

I. FORCE FIELD ATOMS TYPES AND CHARGES

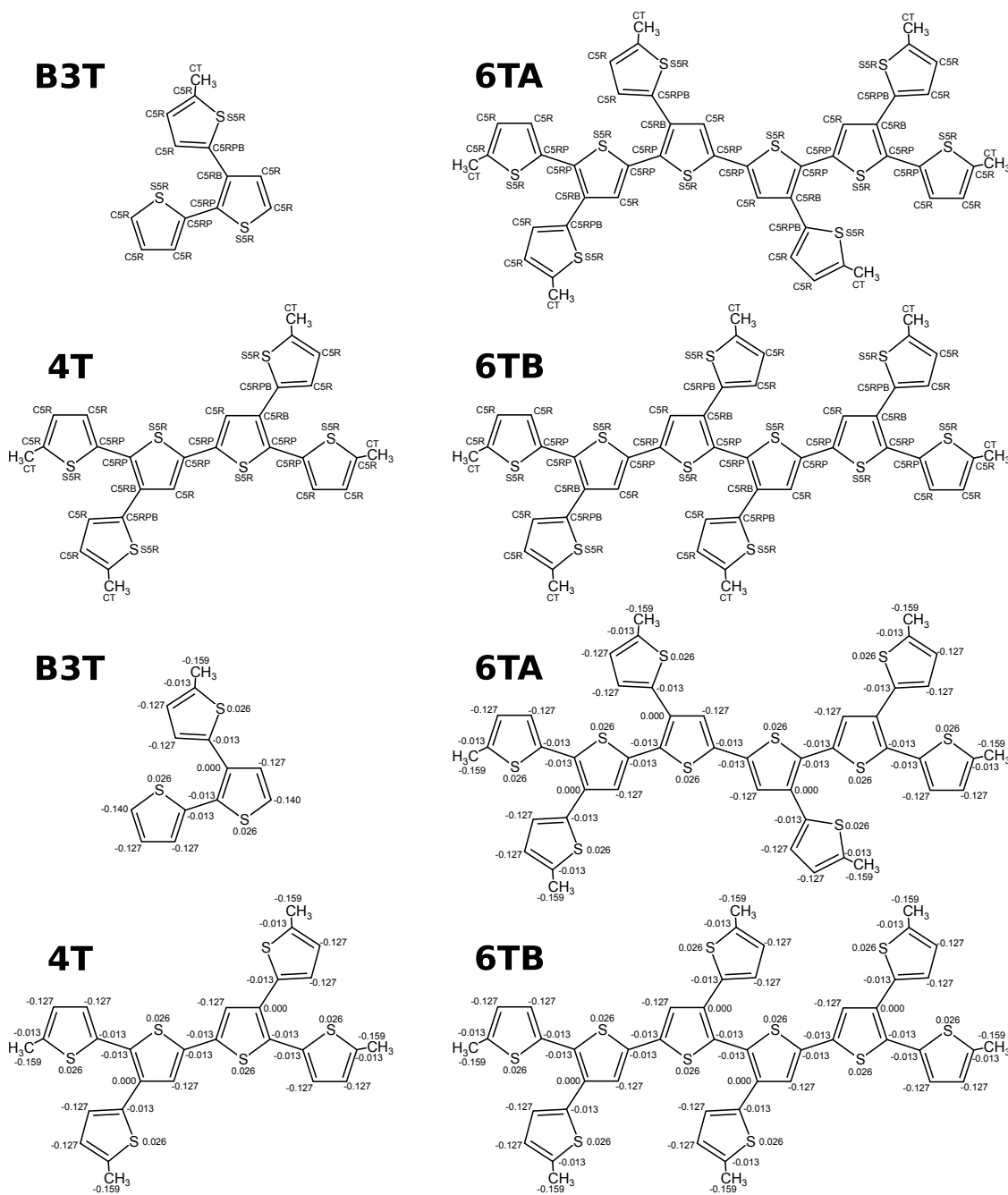


FIG. 1. Atom types and charges used for the branched oligothiophenes in the force field calculations. Aromatic hydrogens have a charge of 0.127 and the methyl hydrogens have a charge of 0.053.

