Molecular and vibrational structure of the extracellular bacterial signal compound N-butyryl-homoserine lactone (C4-HSL)

The molecular and vibrational structure of the title compound (C4-HSL) was studied by experimental and theoretical methods. The infrared (IR) absorption spectrum was measured in the solid state and in CCl4 suspension. The observed absorption bands were compared with transitions obtained with B3LYP/cc-pVTZ density functional theory (DFT) calculations. Two stable molecular conformations were predicted, corresponding to an endo- and an exo-conformer with similar energies. Intermolecular amide-amide hydrogen bonding in the crystal state was approximated by a simple cluster model, leading to excellent agreement with the observed solid state IR spectrum. Due to the low solubility of C4-HSL in common solvents for IR spectroscopy, such as CS2 and CCl4, a liquid solution spectrum of pure, monomeric C4-HSL was not obtained. However, absorbance peaks observed in oversaturated CCl4 solution could be assigned to distinct contributions from suspended micro-crystalline aggregates and dissolved monomeric species. The key vibrational bands of the monomeric form of C4-HSL are reported here for the first time: 3425 cm\(^{-1}\) (\(\nu(\text{N-H})\)), 1784 cm\(^{-1}\) (\(\nu(\text{C=O})\), lactone), 1688 cm\(^{-1}\) (amide I), and 1494 cm\(^{-1}\) (amide II) (CCl4).

General information
State: Published
Organisations: Department of Photonics Engineering, Roskilde University
Contributors: Bak, J., Spanget-Larsen, J.
Pages: 237-241
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Vibrational Spectroscopy
Volume: 49
Issue number: 2
ISSN (Print): 0924-2031
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.55
Web of Science (2017): Impact factor 1.363
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.76
Web of Science (2016): Impact factor 1.74
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.88
Web of Science (2015): Impact factor 1.682
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.1
Web of Science (2014): Impact factor 2.003
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.68
Web of Science (2013): Impact factor 1.547
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.72
Web of Science (2012): Impact factor 1.747
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1