

Structural Dynamics of Chloromethanes through Computational Spectroscopy: Combining INS and DFT

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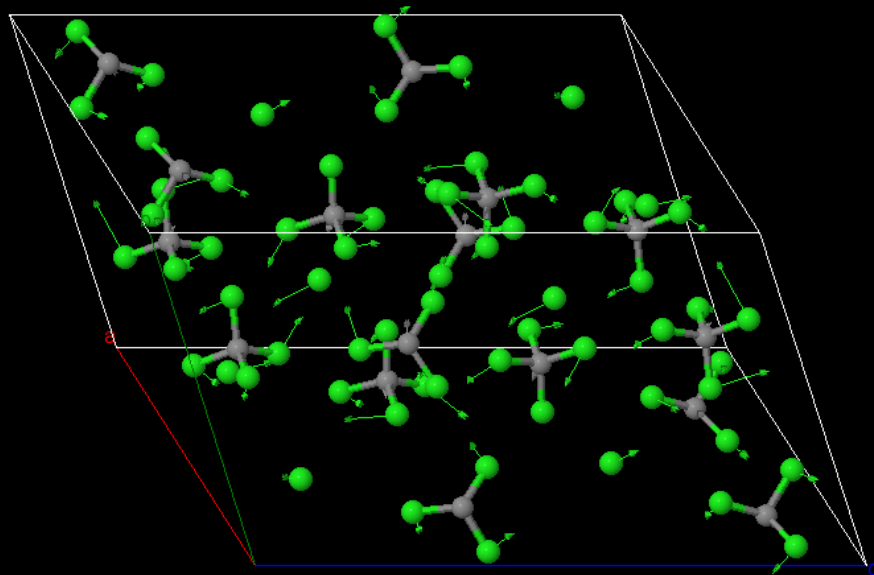
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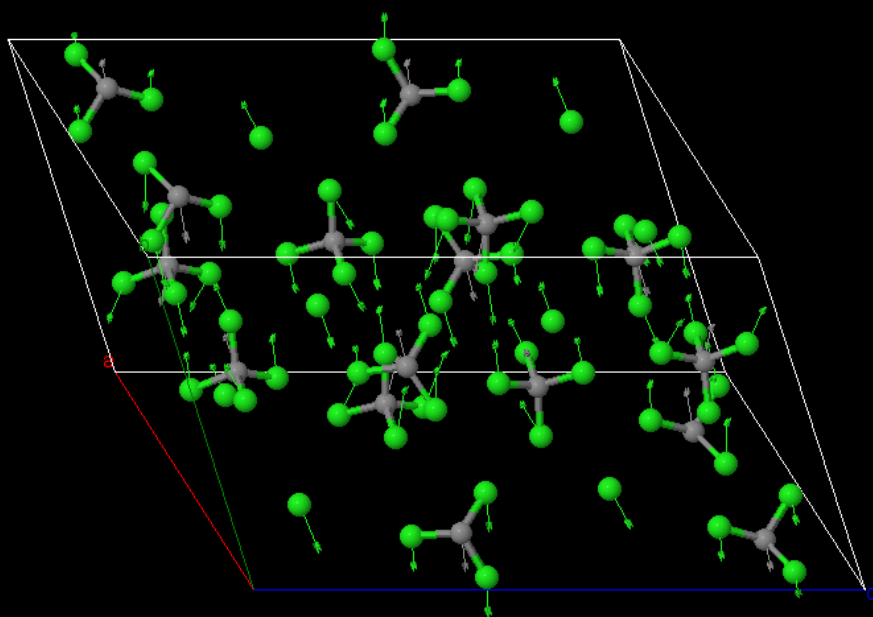
Figure S2. – Atomic displacements of some vibrational modes of trichloromethane, CHCl₃.

Figure S3. – Atomic displacements of some vibrational modes of dichloromethane, CH₂Cl₂.