II. THEORETICAL IR SPECTRA OF 6TA AND 6TB

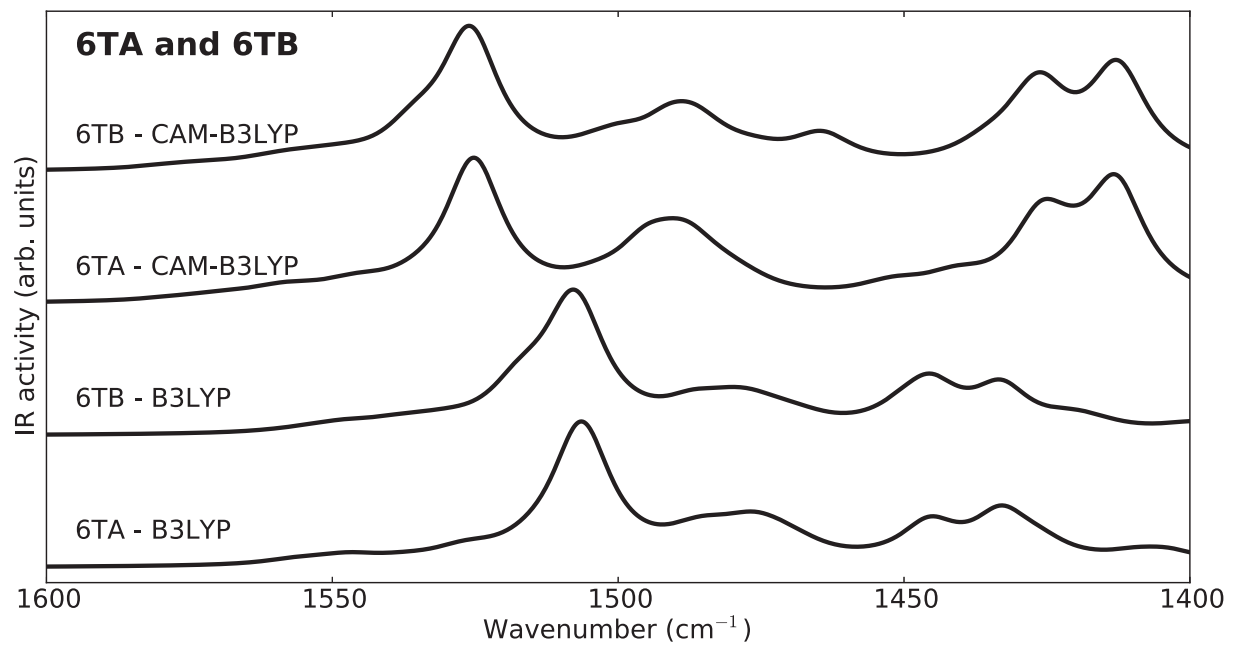


FIG. 2. Theoretical room temperature IR spectra for 6TA and 6TB, weighted by liquid MD statistics.

