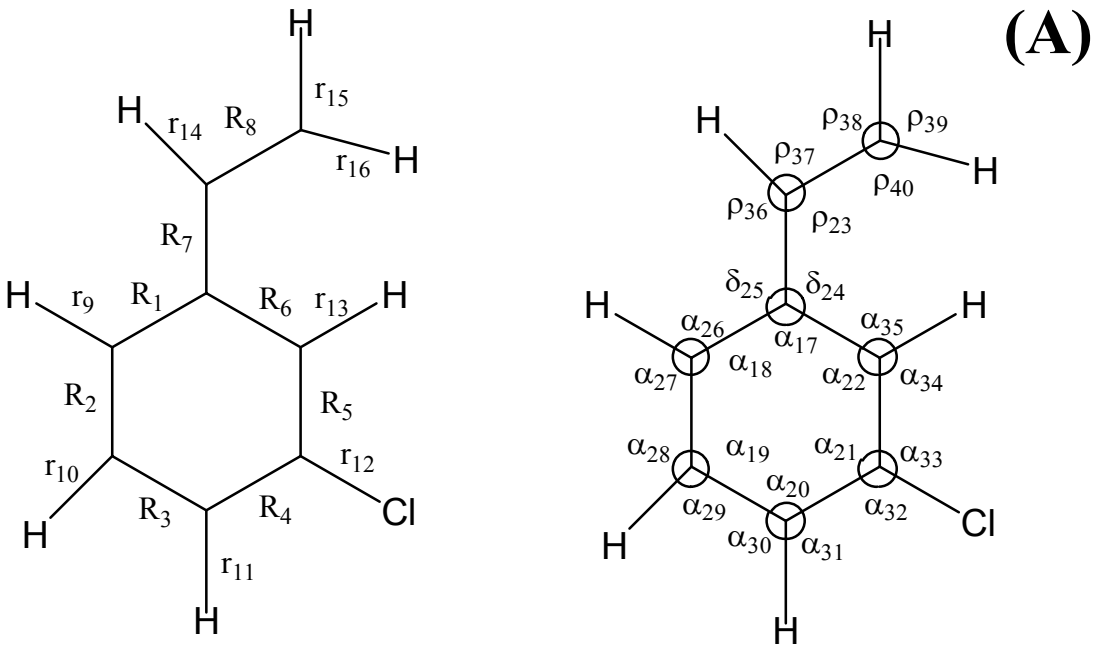
CAPTIONS FOR FIGURES (Supplementary material):

FIG. 1S: Internal coordinates defined for the scaling procedure. (A) in plane coordinates, (B) out of plane coordinates.
FIG. 2S: Observed and calculated IR spectra at the B3PW91 and B3LYP levels with different basis sets. Solid line for the *cis* conformer and dotted line for the *trans* one.
FIG. 3S: Observed (solid line), and calculated (dotted line) INS spectra for the *cis* conformer with different methods and the 6-31G* basis set.
FIG. 4S: Observed (solid line), and calculated (dotted line) INS spectra for the *trans* conformer with different methods and the 6-31G* basis set.
FIG. 5S: Observed (solid line), and calculated (dotted line) INS spectra for the *cis* conformer at the B3PW91 level with different basis sets.
FIG. 6S: Observed (solid line), and calculated (dotted line) INS spectra for the *trans* conformer at the B3PW91 level with different basis sets.
FIG. 7S: Observed (solid line), and calculated (dotted line) INS spectra for the *cis* conformer at the B3LYP level with different basis sets.
FIG. 8S: Observed (solid line), and calculated (dotted line) INS spectra for the *trans* conformer at the B3LYP level with different basis sets.

Figure1S


(A)
H
r15
H
r14
R8
r16
H
R7
H
r9
R1
R6
r13
H
R2
R5
r10
r12
H
R3
R4
Cl
r11
H
H
ρ38
ρ39
H
ρ37
H
ρ40
ρ36
ρ23
δ25
δ24
H
α26
α35
H
α17
α18
α27
α22
α34
α28
α19
α21
α33
α20
α29
α32
Cl
H
α30
α31
H

