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Raman Spectroscopy vs. molecular modeling of polyene pigments

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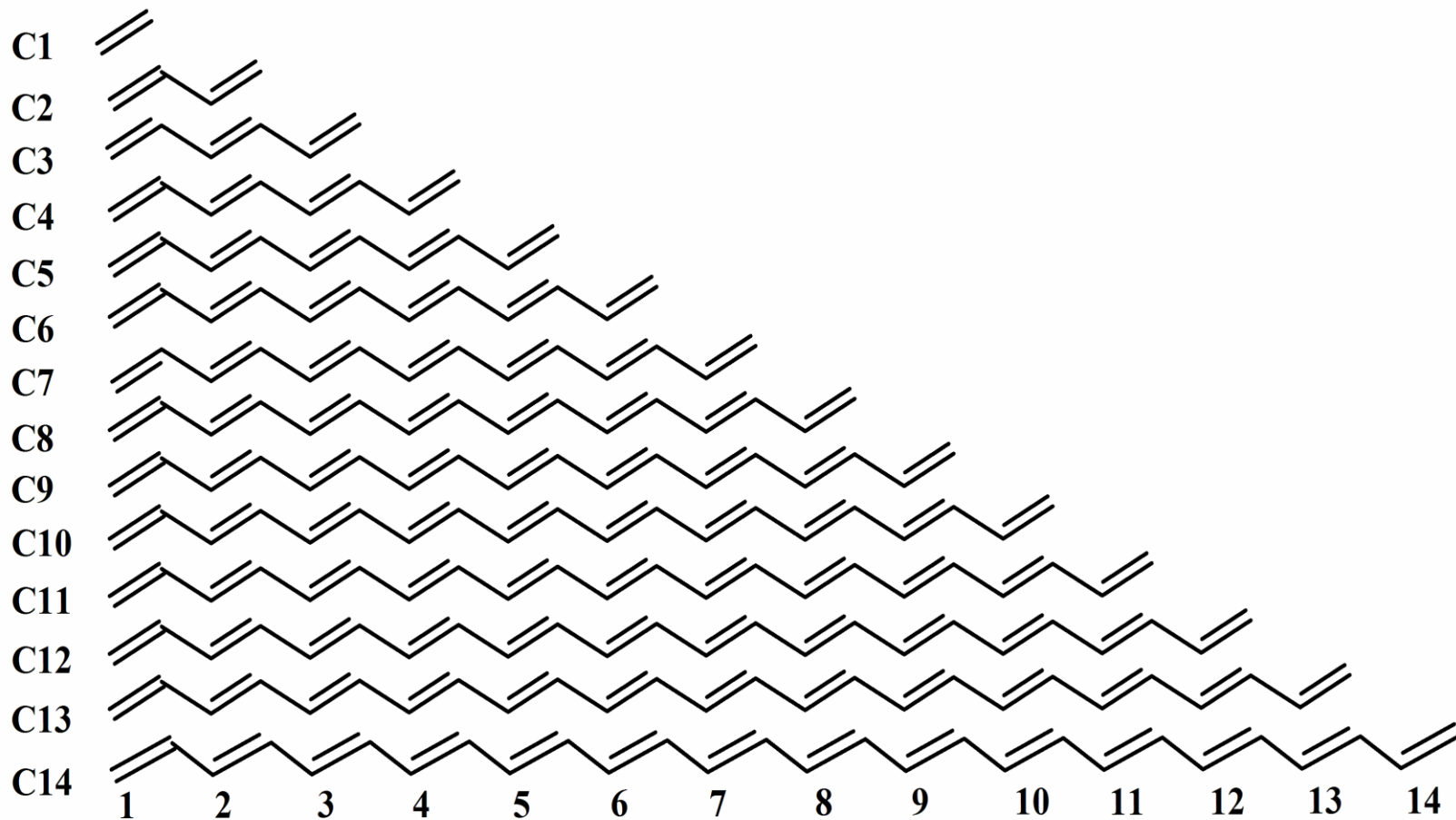
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Polyenes:



