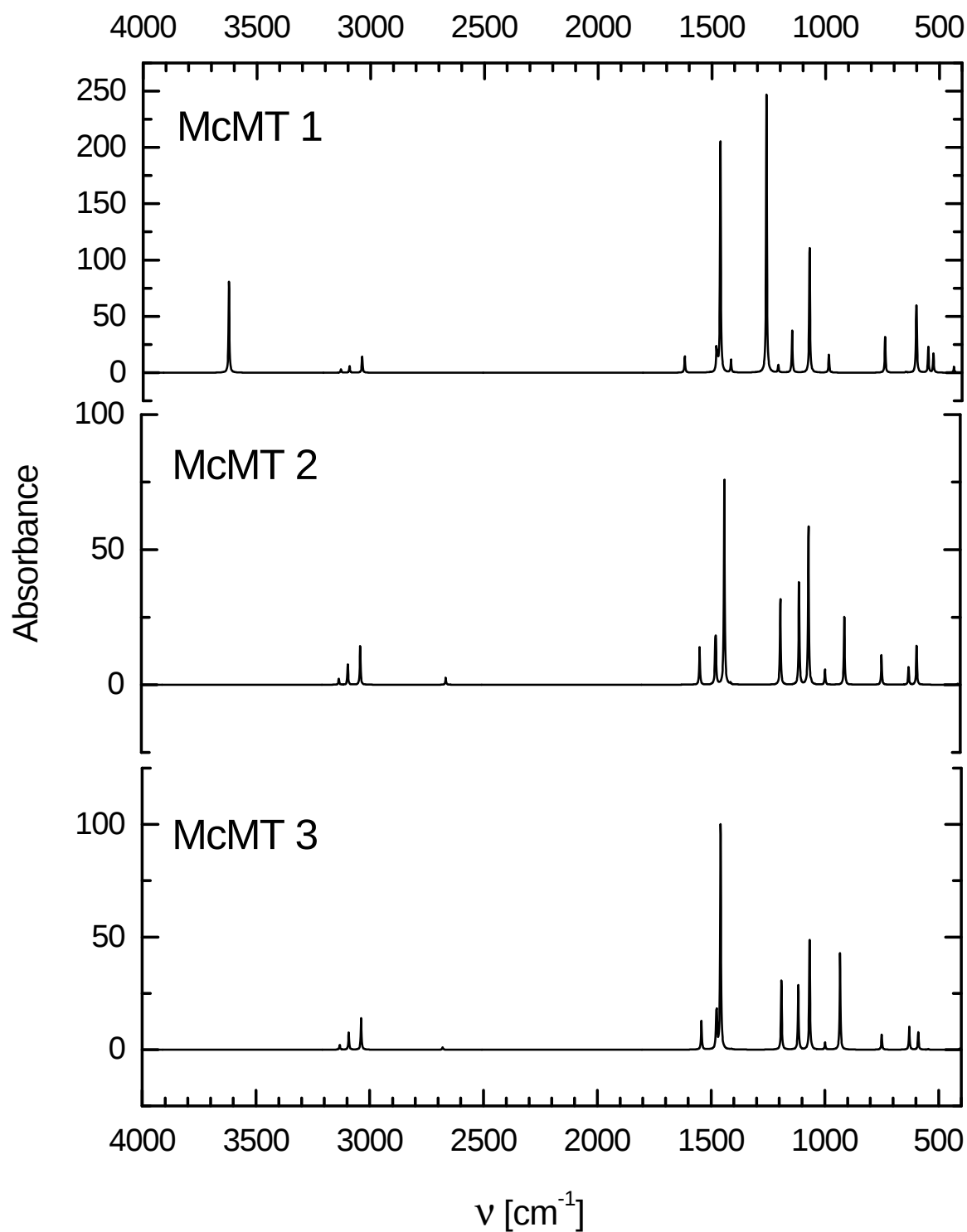
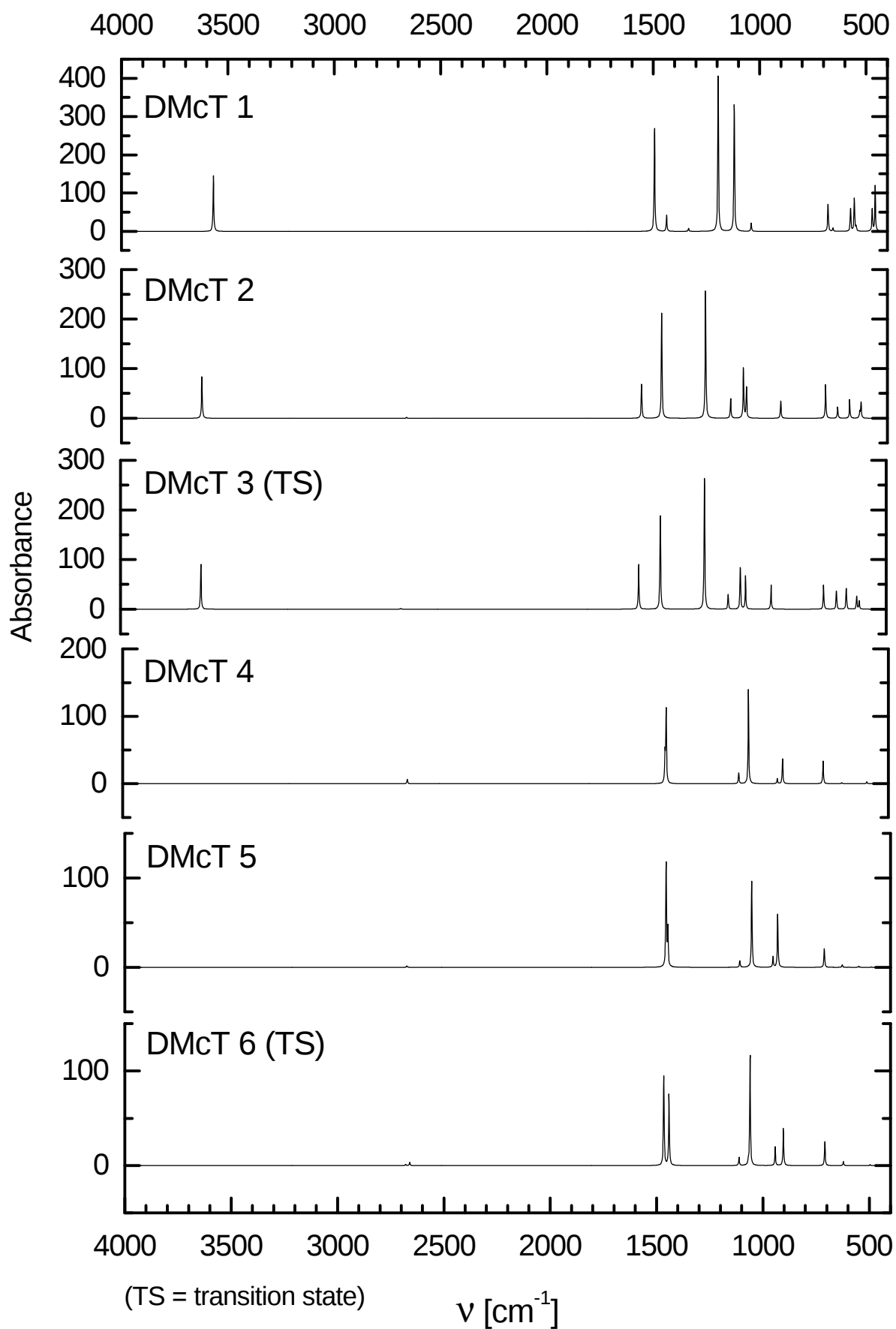




**Theoretical IR spectra for all McMT isomers
calculated at B3LYP/6-311+G(d,p) level, unscaled.**



**Theoretical IR spectra for all DMcT isomers
calculated at B3LYP/6-311+G(d,p) level, unscaled.**