Four-component Relativistic NMR calculations in *trans*-Platinum Complexes

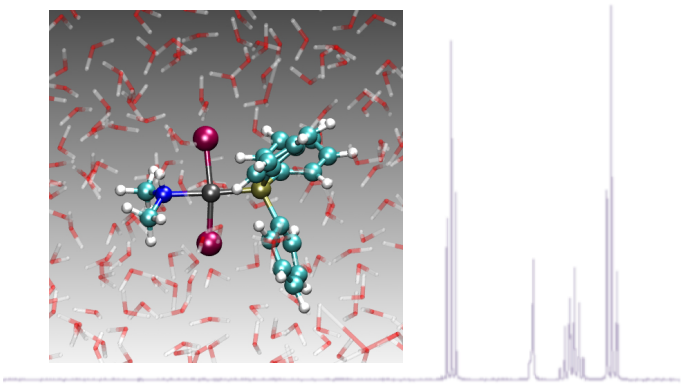
Abril C. Castro,[1] Heike Fliegl,[2] Michele Cascella,[2] Trygve Helgaker[2] and Marcel Swart[1,3]

1. Institut de Química Computacional i Catàlisi, Departament de Química, Universitat de Girona, Campus Montilivi, 17071, Girona, Spain.
2. Centre for Theoretical and Computational Chemistry (CTCC), Department of Chemistry, University of Oslo, P,O, Box 1033 Blindern, N-0315 Oslo, Norway.
3. Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010, Barcelona, Spain.

Our investigation focus on the theoretical determination of the NMR chemical shifts using both "static" and "dynamic" approaches of a number of new *trans*-platinum complexes that have been recently synthesized (See Figure 1).[1] In the last decade, *trans*-platinum complexes have been demostrated to be endowed with antitumor activity. Therefore, these non conventional complexes could lead to the development of better platinum drugs, in an attempt to mimimize the severe side effects of the cisplatin (*cis*-[$PtCl_2(NH_3)_2$]), which is now one of the most important platinum complexes that exhibits antitumor activity.

The ^{31}P-NMR chemical shifts were computed using *ab-initio* molecular dynamics (AIMD) simulations, followed by DFT-NMR calculations on a large series of snapshots. The relativistic calculations were perfomed with the ReSpect (Relativistic Spectroscopy) program, using a four-component Dirac-Coulomb (DC) Hamiltonian including both scalar and spin-orbit corrections.[2] The NMR chemical shifts obtained from the four-component relativistic calculations were also compared with those obtained using the spin-orbit zeroth-order-regular approximation (SO-ZORA), as implemented in the ADF program.

Figure 1. *trans*-[$PtCl_2$(dma)PPh_3] complex.



[1] A. G. Quiroga, *J. Inorg. Biochem*. **2012**, 114, 106-112.
[2] V. G. Malkin, O. L. Malkina, R. Reviakine, A. V. Arbuznikov, M. Kaupp, B. Schimmelpfennig, I. Malkin, M. Repiský, S. Komorovský, P. Hrobárik, E. Malkin, T. Helgaker, and K. Ruud, *ReSpect program*, **2007**.