III. INDIVIDUAL SPECTRA

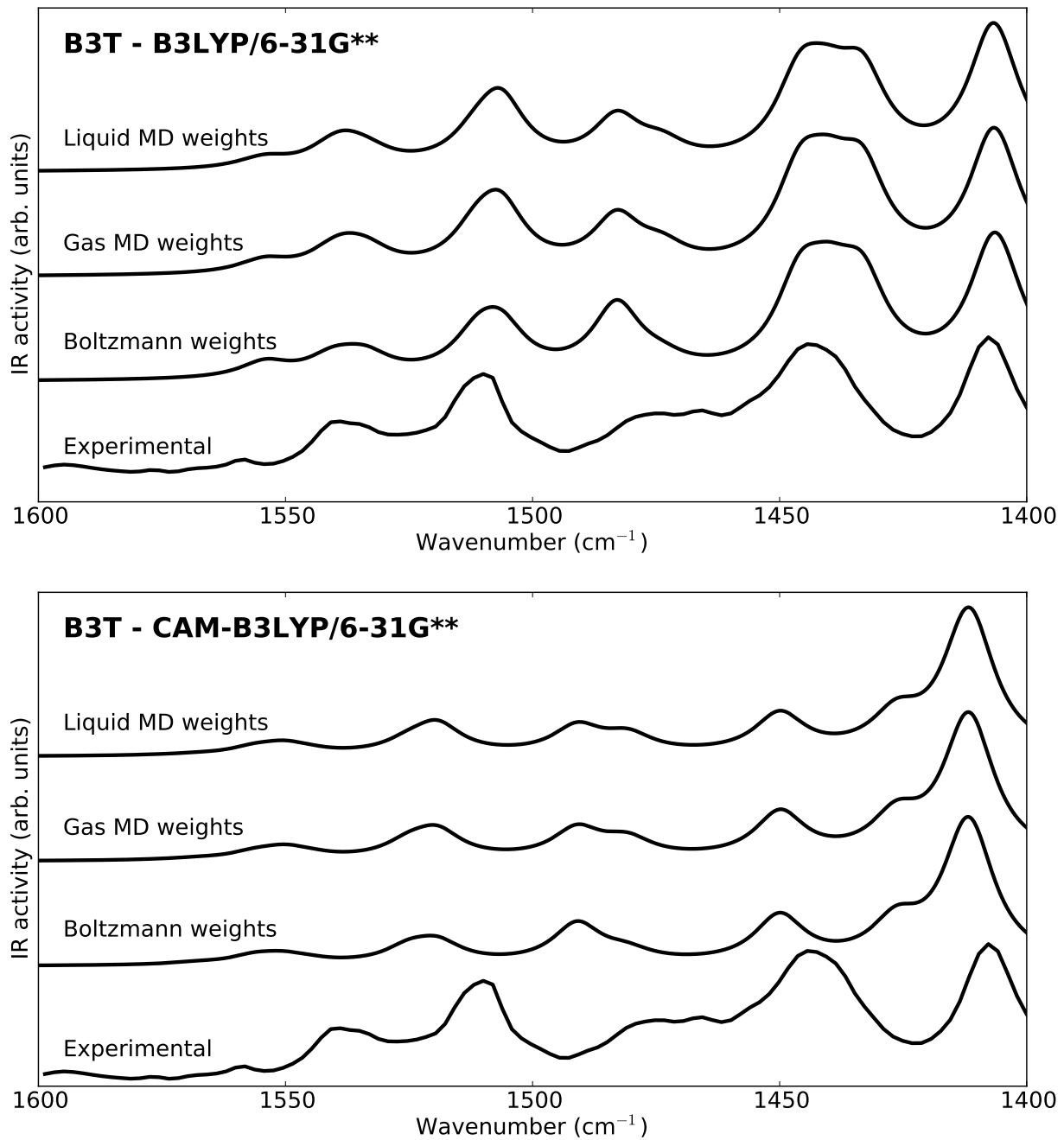


FIG. 3. Theoretical room temperature IR spectra for B3T compared to experimentally measured spectra.

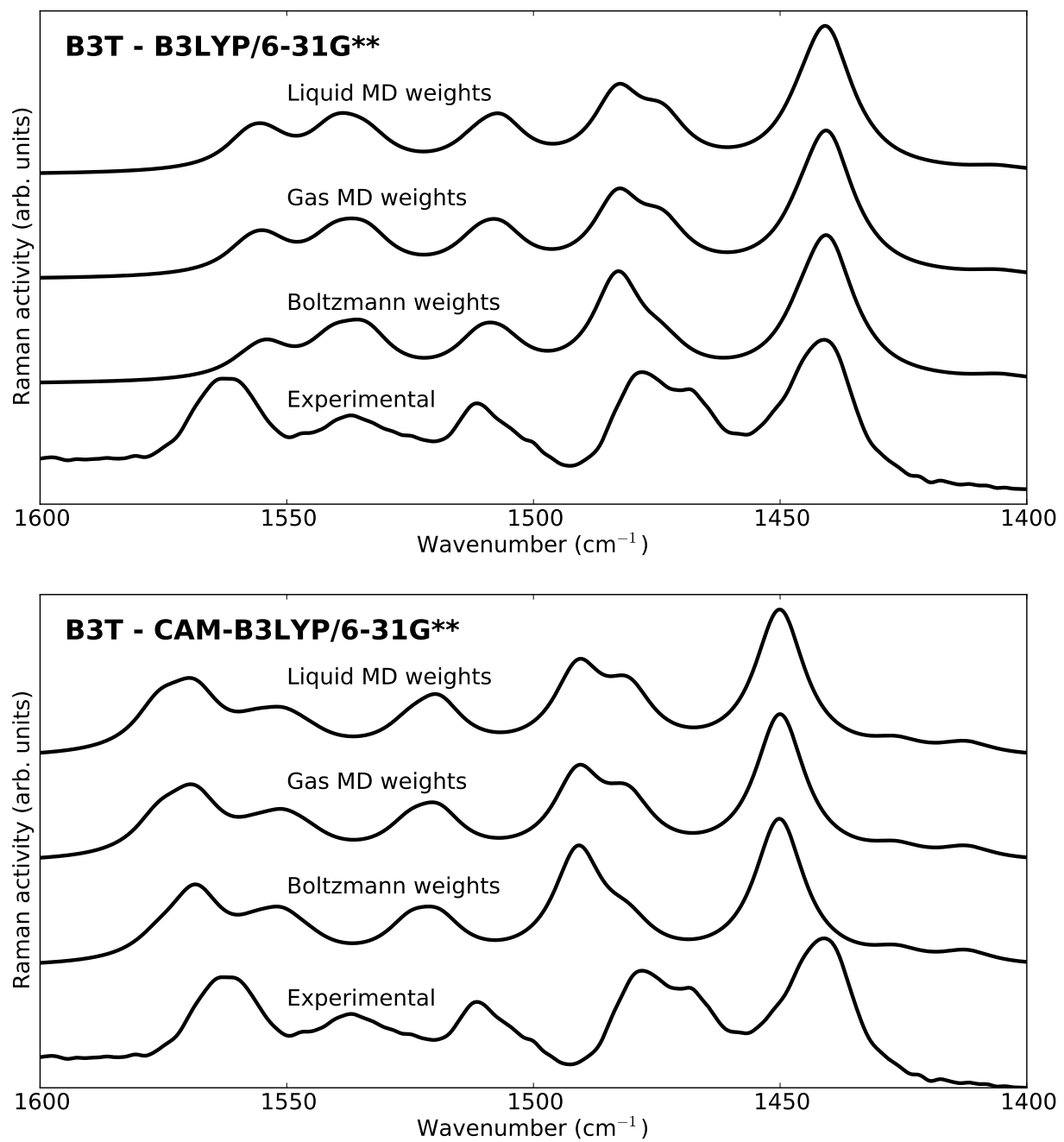


FIG. 4. Theoretical room temperature Raman spectra for B3T compared to experimentally measured spectra.

