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(understanding what goes into calculation)
Understanding which parameter exist and what they do (aimed at Gaussian)

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sufficiently well developed that it can be automated for implementation on a computer. Note that the words exact and perfect do not appear in these definitions.

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chemistry that uses
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approximations, Journal
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10.1002/jcc.26126, 41,

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that as many terms used are either unique to computational chemistry or have a unique meaning in this context a glossary of these terms, which will appear in bold face is given at the end. Also the ...

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