Density Functional Calculation of THz Spectra of Glucose Anomers

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Especially in the organic material analysis field the distinction between different anomers, as well as between D- and L - enantiomers of chiral molecules is an important issue in biological and medical applications. Recently, THz domain spectroscopy has been suggested as a new technique for structural identification of organic isomers[1]. We have found that THz spectra of commercial D- and L-glucose samples have clearly distinct THz spectra, with a particularly large difference in the 9-10 THz region. However, commercial L-glucose samples are mixtures of α and β anomers, so we have computed the vibrational modes and far infrared spectra of α- and β-glucose in crystal form using density functional theory. Despite the fact that the two anomers differ only in the orientation of a single OH group, the THz spectra are markedly different around 9 THz where β-glucose has a strong absorption band while the absorption of α-glucose is negligible, see Figure 1. We show that a 50-50% combination gives excellent agreement with experiment. We discuss the spectral differences in terms of the vibrational modes of the single molecules and their coupling through intermolecular interaction in the two different crystal structures.

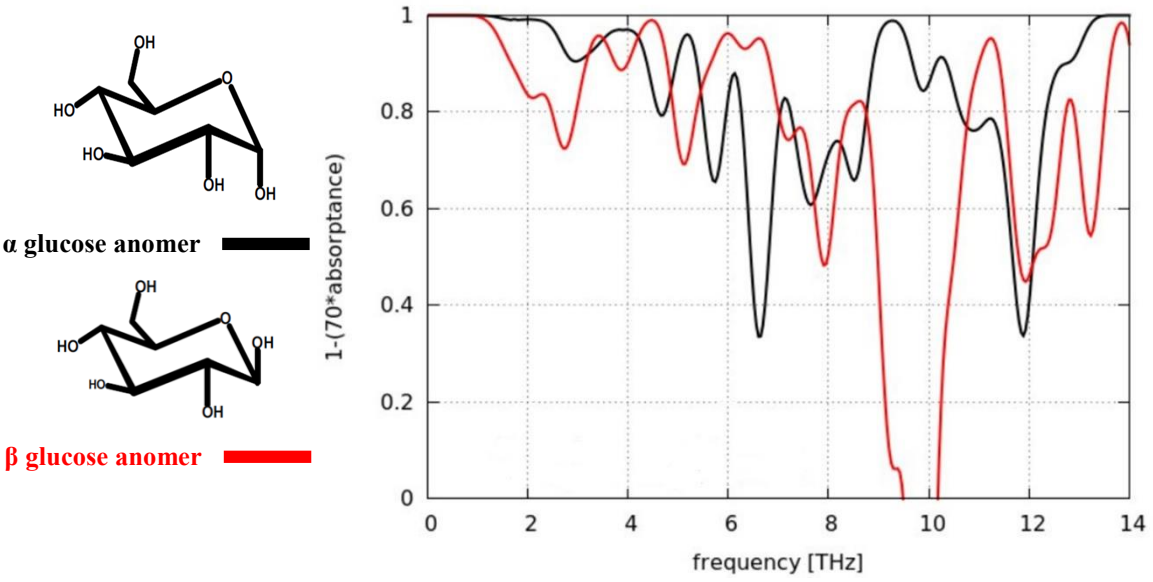

Figure 1 FIR Spectra of α and β glucose crystal

[1] W. Chen et al., *Isomers Identification of 2-hydroxyglutarate acid disodium salt (2HG) by Terahertz Time-domain Spectroscopy,* Sci. Rep. **7** (2017) 12166.