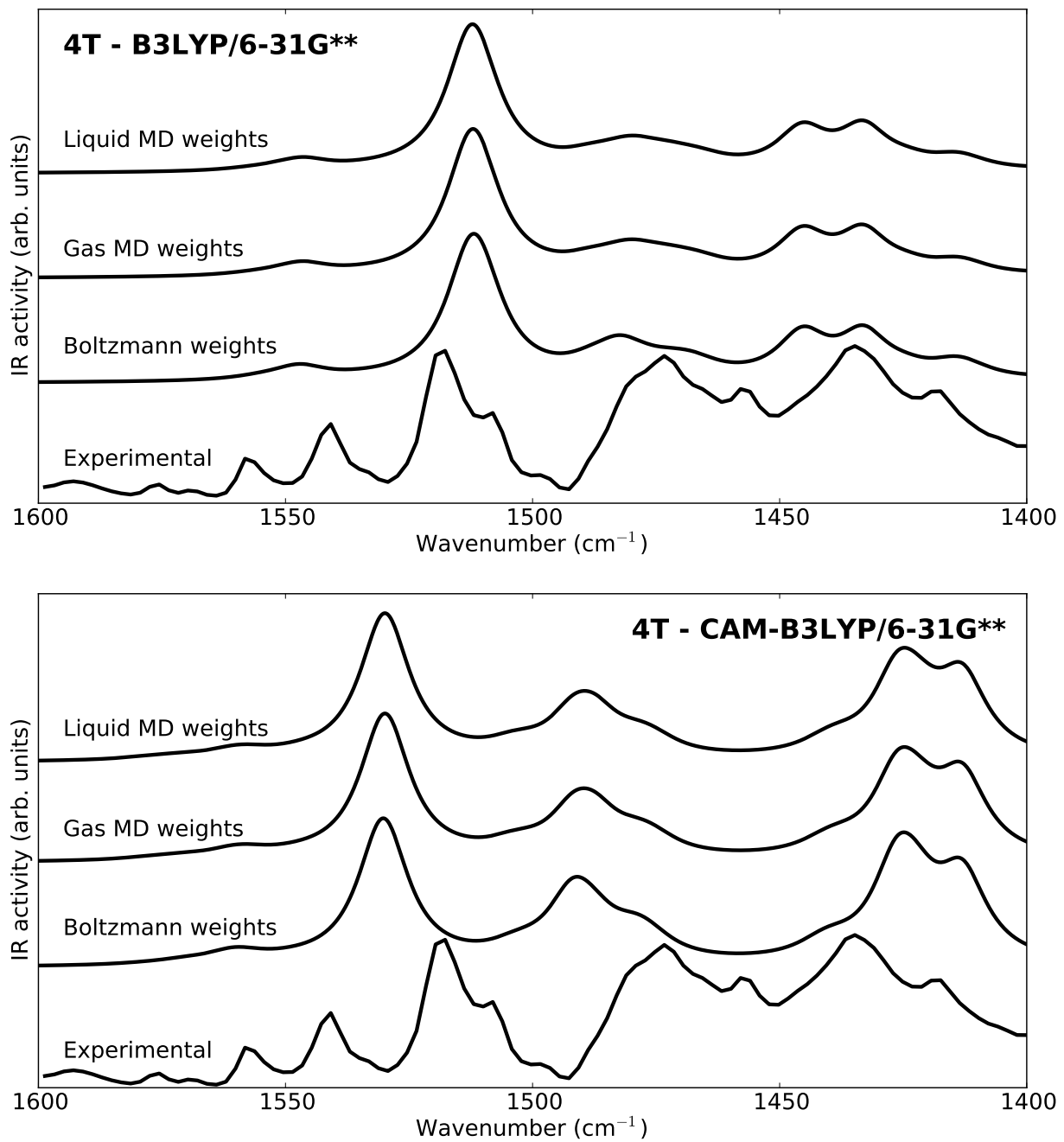


FIG. 5. Theoretical room temperature IR spectra for 4T compared to experimentally measured spectra.