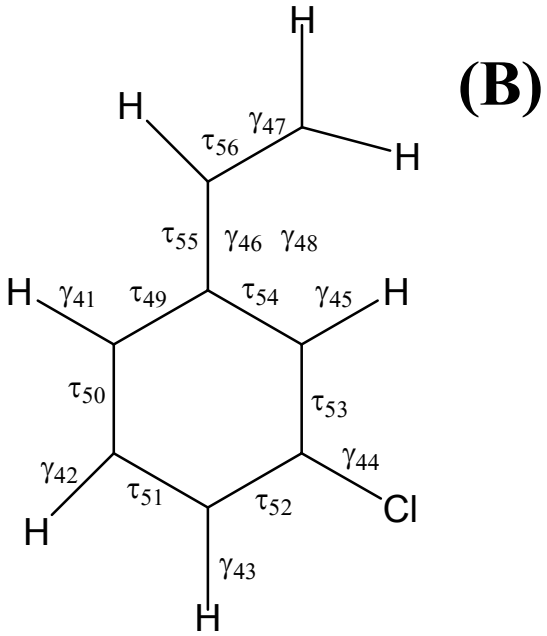

(B)
H
H
γ47
τ56
H
τ55
γ46
γ48
H
γ41
τ49
τ54
γ45
H
τ50
τ53
γ44
γ42
τ51
τ52
Cl
H
γ43
H