In analogy to the estimation of energy in the complete basis set limit (CBS), the structural and spectroscopic parameters $Y(n)$ changes upon increasing the chain length ($n=1,2,3,\dots \infty$, where n is the number of C=C units) were estimated toward infinity using an exponential-type three-parameter function [43,44]:

$$Y(n) = Y(\infty) + A \exp(-n/B) \tag{1}$$

In this formula A and B are fitting parameters and $Y(\infty)$ is the estimated value of C=C, C-C bond lengths or $\nu(\text{C}=\text{C})$ and $\nu(\text{C}-\text{C})$ frequencies for polyene systems containing “ $n = \infty$ ” C=C units.

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2
3 **Modeling red coral (*Corallium rubrum*) and African snail (*Helixia aspersa*) shell**
4 **pigments: Raman spectroscopy vs. DFT studies**
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8 Teobald Kupka,^{a*} Aneta Buczek,^a Małgorzata A. Broda,^a Roman Szostak,^b Hong-Ming Lin,^{c*}
9 Lu-Wei Fan,^d Roman Wrzalik^e and Leszek Stobiński^f
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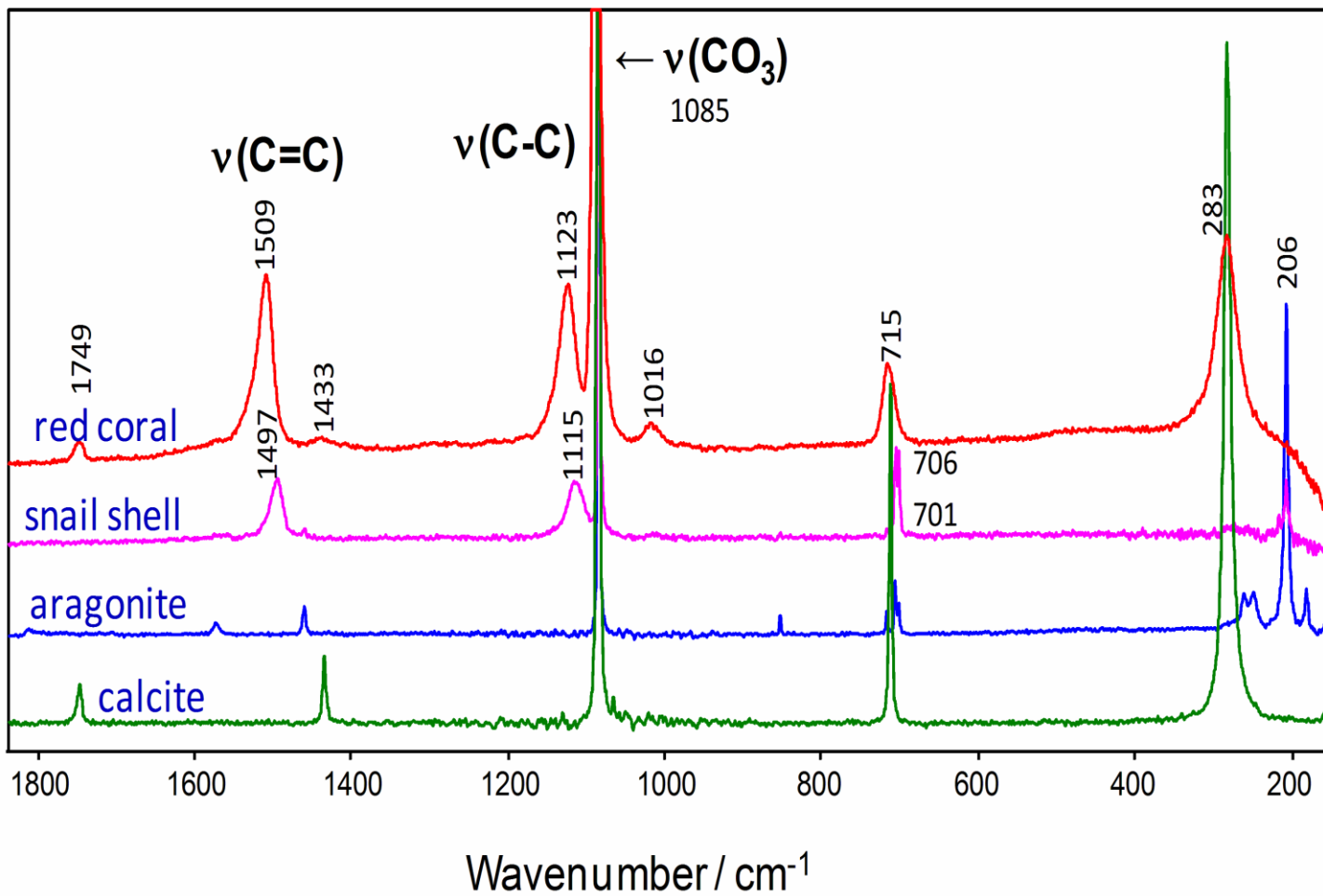
11
12 **Abstract**
13