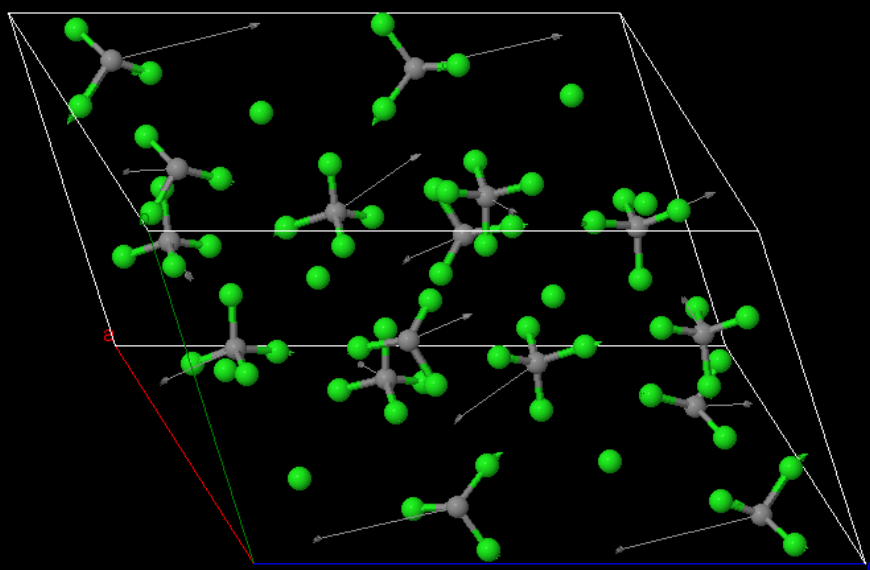
Figure S1. – Atomic displacements of some vibrational modes of carbon tetrachloride, CCl_4 .