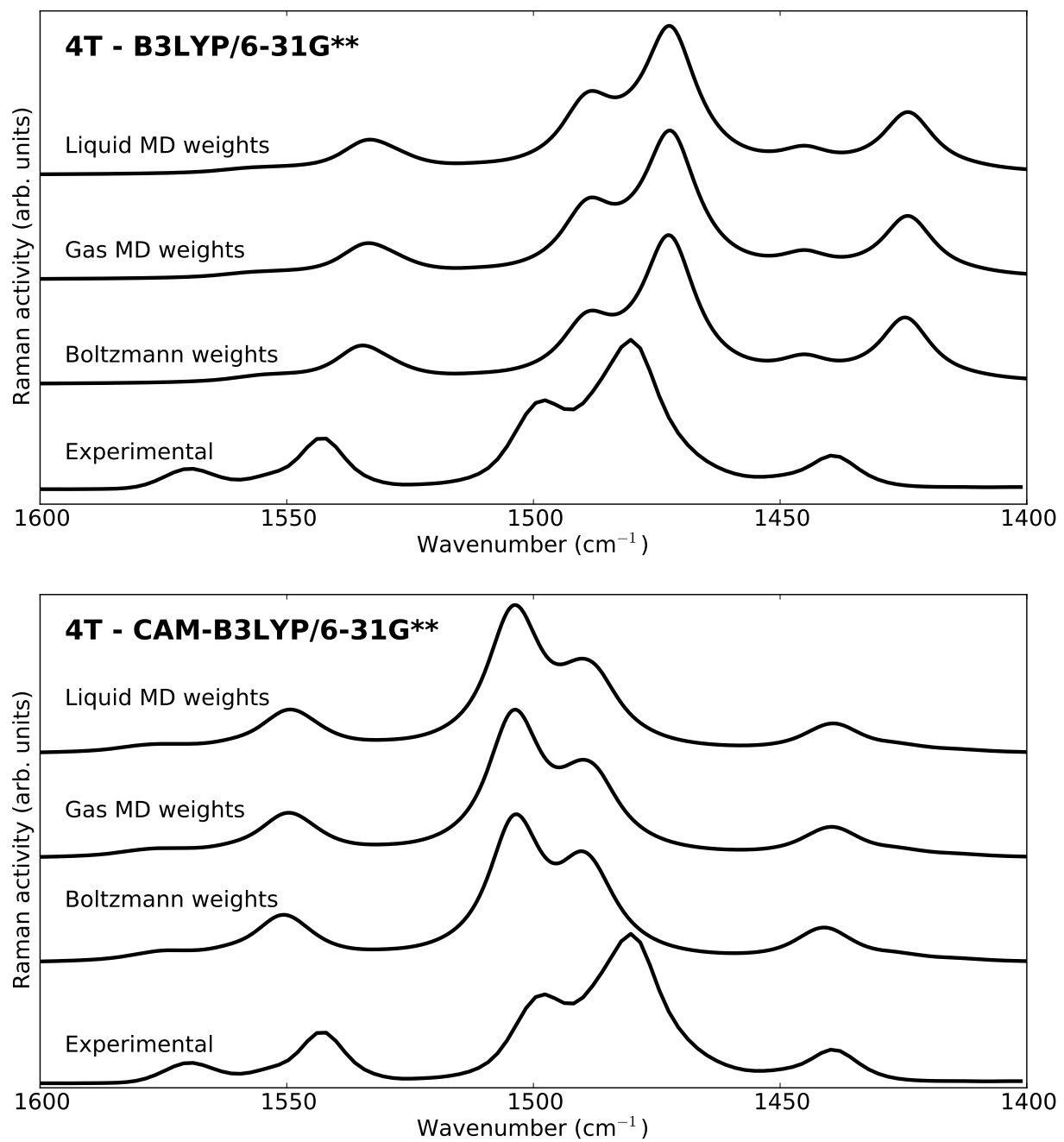


FIG. 6. Theoretical room temperature Raman spectra for 4T compared to experimentally measured spectra.

