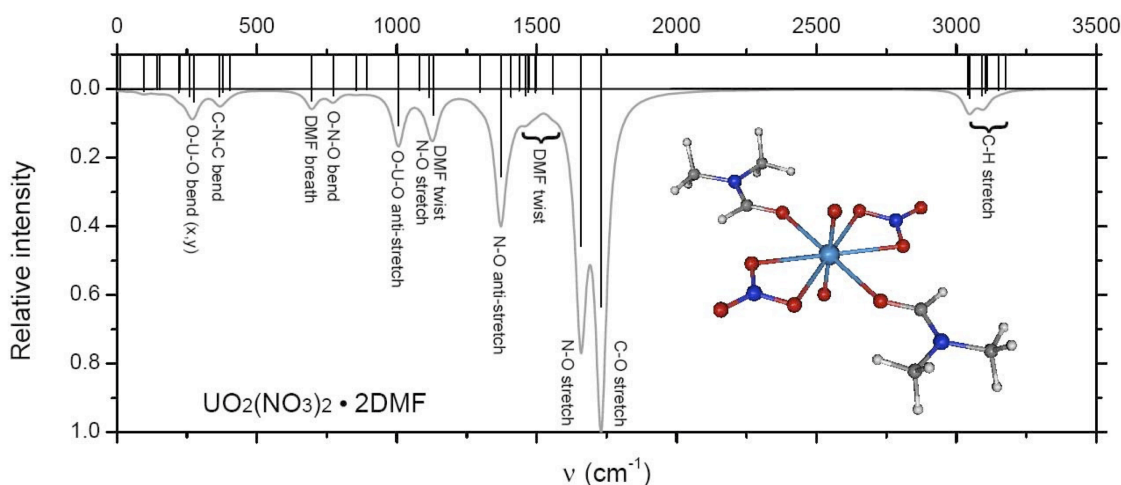


Calculation of response properties with the normalized elimination of the small component (NESC) method

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The NESC method, originally developed by Dyall and improved by Zou, Filatov and Cremer [1-5], is a first principles 2-component approach (positron components are eliminated) fully equivalent to the exact 4-component approach based on the Dirac equation. In view of the fact that NESC provides the exact 2-component relativistic description of one-electron systems, it is an ideal starting point for developing a repertoire of methods, by which routinely first and second order response properties can be calculated. Previously, we have pointed out the relationship between IORA (infinite order regular approximation) and NESC and have used this for a rapid iterative solution of the NESC equations. In this work, we present algorithm and methods for the calculation of molecular geometries, dipole moments, hyperfine structure constants, vibrational frequencies, force constants, electric polarizabilities, infrared intensities, and other response properties. We also discuss the impact of spin-orbit coupling on molecular properties. Applications are presented for mercury containing molecules and some other molecular systems containing transition metals, which require a relativistic treatment. A simple way is sketched how to obtain a quantitative characterization of the bond strength involving heavy atoms with strong relativistic effects.



- [1] Zou, W., Filatov, M., Cremer, D. *Theor. Chem. Acc.* 130:633–644, 2011.
- [2] Zou, W., Filatov, M., Cremer, D. *J. Chem. Phys.* 134:244117.1-11, 2011.
- [3] Zou, W., Filatov, M., Cremer, D. *J. Chem. Theory Comput.* 8:2617, 2012.
- [4] Zou, W., Filatov, M., Cremer, D. *J. Chem. Phys.* 137:084108, 2012.
- [5] Filatov, M., Zou, W., Cremer, D. *J. Chem. Phys.* 139:014106, 2013.