Figure2S

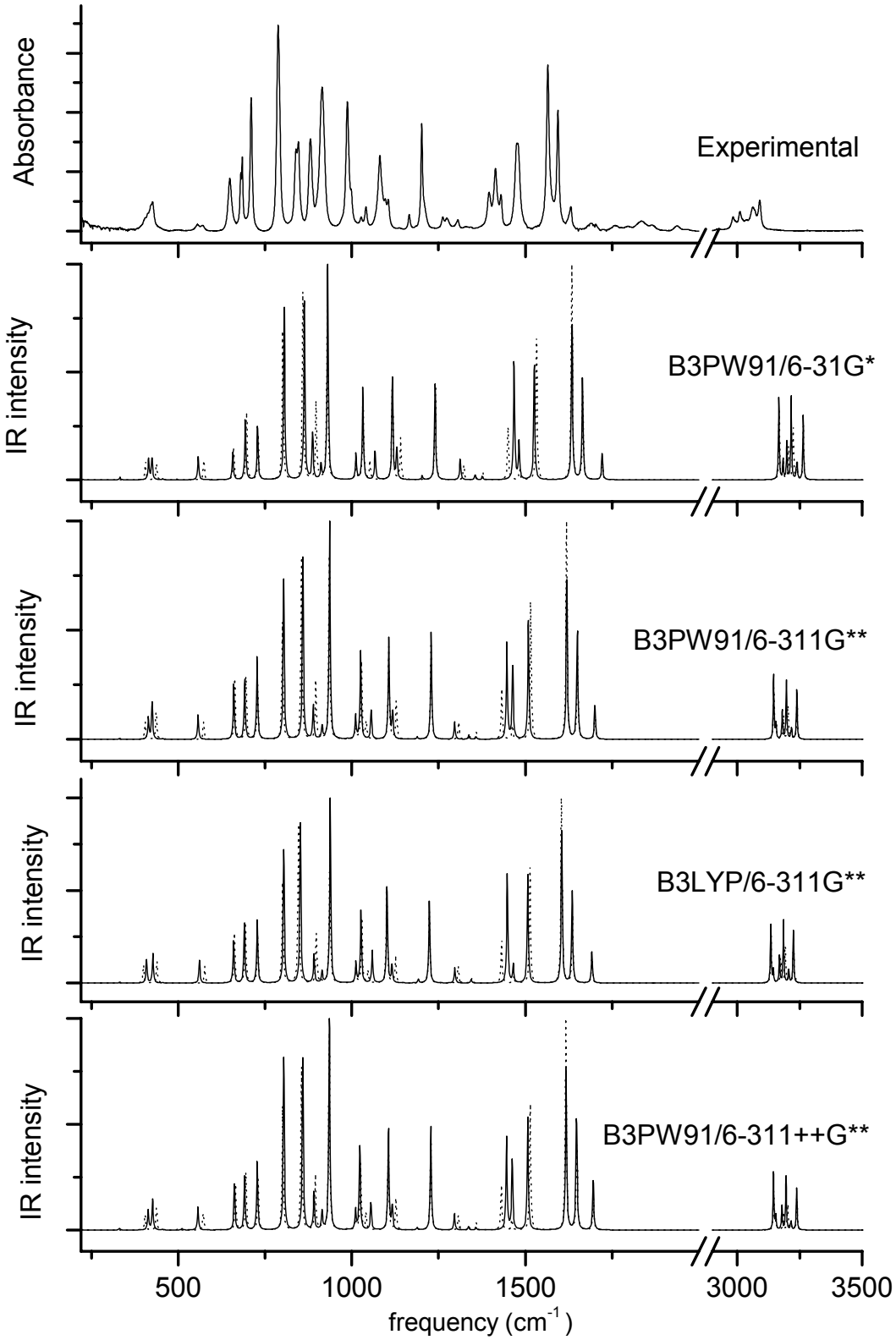

Absorbance
Experimental
IR intensity
B3PW91/6-31G*
IR intensity
B3PW91/6-311G**
IR intensity
B3LYP/6-311G**
IR intensity
B3PW91/6-311++G**
500
1000
1500
3000
3500
frequency (cm-1)