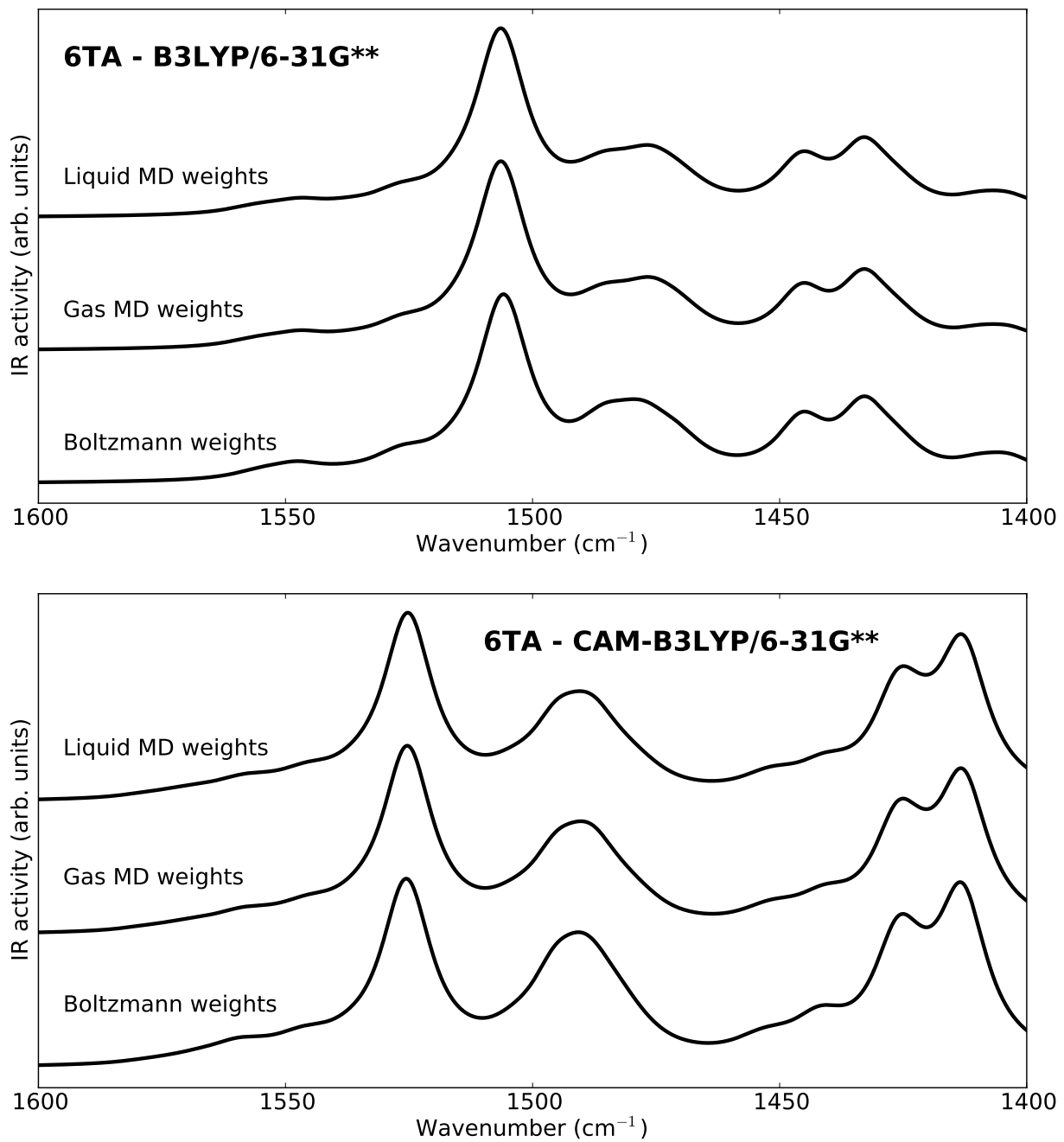


FIG. 7. Theoretical room temperature IR spectra for 6TA.