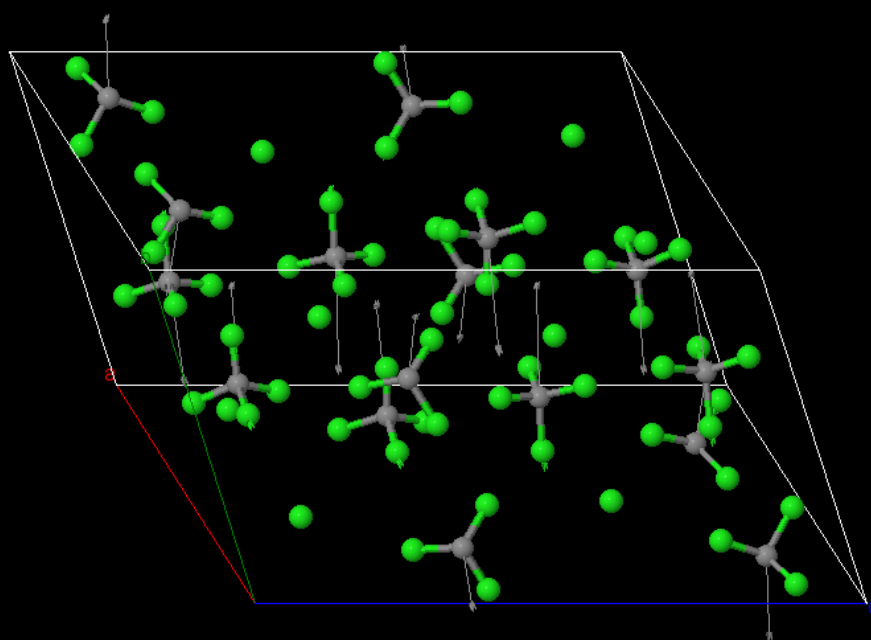
a) Librational mode, 20 cm^{-1}



b) translational mode, 44 cm^{-1}

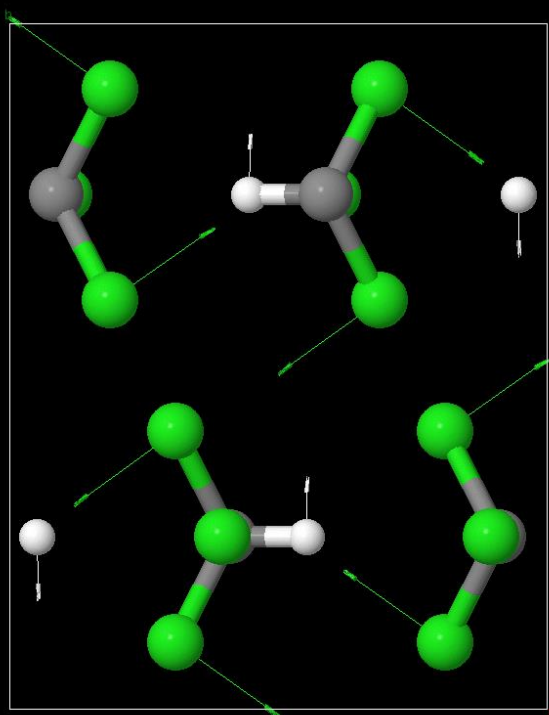


c) v_3 Lowest component

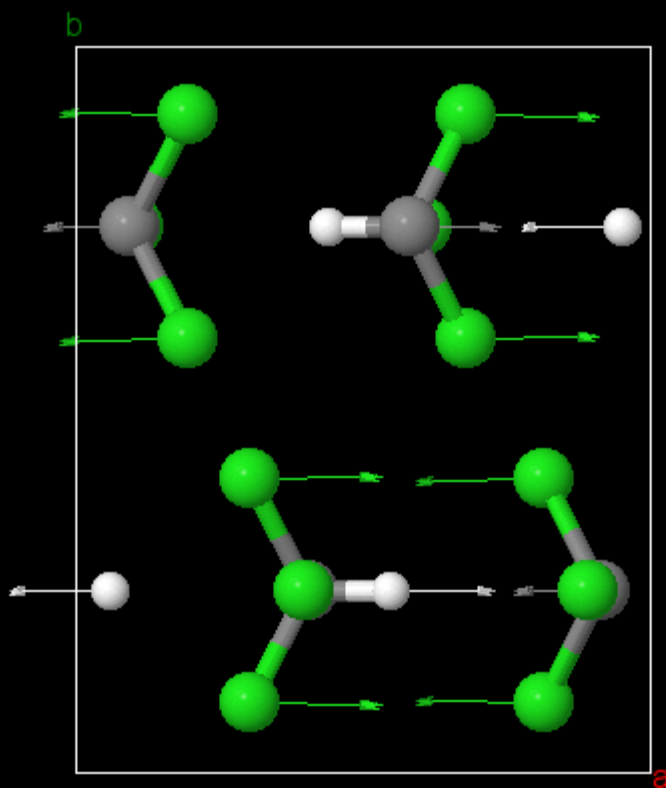


d) v_3 highest component

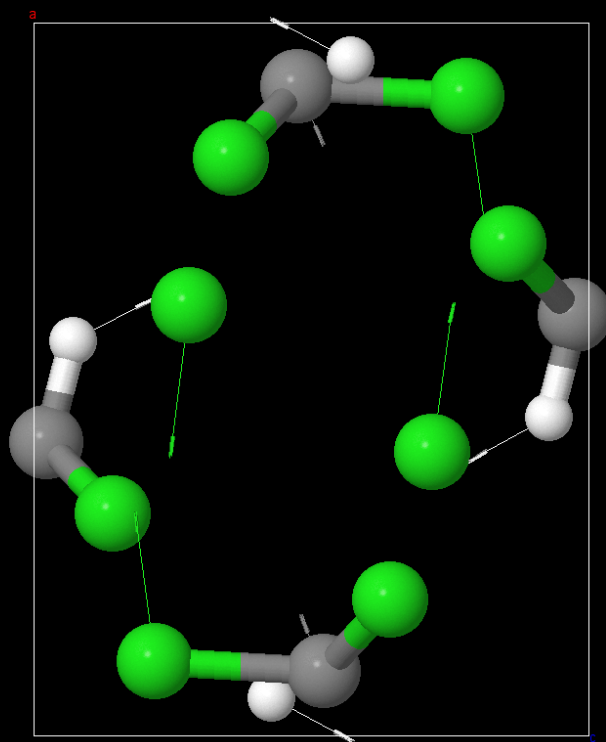
Figure S2. – Atomic displacements of some vibrational modes of trichlorometane, CHCl_3 .



