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June 4th, 2020 - an orbital is just a bit of space where there is a 95 chance of finding that particular electron if an electron is in a

particular orbital you know about its energy but there is no way of knowing how it is moving around within that orbital the big problem in all of this to my mind is the confusion in the words orbit and orbital'

'turbomole modular program suite for ab initio quantum

June 4th, 2020 - from turbomole s beginnings code development was accompanied by basis set development an overview with typical applications for the different basis set families developed with turbomole is given in table i the turbomole or karlsruhe basis set family currently consists of four types the now outdated def basis sets 20 114 116 20 k'

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