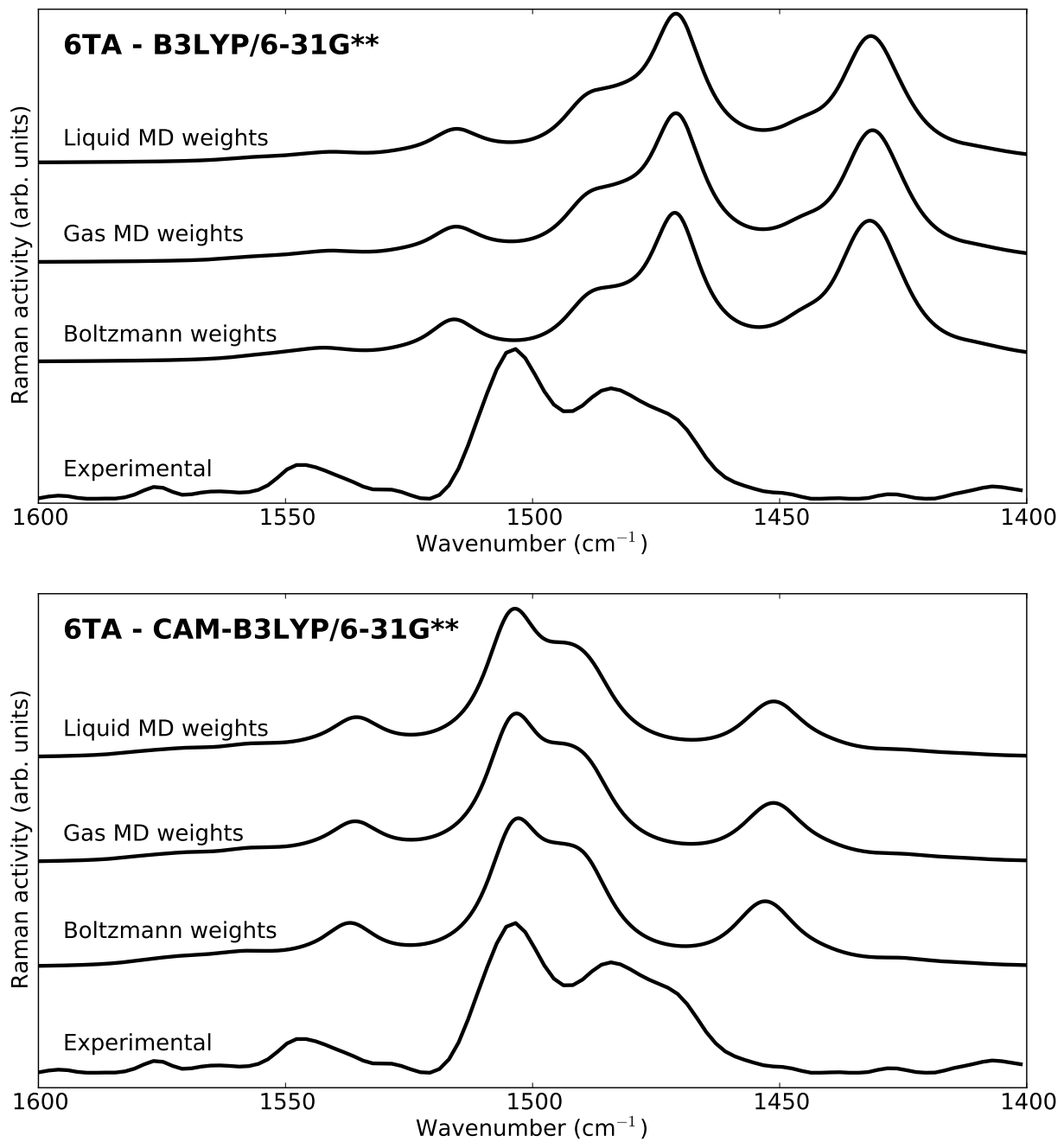


FIG. 8. Theoretical room temperature Raman spectra for 6TA compared to experimentally measured spectra.