Figure3S

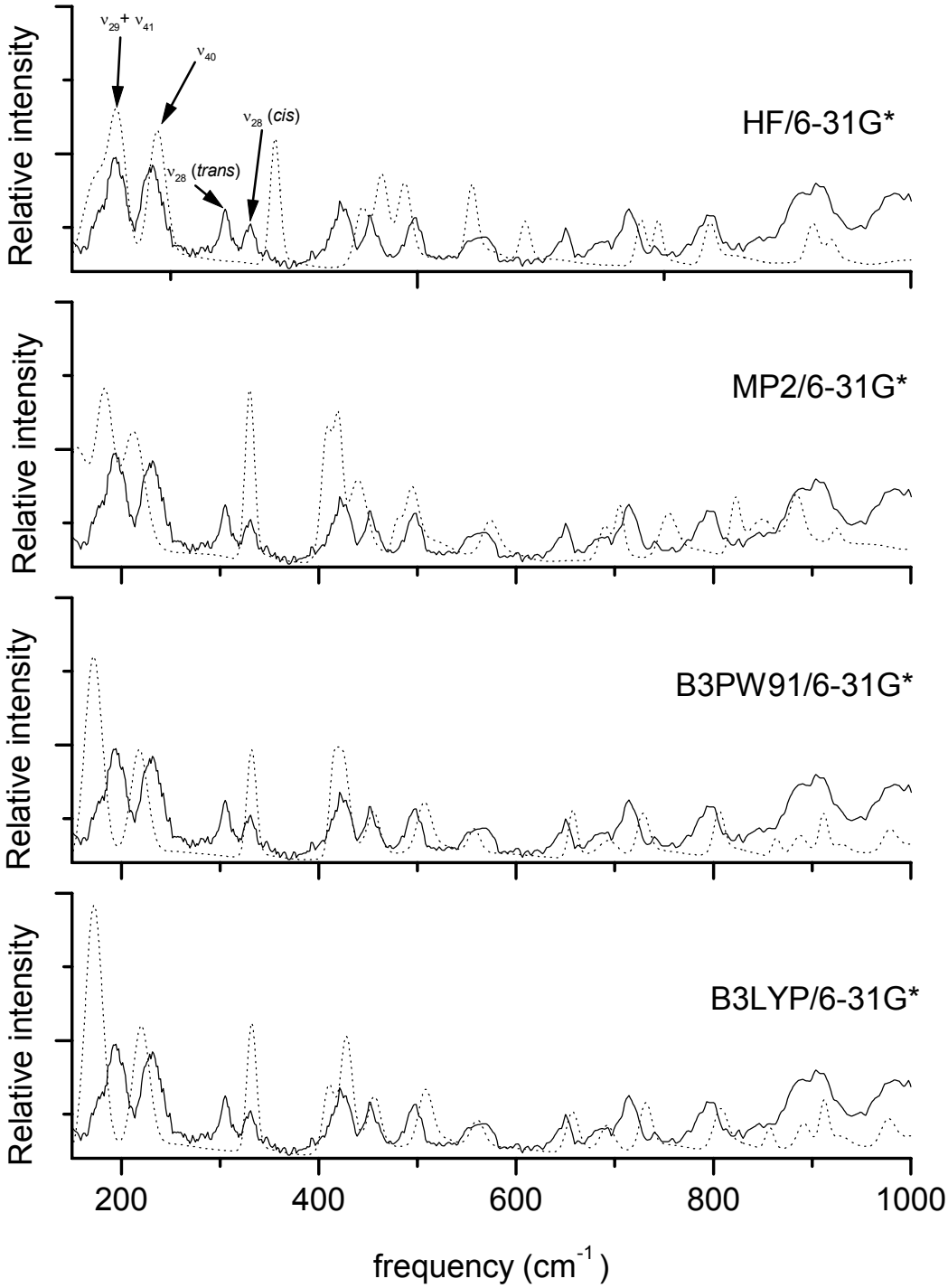

ν29+ ν41
ν40
ν28 (cis)
ν28 (trans)
HF/6-31G*
MP2/6-31G*
B3PW91/6-31G*
B3LYP/6-31G*
Relative intensity
200
400
600
800
1000
frequency (cm-1)