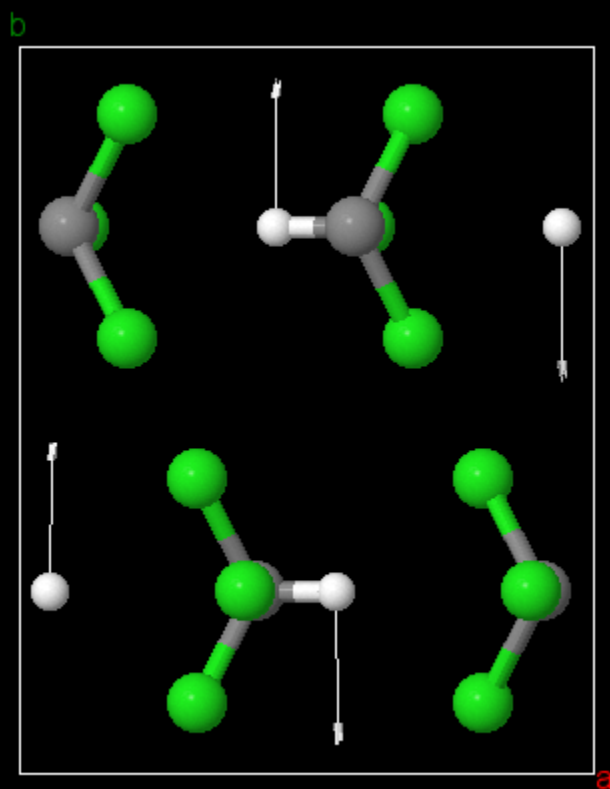
a) Librational mode, 45 cm^{-1}



b) Translational mode, 66 cm^{-1}

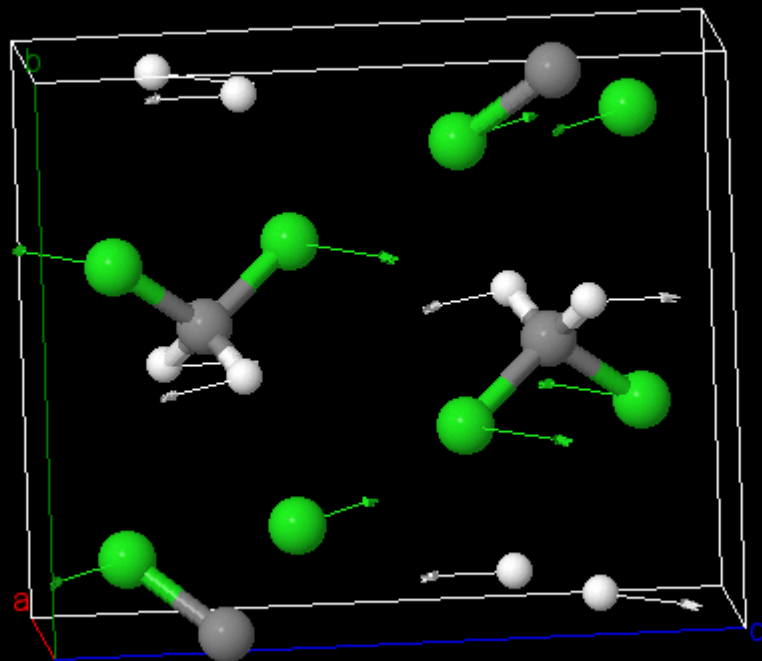


c) Librational mode, 93 cm⁻¹

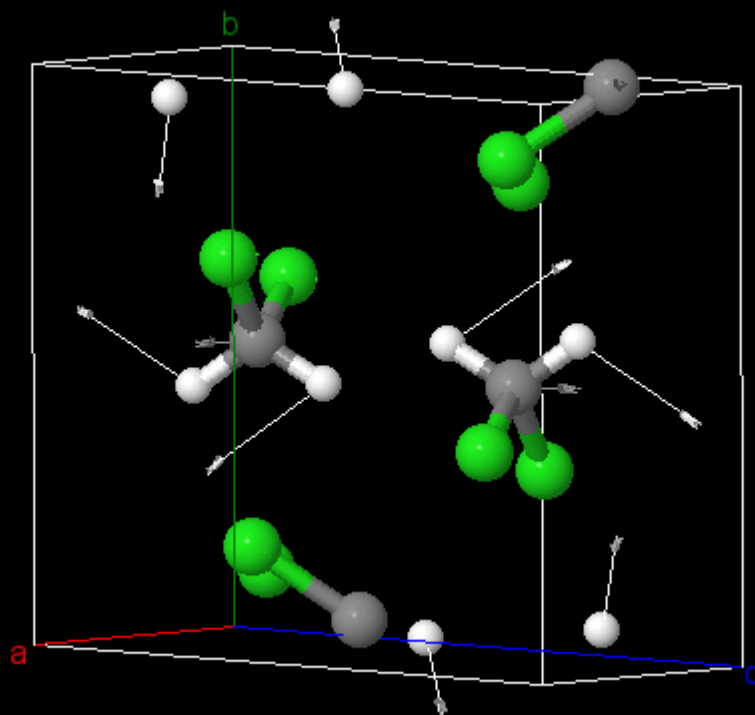


d) CH bending mode, 1180 cm⁻¹

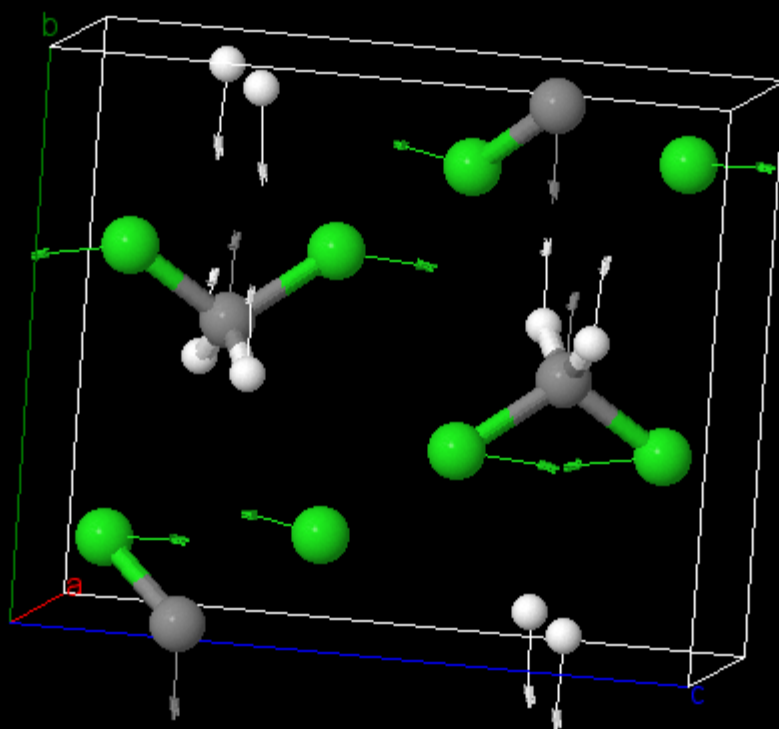
