



Biography

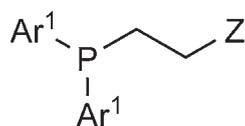
Dr. Johannes Teichert studied at Philipps-Universität Marburg, Germany, and at Université Paul Sabatier, Toulouse, France. After obtaining his diploma thesis with Prof. Gerhard Hilt, he joined the group of Prof. Ben Feringa at Rijksuniversiteit Groningen, the Netherlands, to obtain his PhD. After postdoctoral studies with Prof. Jeffrey Bode at ETH Zürich, Switzerland, he moved to the Technische Universität Berlin, Germany to set up an independent research group. His research interests include transition-metal catalysis, organometallic chemistry and synthesis.

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Abstract

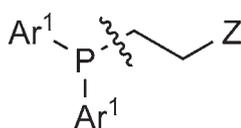
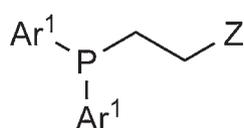
The *Science of Synthesis* database search has been used to identify possible synthetic approaches to a relatively broad ligand library of phosphine ligands bearing heteroatoms in the carbon backbone (Scheme 1). In particular, the structure-based query was found to be a useful tool to quickly identify various synthetic approaches for the compounds of interest.



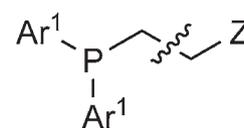
Scheme 1 Phosphine Ligand Bearing Heteroatoms in the Carbon Backbone

Discussion

In this case study, the *Science of Synthesis* database has been used to identify possible synthetic approaches to phosphine ligands bearing heteroatom substituents in the β -position to phosphorus (Scheme 2). The aim of this investigation was to obtain an overview of the known synthetic approaches to be able to quickly synthesize a small library of phosphorus compounds that could subsequently be tested in transition-metal catalysis.



disconnection A



disconnection B



Scheme 2 General Structure of Phosphorus-Based Ligands and Possible Disconnections

The general structure of the synthetic targets was searched for using the online structure query tool. This is easy and intuitive to use. Even though no placeholder option for substructure search is provided, the query automatically located substructures in the results, which was helpful for such an explorative search. A variety of (sub)chapters of the database were located, which highlights the usefulness of the structure search. The query of this case study would otherwise be difficult to carry out using solely a text-based search, as the products are located in many different (as a matter of fact not necessarily related) chapters. In addition, the object of this search was to get an overview of a relatively broad field (with various substituents and substitution patterns), which would have complicated the text-based search even further. The fact that the precise sorting of the information into the subchapters of the database is visible to the user adds to the user-friendliness of the database.

The query ($\text{Ar}^1 = \text{Ph}$, $\text{Z} = \text{OH}$) delivered some general chapters of interest as well as subchapters in other categories that were helpful for the desired synthetic information. Three major chapters easily localized were 31.42 (Arylphosphines and Derivatives), 6.1.16 (Phosphinoboranes and Borane-Phosphine Complexes), and 4.4.22 (Silyl Phosphines). These chapters provided a good overview of the general approaches to heteroatom-derived phosphine ligands. Even though these chapters are densely packed with information, they are easy to navigate through their thorough and logical subdivision into subchapters, so that the necessary information could quickly be located. This is especially helpful when the researcher does not have much previous knowledge about a compound class of interest. In particular, the fact that general experimental details are given for the most important reactions helps to quickly derive conditions for the envisaged (as yet unknown) target. Therefore, these chapters provide an ideal starting point for a practical investigation. In this case study, different approaches using various phosphorus-based starting materials could be identified using this search. For example, possible P-based nucleophiles (deprotonation of phosphines, silyl phosphines as P-nucleophiles) as well as possible protecting groups (phosphine–borane complexes) could be identified. As a result of this structure search, two possible disconnection approaches to the desired ligand structures could be identified (Scheme 1). It should be noted that next to the general chapters as mentioned above, the query delivered other helpful examples in other chapters (42.10.2.1.4.2 to 42.10.2.1.4.5, 36.10.1.1.4, and 3.18.1.3.6). Again, the well-organized structure of the *Science of Synthesis* database with its detailed and precise subdivision of contents was very helpful in generalizing the information for the researcher. The fact that in some cases the information given is redundant should be seen as a positive aspect, as some of the reactions can be categorized in different ways.

Expansion of the original query to other heteroatoms ($\text{Z} = \text{NH}_2$, SH) interestingly delivered mostly the same chapters as the original query, which shows that the information in the actual chapters is already structured in a useful and easy-to-locate fashion. Nevertheless, especially for the nitrogen-derived compounds, it should be noted as an additional feature that via this query, other oxidation states of the desired targets (amides in addition to amines and anilines) could also easily be located.

Conclusion

The structure-based query feature of the Science of Synthesis database, was applied in this case study to locate synthetic procedures for a class of heteroatom-substituted phosphorus-based ligands. This was found to be a highly useful tool for obtaining a good overview of the synthetic methods available. With the highly ordered and detailed information given in the chapters, the database serves as an ideal starting point for explorative synthetic studies. This is especially true for the acquisition of experimental details for a relatively broad spectrum of desired products, in this example a ligand library.

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