



SubTHz absorption spectra of vibration modes of tubulin

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Proteins, vital to cellular life, perform diverse functions like catalyzing reactions and transporting molecules through conformational changes are thought to be enabled by normal vibrational modes [1]. While spectroscopic detection is challenging [2], these modes can be calculated using normal mode analysis [3], visualized as oscillatory protein structure deformations. This study explores the normal vibration modes of tubulin, a 110 kDa heterodimeric protein forming microtubules crucial to the cytoskeleton. Microtubules play structural and functional roles in cells, generating force for division and transport. In this work, all-atom normal mode analysis reveals low-frequency vibration modes of tubulin heterodimer. Interestingly, frequency distribution of these modes (40-175 GHz) coincides with 5G and 6G communication technologies. The study also highlights the impact of water layers on protein atom dipole moments and frequency values – involving more water layers around the tubulin in the normal mode analysis causes shift of the absorption spectra.

- [1] C. M. Cheatum, “Low-Frequency Protein Motions Coupled to Catalytic Sites,” *Annu. Rev. Phys. Chem.*, vol. 71, no. 1, pp. 267–288, Apr. 2020, doi: 10.1146/annurev-physchem-050317-014308.
- [2] A. G. Markelz and D. M. Mittleman, “Perspective on Terahertz Applications in Bioscience and Biotechnology,” *ACS Photonics*, vol. 9, no. 4, pp. 1117–1126, Apr. 2022, doi: 10.1021/acsp Photonics.2c00228.
- [3] A. Nicolai, P. Delarue, and P. Senet, “Theoretical Insights into Sub-Terahertz Acoustic Vibrations of Proteins Measured in Single-Molecule Experiments,” *The Journal of Physical Chemistry Letters*, vol. 7, no. 24, pp. 5128–5136, Dec. 2016, doi: 10.1021/acs.jpclett.6b01812.

Authors acknowledge support from the Czech Science Foundation p.no. GA20-06873X. Part of the text was edited by ChatGPT 3.5.