Figure4S

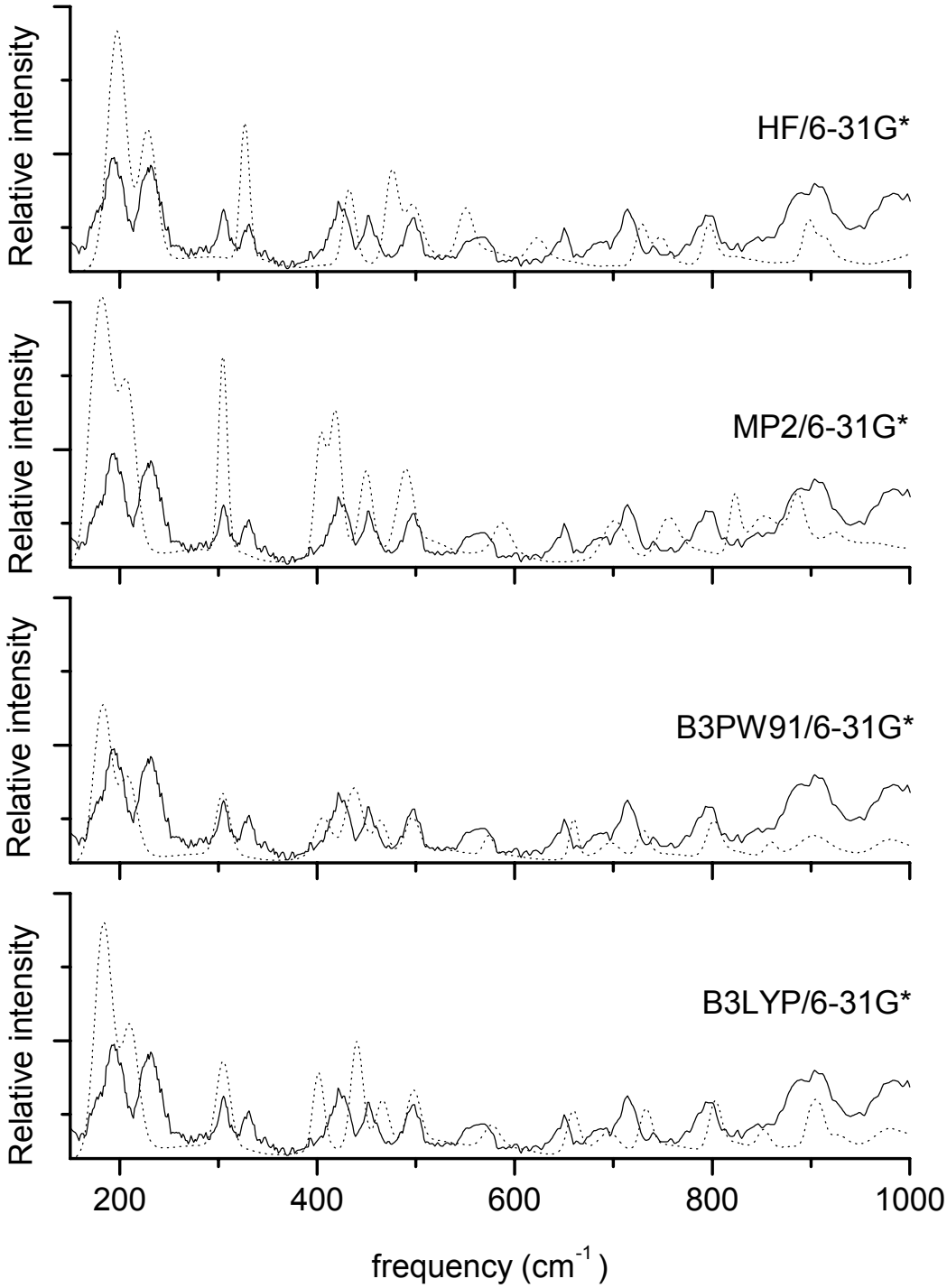

Relative intensity
HF/6-31G*
Relative intensity
MP2/6-31G*
Relative intensity
B3PW91/6-31G*
Relative intensity
B3LYP/6-31G*
200
400
600
800
1000
