Content of the Electronic Supplementary Information.

1. Output file of the calculated vibrational frequencies of DL-alanine, from the CRYSTAL17 software. This includes the calculated modes and the geometry of the unit cell atoms using the B97-3c functional. This file can be read by freely available Notepad++ software, for example. Additionally, this output file can be uploaded to CRYSPLOT, the free online visualisation software for CRYSTAL17:
http://crysplot.crystalsolutions.eu/web_pages_yves3/vibration.html
Here the infrared calculated spectrum can be observed, and the vibrational origin of each mode visually analysed.

2. Media files (GIF) for the molecular vibrational modes of the four lowest energy absorptions. These files animate the motions indicated in Fig 13.