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Editorial

Foreword to special issue on "Theory and Mechanistic Studies"

For a long time, theoretical inorganic/metal-organic chemistry depended on empirical models like ligand field or extended Huckel theory. Contrary to the situation in organic chemistry, Hartree–Fock calculations on small model systems gave more-or-less useless results. For transition metals the error which was introduced due to the missing correlation energy was too big to describe the systems in a correct way. But with the availability of density functional theory (DFT) methods for transition metals the number of papers which address mechanistic questions has steadily increased during the last couple of years. As can be seen from Fig. 1, around the turn of the century the number of papers with a theoretical content in the *Journal of Organometallic Chemistry* significantly increased.

Computational transition metal chemistry is nowadays dominated by DFT-methods, which is reflected by this issue. Molecules with even larger sizes can be treated by good-quality basis sets and the resulting accuracy lead to a general acceptance of density functional methods.

Faster algorithms and the increasing compute power along with decreasing costs made the necessary tools available. Programs with user–friendly interfaces have become widely available, in some cases even free within the academic community. Additionally the number of courses where quantum chemistry and its applications are taught increase constantly all over the world. It can therefore be expected that the trend will continue.

The present special issue on "Theory and Mechanistic Studies" gives examples from several fields and highlights the usefulness of DFT-calculations for mechanistic studies.

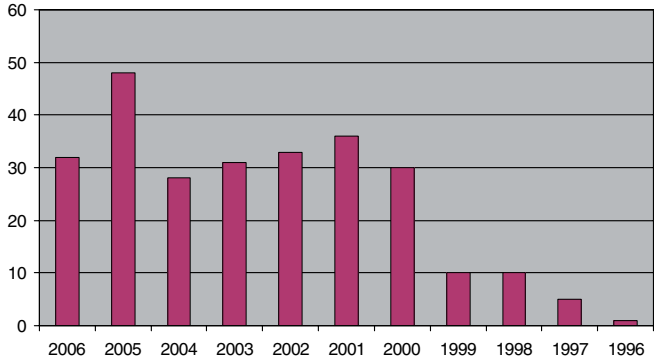

Fig. 1. Papers including DFT-calculations published in the *Journal of Organometallic Chemistry*.

We hope that the readers of this issue will enjoy the present selection of papers from this important and rapidly developing field.

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