Figure S3. – Atomic displacements of some vibrational modes of dichlorometane, CH_2Cl_2 .



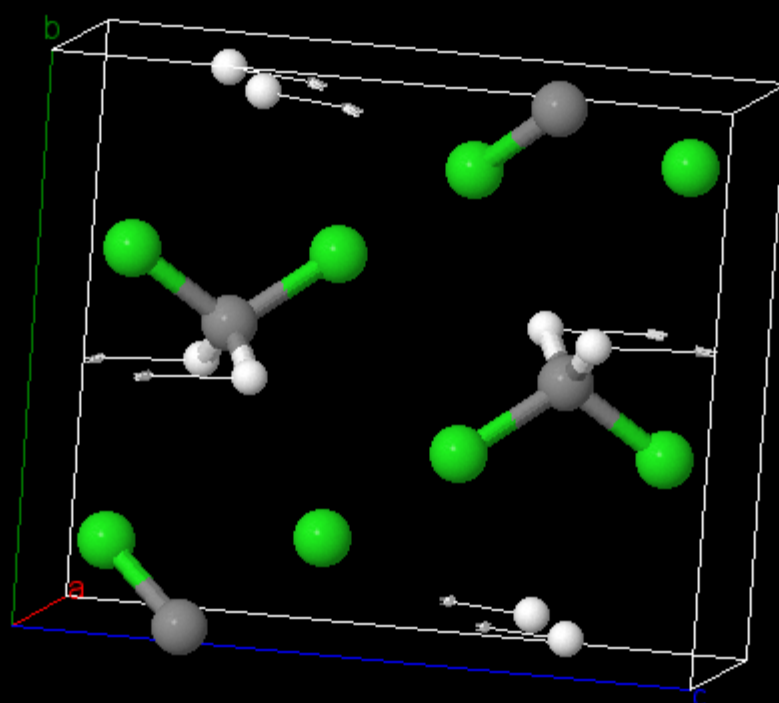
a) Librational mode, 117 cm^{-1}



b) Librational mode, 132 cm^{-1}



c) CCl₂ bending mode, 283 cm⁻¹



d) CH₂ rocking mode, 1230 cm⁻¹