

## **4-COMPONENT CALCULATIONS FOR MOLECULES WITH HEAVY ATOMS**

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Practical experiences with 4-component relativistic calculations for molecules will be discussed. Due to the kinetic balance requirements the feasibility of such calculations depend strongly on the availability of good and cost-effective basis sets. But very little is known about the requirements for a good basis set for 4-component calculations. The recently derived “double-zeta plus” series of basis sets are offer one approach, but there is a need to experiment in order to clarify whther these atom-optimized sets need to be extended for molecular applications.

Calculations on the heavy methane analogs as wll as on Tl compounds will be presented.