frequency (cm-1)

Figure5S

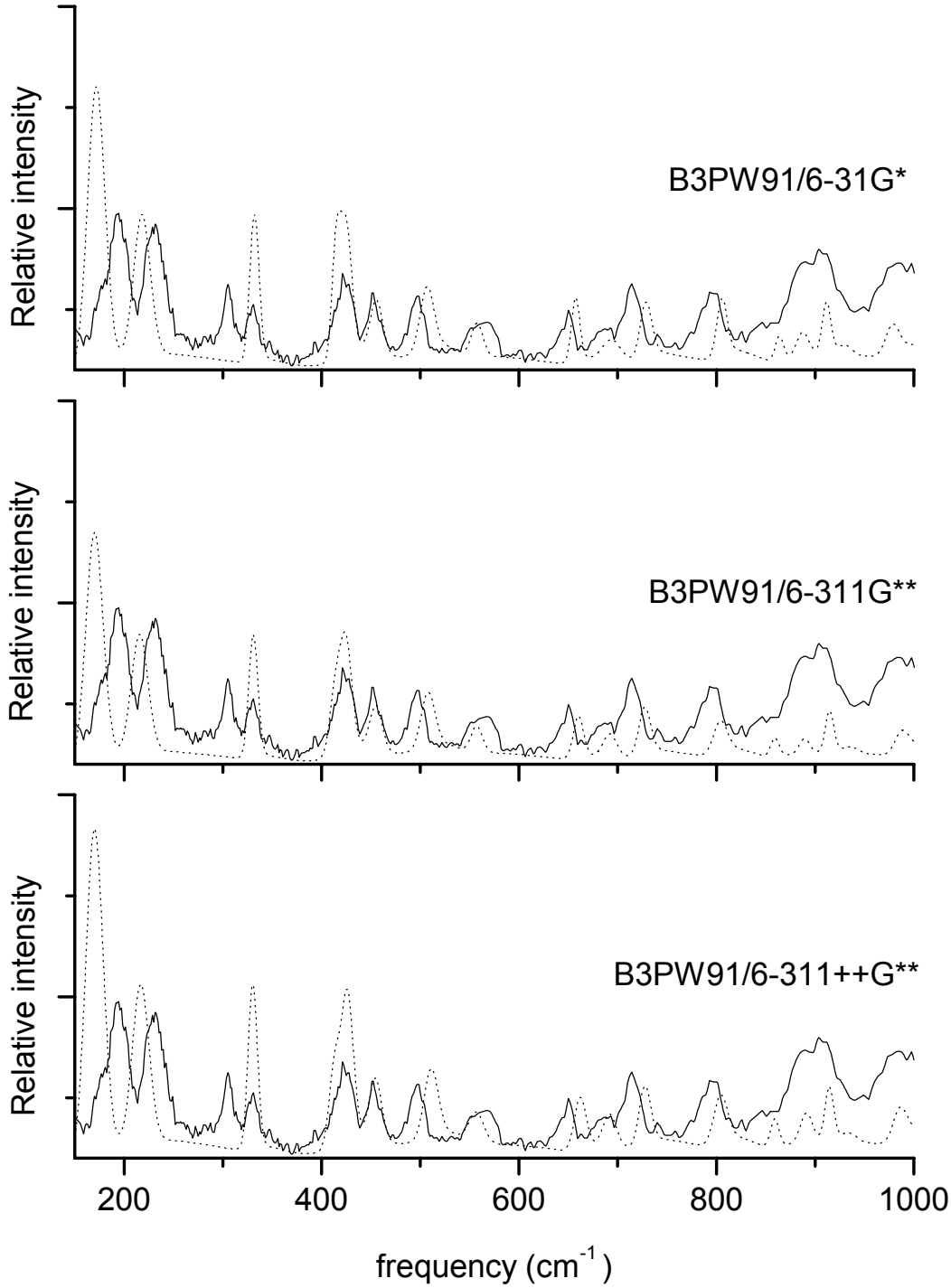

Relative intensity
B3PW91/6-31G*
Relative intensity
B3PW91/6-311G**
Relative intensity
B3PW91/6-311++G**
200
400
600
800
1000
frequency (cm-1)

