# Appendix 1. Abbreviations and Acronyms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMBER</td>
<td>assisted model building with energy refinement; a MM-force field</td>
</tr>
<tr>
<td>B3LYP</td>
<td>hybrid density functional consisting of 20% Hartree-Fock and 80% Becke88 exchange combined with the Lee-Yang-Parr correlation functional</td>
</tr>
<tr>
<td>BLYP</td>
<td>GGA density functional consisting of the Becke approximation for exchange and the Lee-Yang-Parr functional for correlation</td>
</tr>
<tr>
<td>BP or BP86</td>
<td>GGA density functional consisting of the Becke approximation for exchange and the Perdew expression for correlation</td>
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<tr>
<td>cam</td>
<td>camphor</td>
</tr>
<tr>
<td>CASPT2</td>
<td>Complete Active Space with Second-order Perturbation Theory</td>
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<tr>
<td>CASSCF</td>
<td>Complete Active Space Self-Consistent Field Theory</td>
</tr>
<tr>
<td>cc-pV(D,T,Q)Z</td>
<td>correlation-consistent polarized (double, triple, or quadruple)-split valence basis set</td>
</tr>
<tr>
<td>CHARMM</td>
<td>chemistry at Harvard molecular mechanics; a MM-force field</td>
</tr>
<tr>
<td>CI</td>
<td>configuration interaction (a post Hartree-Fock method)</td>
</tr>
<tr>
<td>DFT</td>
<td>density functional theory</td>
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<tr>
<td>DZ</td>
<td>double zeta (basis set)</td>
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<tr>
<td>DZP</td>
<td>double zeta + polarization (basis set)</td>
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<tr>
<td>ENDOR</td>
<td>electron-nuclear double resonance spectroscopy</td>
</tr>
<tr>
<td>ESR</td>
<td>electron spin resonance spectroscopy</td>
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<tr>
<td>G2</td>
<td>Gaussian-2 theory (the second in a series of Gx methods for calculation of total energies of a given molecular species using a composite technique in which a sequence of well-defined ab initio molecular orbital calculations is performed)</td>
</tr>
<tr>
<td>G3</td>
<td>Gaussian-3 theory (the third in a series of Gx methods for calculation of molecular energies, see also G2)</td>
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<tr>
<td>GGA</td>
<td>generalized density gradient approximations</td>
</tr>
<tr>
<td>HF</td>
<td>Hartree-Fock</td>
</tr>
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<td>Abbreviation</td>
<td>Description</td>
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<tr>
<td>HOMO</td>
<td>Highest occupied molecular orbital</td>
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<tr>
<td>KIE</td>
<td>kinetic isotope effect</td>
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<tr>
<td>k_x</td>
<td>rate constant for a certain reaction x</td>
</tr>
<tr>
<td>LACVP</td>
<td>Los Alamos Effective Core Valence Potential (basis set)</td>
</tr>
<tr>
<td>LDA</td>
<td>Local density approximation</td>
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<tr>
<td>LUMO</td>
<td>Lowest occupied molecular orbital</td>
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<tr>
<td>LYP</td>
<td>Lee-Yang-Parr Correlation functional</td>
</tr>
<tr>
<td>meta-GGA</td>
<td>Meta Generalized Gradient Approximation</td>
</tr>
<tr>
<td>MM</td>
<td>molecular mechanics</td>
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<tr>
<td>MO</td>
<td>molecular orbital</td>
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<tr>
<td>MRMP</td>
<td>multireference Møller-Plesset</td>
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<tr>
<td>OPLS</td>
<td>optimized potentials for liquid simulations</td>
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<tr>
<td>OPTX</td>
<td>Handy-Cohen Optimized Exchange Functional</td>
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<tr>
<td>P450</td>
<td>Cytochrome P450 protein</td>
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<tr>
<td>PBE</td>
<td>Perdew–Burke–Ernzerhof Correlation functional</td>
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<tr>
<td>SCF</td>
<td>Self-Consistent Field approach; in an SCF calculation the wavefunction is gradually refined until self-consistency is achieved</td>
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<tr>
<td>STO</td>
<td>Slater type orbital</td>
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<tr>
<td>THF</td>
<td>tetrahydrofuran (oxacyclopentane)</td>
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<tr>
<td>TZ</td>
<td>triple zeta (basis set)</td>
</tr>
<tr>
<td>TZP</td>
<td>triple zeta + polarization (basis set)</td>
</tr>
<tr>
<td>ZORA</td>
<td>a relativistic zeroth-order regular approximation</td>
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</table>