A Quantum Leap Into the Future of Chemistry

What's New in Q-Chem

EFP Library of Common Fragments

Developers: Dmytro Kosenkov and Lyudmila Slipchenko

Q-Chem offers a user-friendly library of standard EFP fragments with precomputed parameters, which simplifies the EFP job setup. The library contains validated parameters for common organic solvents and DNA bases, and will be constantly updated to include more fragments.

Publications: D. Ghosh, D. Kosenkov, V. Vanovschi, C. Williams, J. Herbert, M. Gordon, M. Schmidt, L. Slipchenko, A. Krylov, "*Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers*"
J. Phys. Chem. A, 2010, 114 (48), pp 12739–12754


Lyudmila Slipchenko


Dmytro Kosenkov

For more new features, visit:
www.q-chem.com/whatsNew4.html

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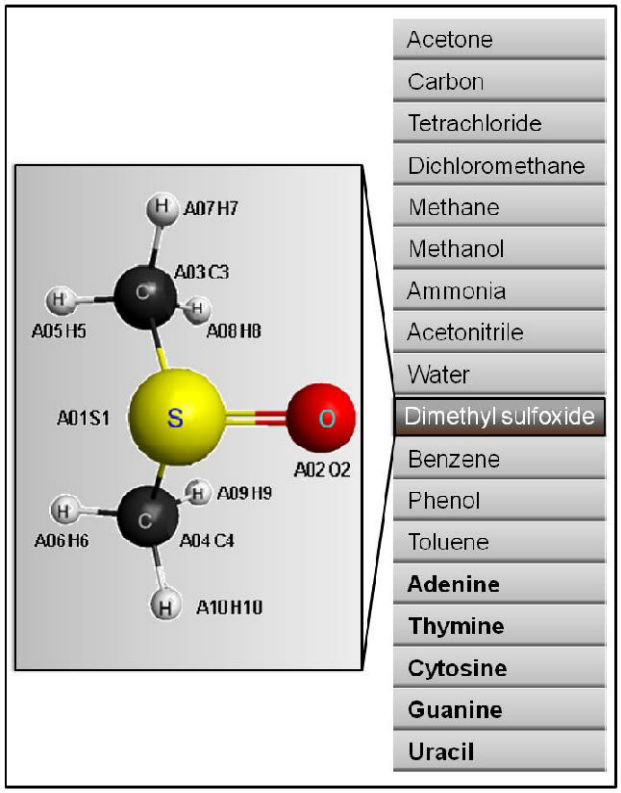
What's New in Q-Chem

EFP Library of Common Fragments (continued)



The EFP fragments included in the library. The library file for each fragment includes coordinates of the atoms, coordinates of the multipar expansion points, the distributed multipole moments (up to octopoles), the electrostatic screening parameters, the coordinates of the LMO centroids, the static and dynamic polarizability tensors at the LMO centroids, the wave function and Fock matrix elements, and the atomic labels of the EF atoms.

For more information on how to use this feature, refer to the Q-Chem Manual, Section ____:

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