Figure6S

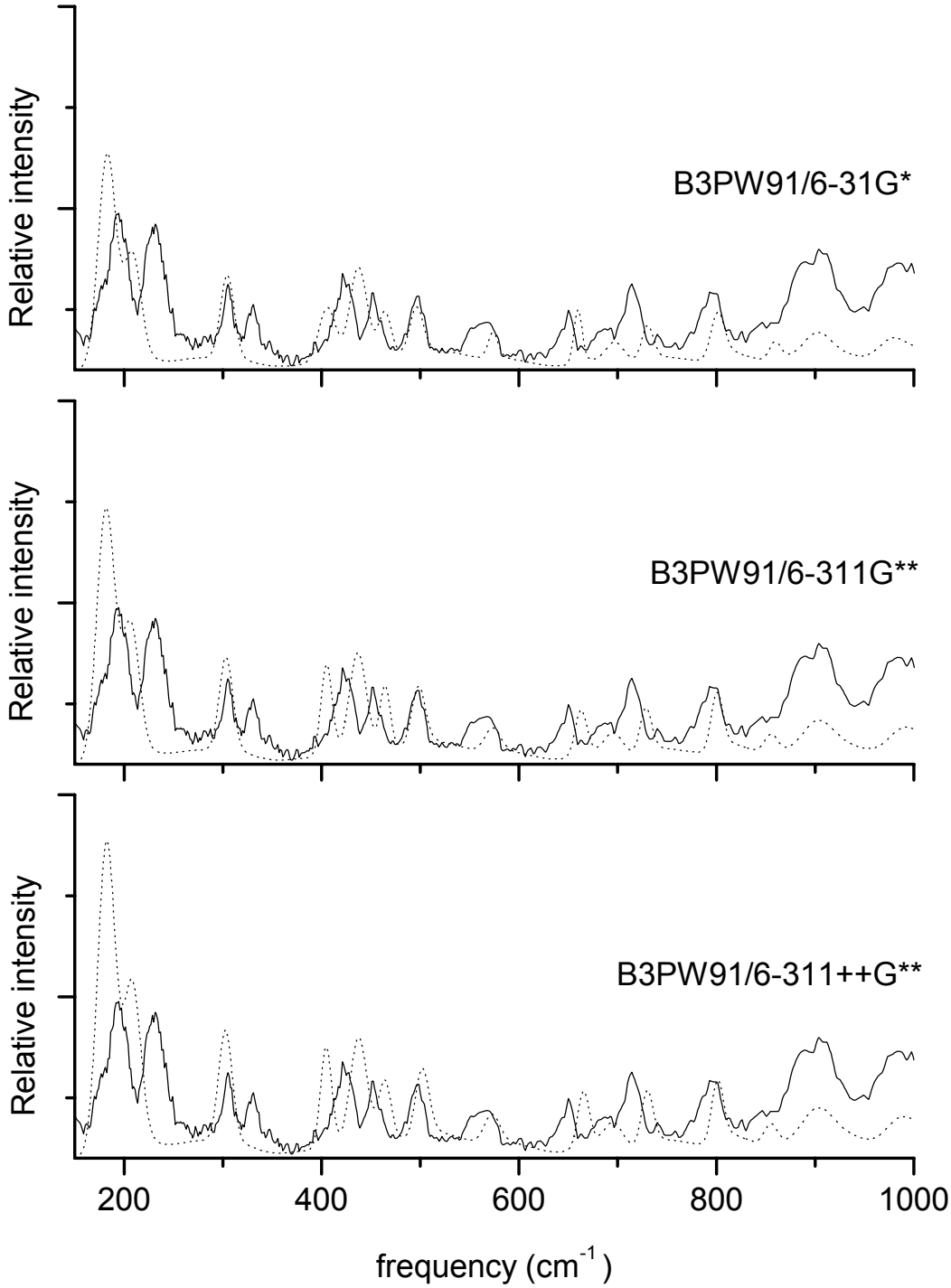

Relative intensity
B3PW91/6-31G*
Relative intensity
B3PW91/6-311G**
Relative intensity
B3PW91/6-311++G**
200
400
600
800
1000
frequency (cm-1)

