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'Molecular Quantum Mechanics And Molecular Spectra ... ETH Zürich, Laboratory Of Physical Chemistry, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland, Email: Martin@Quack.ch Reprinted From "Handbook Of High-Resolution Spectroscopy", Vol. 1, Chapter 1, Pages 1-55 ... The Jan 12th, 2024.

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