実験および理論の連携と融合による新規有機化学研究法の確立と弱い相互作用への応用

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研究の柱と展開

有機化学における亜鉛原素側鎖结合の役割と応用　高分子科学・合成化学における展開　高分子物性を高分子物性を抑制または計測するための方法論（計量化学）の展開

 AIMによる有機分子の評価・分解法の提案

 AIMの亜鉛原素側鎖結合への応用

 반응子の値および反応子側鎖結合・相互作用の研究

実験および理論の連携・融合による新規有機化学研究法の確立と弱い相互作用への応用
新しいNMR解析法の提案：NMR化学シフトの各支配因子への分解

相対論効果の適用

\[
\begin{align*}
\text{R antagonistic effect on o(S):} & = 0.90 \\
\text{R antagonistic effect on o(R):} & = 0.50
\end{align*}
\]

1. Relativistic effect on o(S) is evaluated separately by scalar relativistic and spin-orbit terms in the framework of ZORA.
2. Ranges of the effect with ZQ4PA at the spin-orbit ZORA level is 0.40.
3. Changes in bond distances and angles affect on o(S).
4. However, the magnitudes of the relativistic terms seem not so large.

5. The (o+S) values containing the scalar and spin-orbit relativistic terms correlate well with the observed values.
6. Basis sets of T2Pac were also employed for usual calculations.
7. Factors to affect on (o+S) and (o+S) are considered.

反応性の低い酸化脱水素水素を自由に線想する開発


Highly Regioselective Amination of Unactivated Alkenes by Hypervalent Sulfonylimino-\(^3\)-Bromane

Antion of alkene has generally required metal catalysis and/or high temperatures. Here we report that simple exposure to a small amount of sulfonylimino-\(^3\)-bromane at ambient temperature results in C=C insertion of the nitrogen functionality to afford trifluoromethylated alkene. Riched regioselectivity by varying weathered C=C bonds was observed. Primary mixed C=C bonds were inert. Addition of heterocycle to inhibit deactivation of \(^3\) dramatically improved the C=C addition efficacy. Second order kinetic, activation parameters (negative activation entropy), kinetic isotope effects, and theoretical calculations support a concerted asynchronous insertion mechanism for the metal-free C=C addition event.

Alkanes to amines by bromine

Chromat has been seeking simple ways of inserting nitrogen to other elements into alkanes—simple hydrocarbons with single bonds—to turn them into more molecules, such as drugs. Now Masahito Ouchita at the University of Tokushima in Japan and his colleagues have found that a reactive bromine-based compound can be used for the insertion of nitrogen without the traditional need for a metal catalyst or high temperature. They used trifluorimino-\(^3\)-bromine to insert nitrogen into a variety of alkanes at room temperature. Not only did this reaction achieve reasonable yields, in many cases it also selectively added nitrogen in one of two possible positions.

まとめ

1. 抗酸化作用の有効性を評価するための二極象を利用した新しい相対論効果の提案を行った。
2. ベタクエン化への適用により、機能の分子設計が可能となった。
3. オーバーサイド（オーバーサイド）効果による機能合成が期待される。
4. 新型的機能合成モジュールの開発を計画する。
5. 期待される機能を発現させるための有効な相対論効果の組み合わせに関する指針を示す。