Figure7S

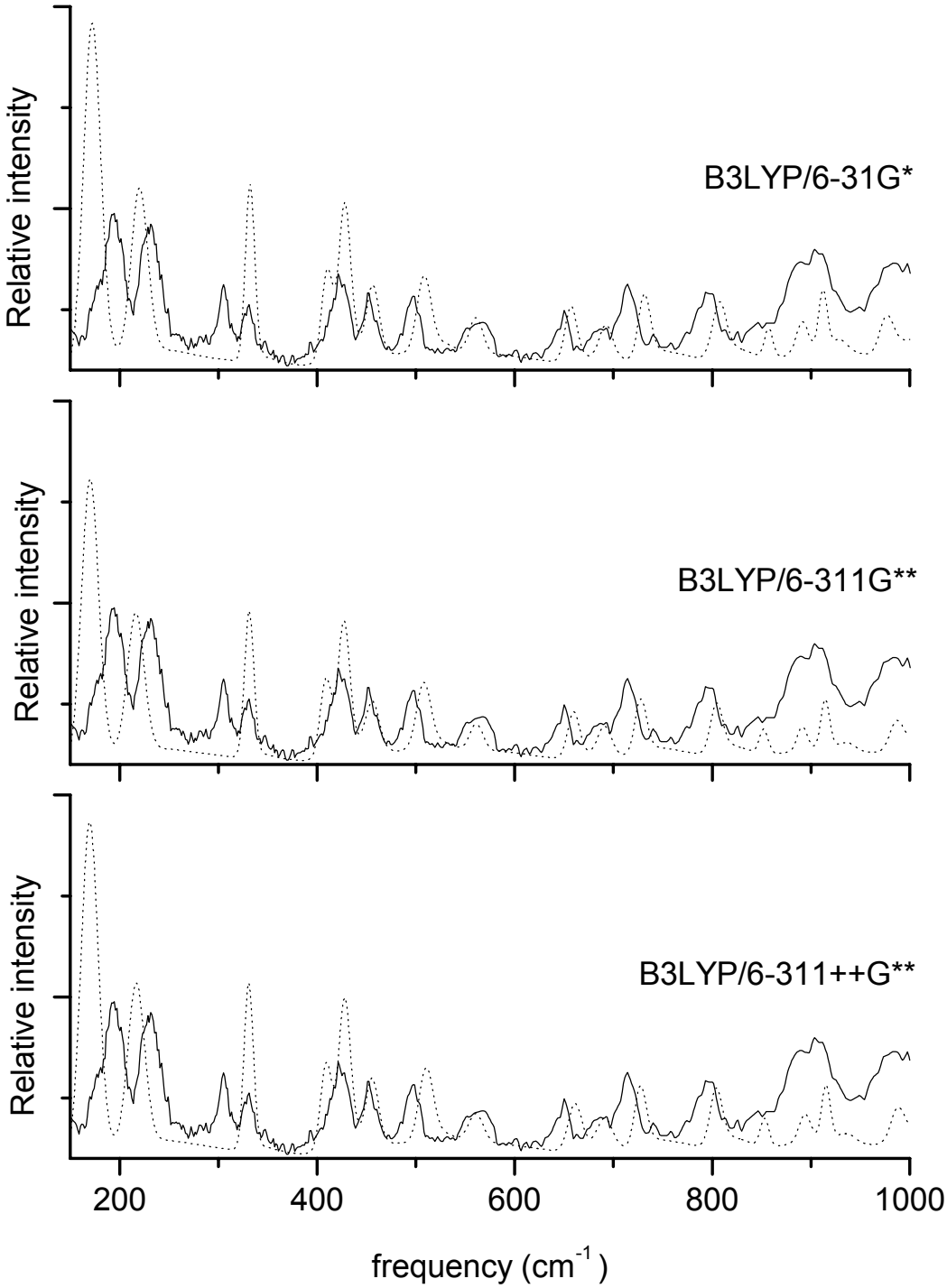
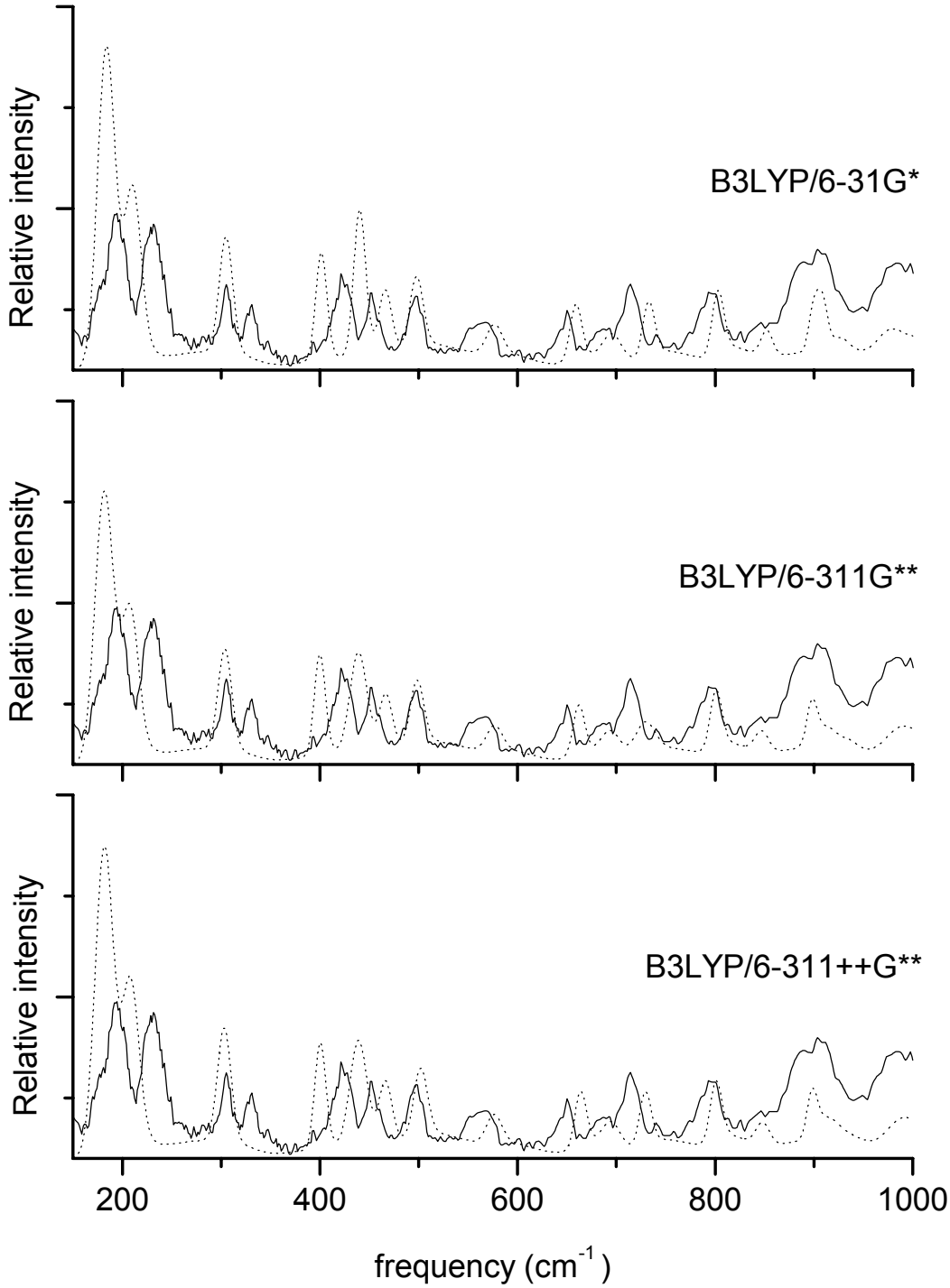

Relative intensity
B3LYP/6-31G*
Relative intensity
B3LYP/6-311G**
Relative intensity
B3LYP/6-311++G**
200
400
600
800
1000
frequency (cm-1)

Figure8S


Relative intensity
B3LYP/6-31G*
Relative intensity
B3LYP/6-311G**
Relative intensity
B3LYP/6-311++G**
200
400
600
800
1000
frequency (cm-1)