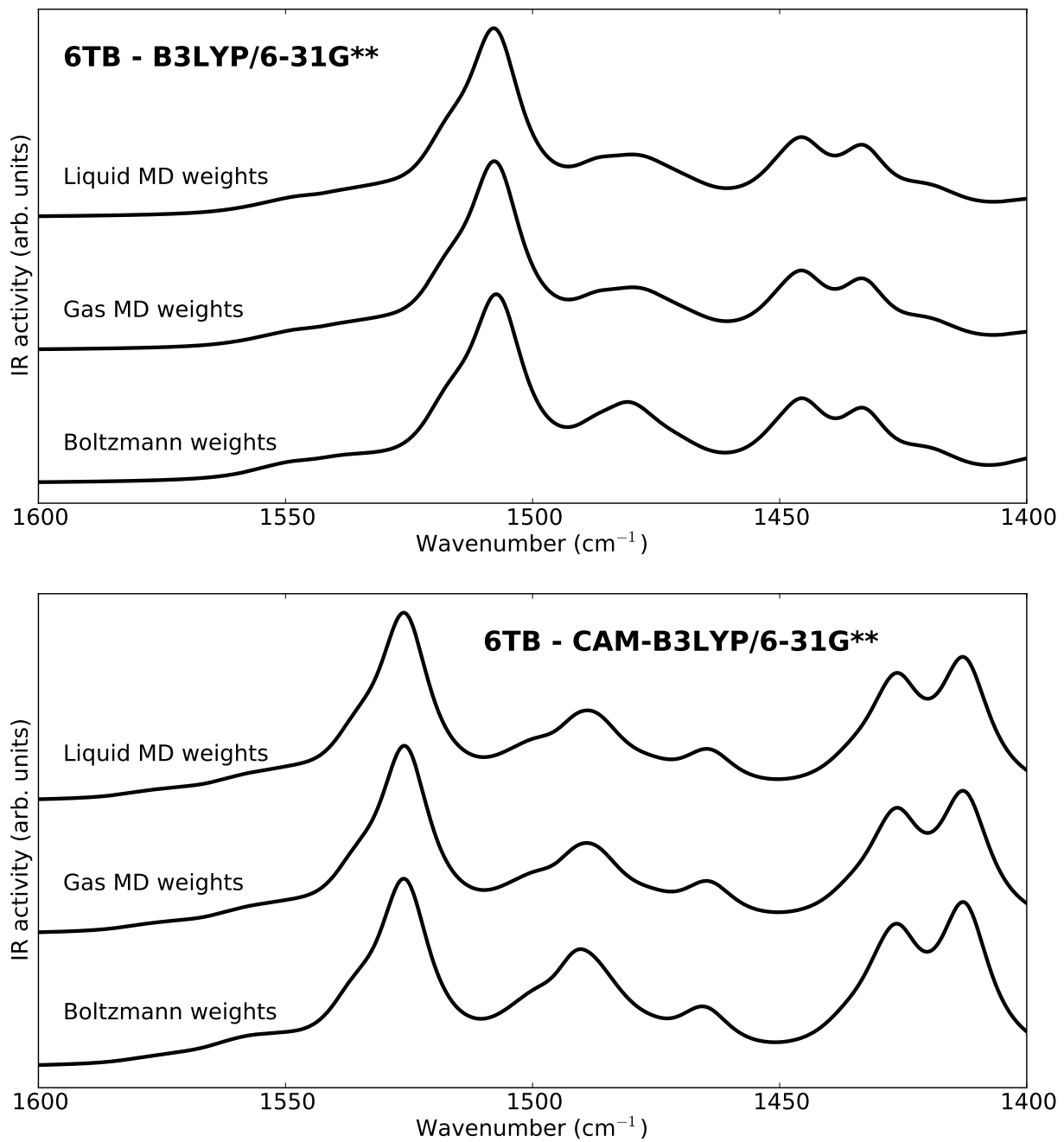


FIG. 9. Theoretical room temperature IR spectra for 6TB.

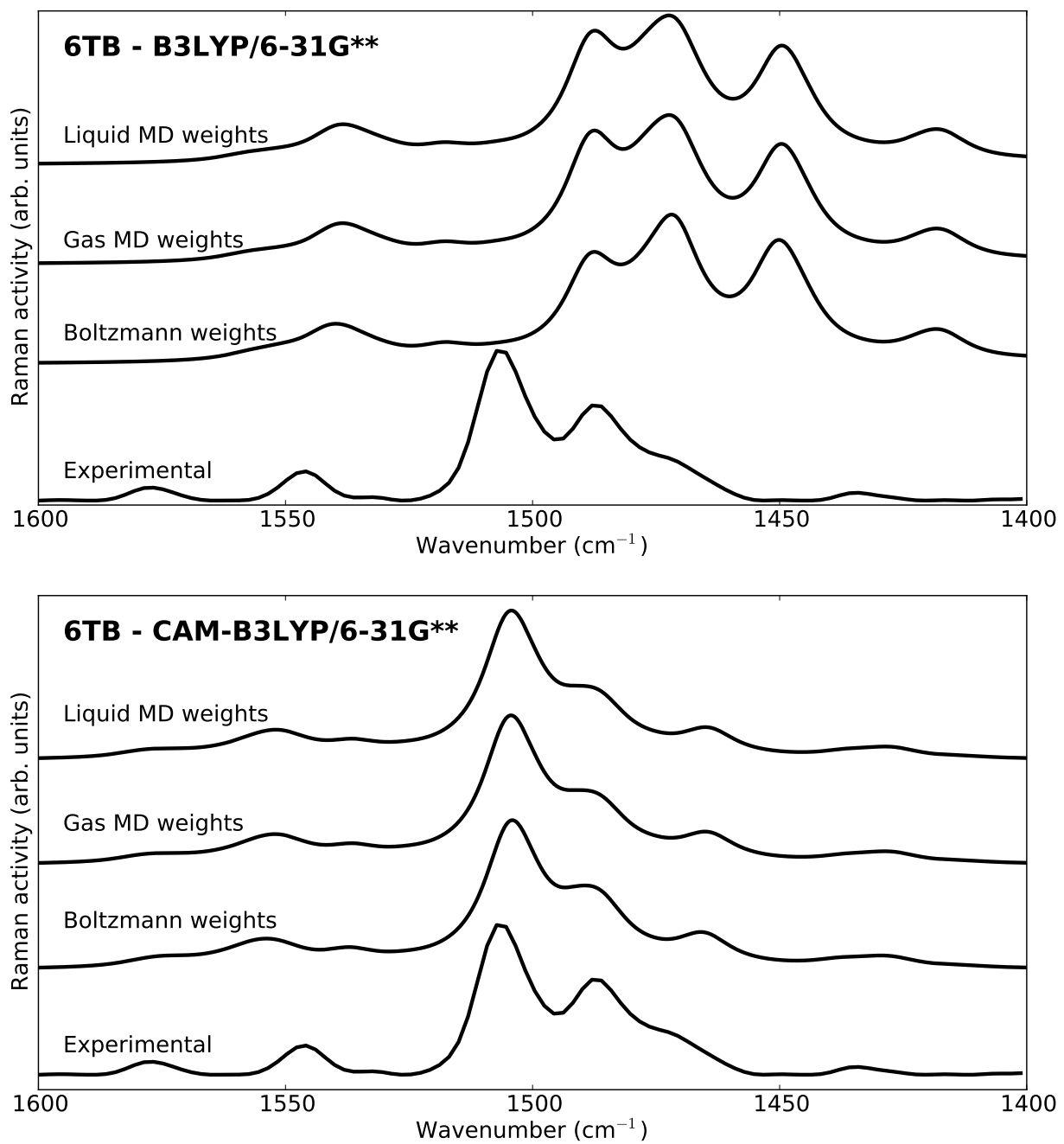


FIG. 10. Theoretical room temperature Raman spectra for 6TB compared to experimentally measured spectra.