.; Lenardão, E. J. *Molecules*, **2023**, v. 28, p. 7349-7394. d) Birmann, P. T.; Casaril, A. M.; Abenante, L.; Penteado, F.; Brüning, C. A.; Savegnago, L.; Lenardão, E. J. *Curr. Med. Chem.*, **2023**, v. 30, p. 2357-2395.
- 3) a) Velde, G. T.; Bickelhaupt, F. M.; Baerends, E. J.; Guerra, C. F.; Van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. *J. Comput. Chem.*, **2001**, v. 22, p. 931-967. b) Rosenau, C. P.; Jelier, B. J.; Gossert, A. D.; Togni, A. *Angew. Chem., Int. Ed.*, **2018**, v. 57, p. 9528-9533.
- 4) Bartz, R. H.; Hellwig, P. S.; Perin, G.; Iarocz, L. E. B.; Madabeni, A.; Orian, L.; Silva, M. S. *New J. Chem.*, **2024**, v. 89, p. 284-287.