14 Pigments from red coral (*Corallium rubrum*) and African snail (*Helixia aspersa*) shell were
15 studied non-invasively using Raman spectroscopy with 1064 nm laser beam. The two
16 observed bands due to organic pigments confined in biomineralized CaCO₃ matrix at about
17
18 observed bands due to organic pigments confined in biomineralized CaCO₃ matrix at about
19 1500 and 1100 cm⁻¹ were assigned to $\nu(\text{C}=\text{C})$ and $\nu(\text{C}-\text{C})$, respectively. Both signals originate
20
21

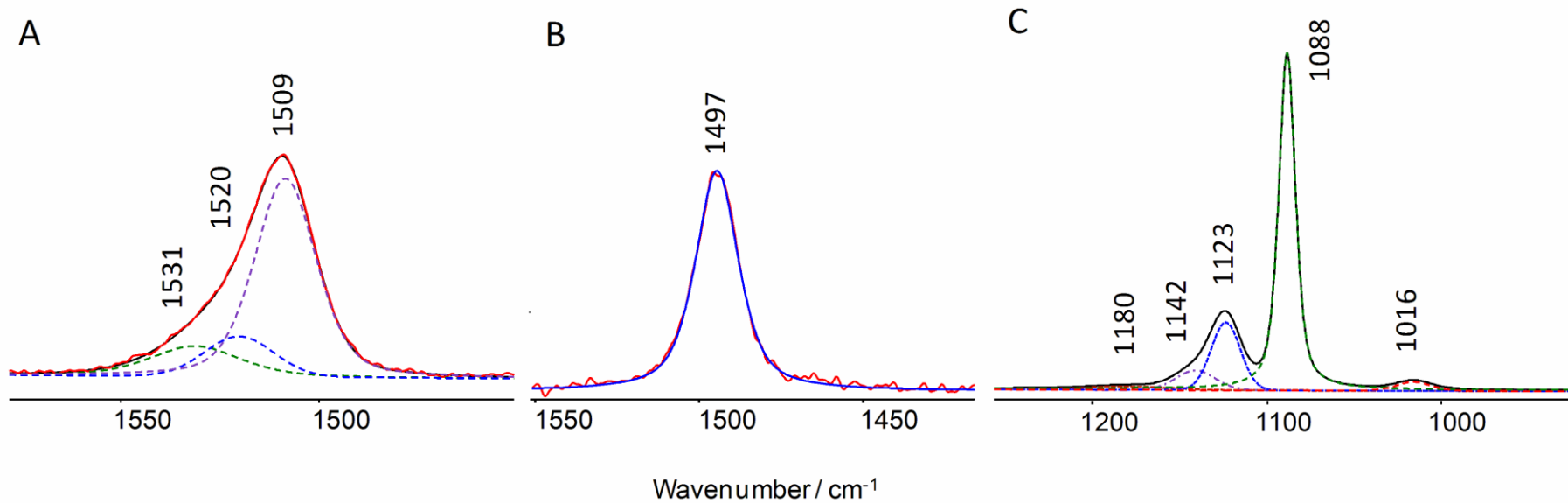
Samples of coral and snail shells



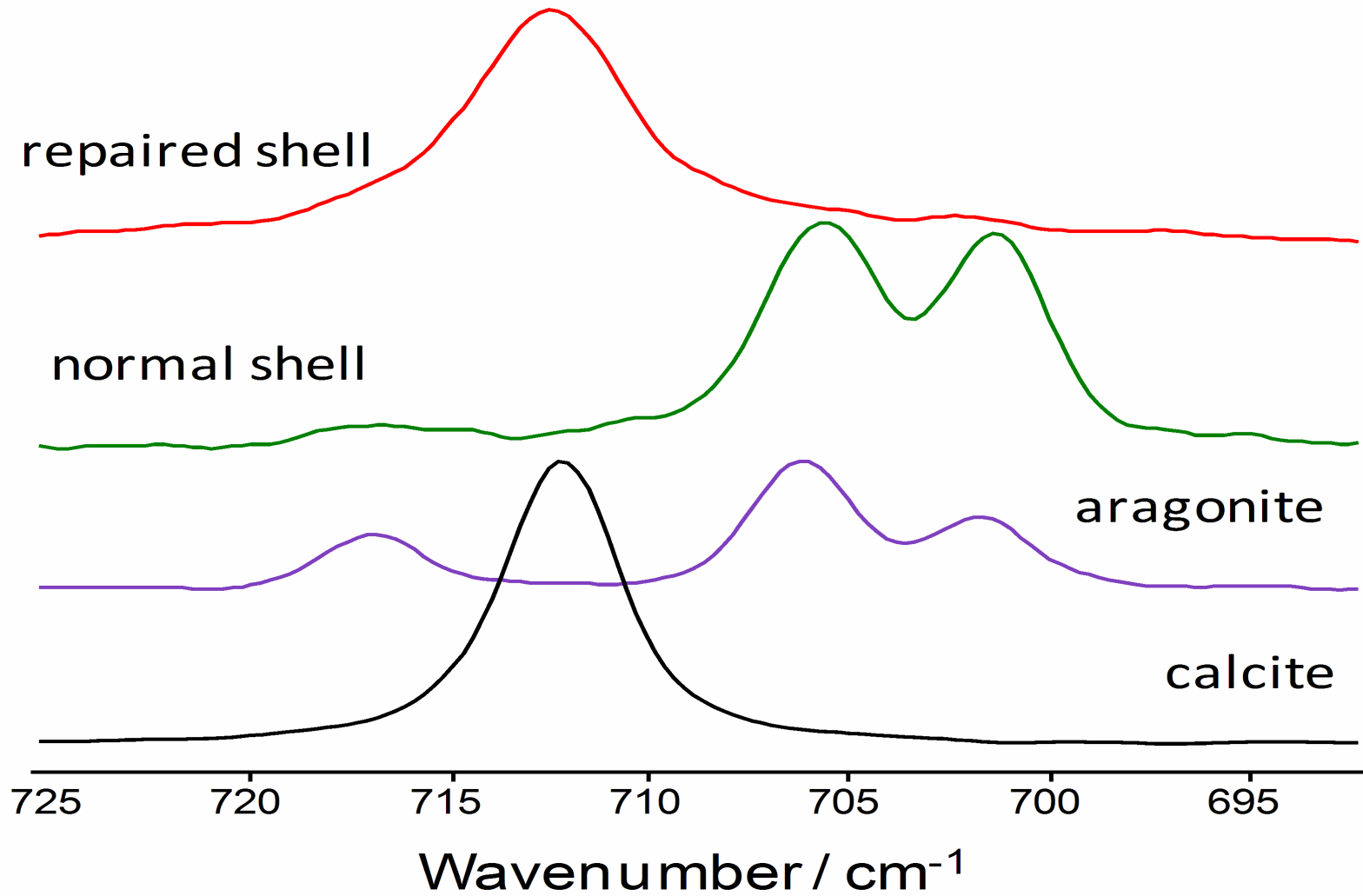
Raman spectra



Raman spectra

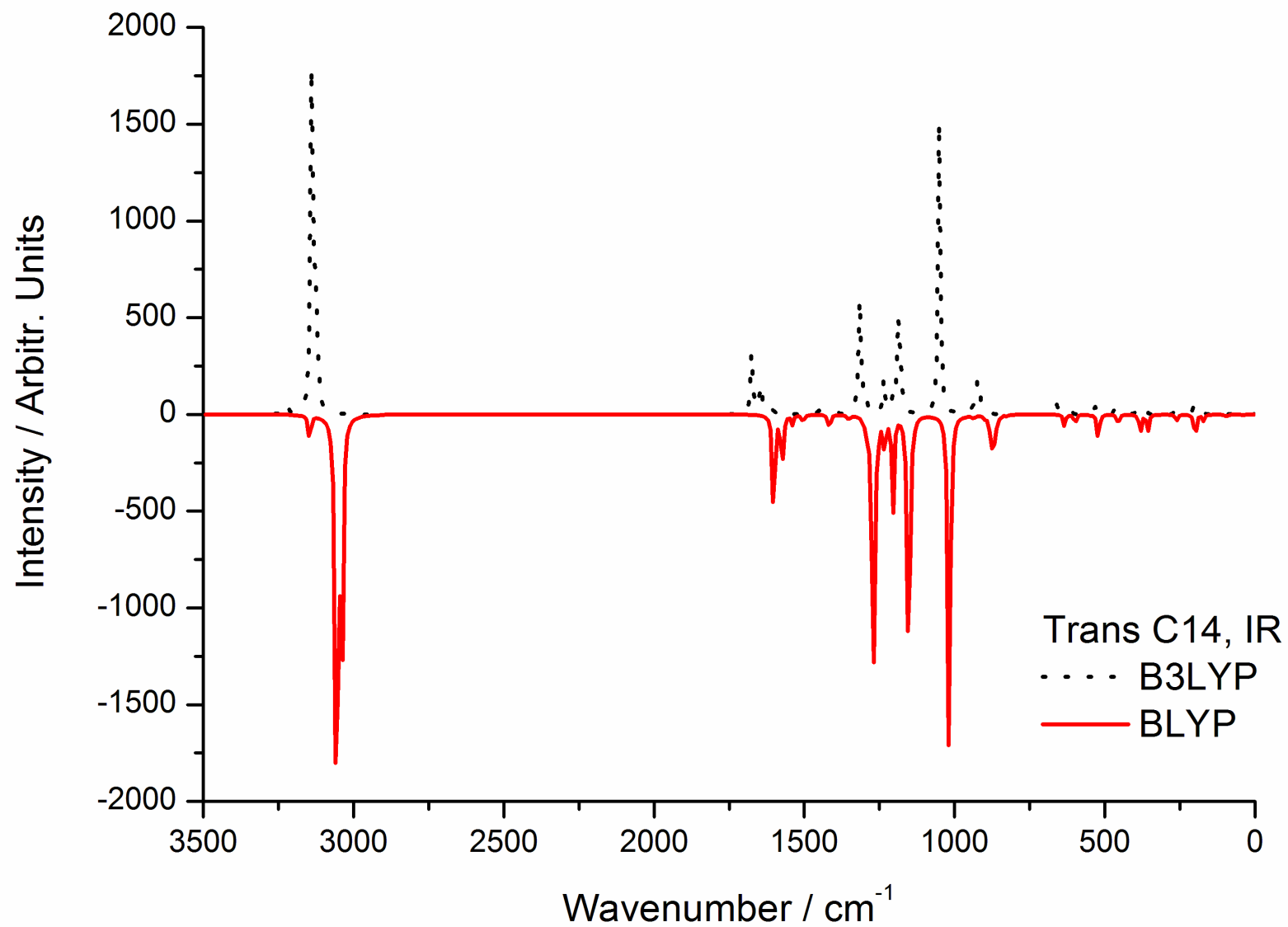


Raman spectra



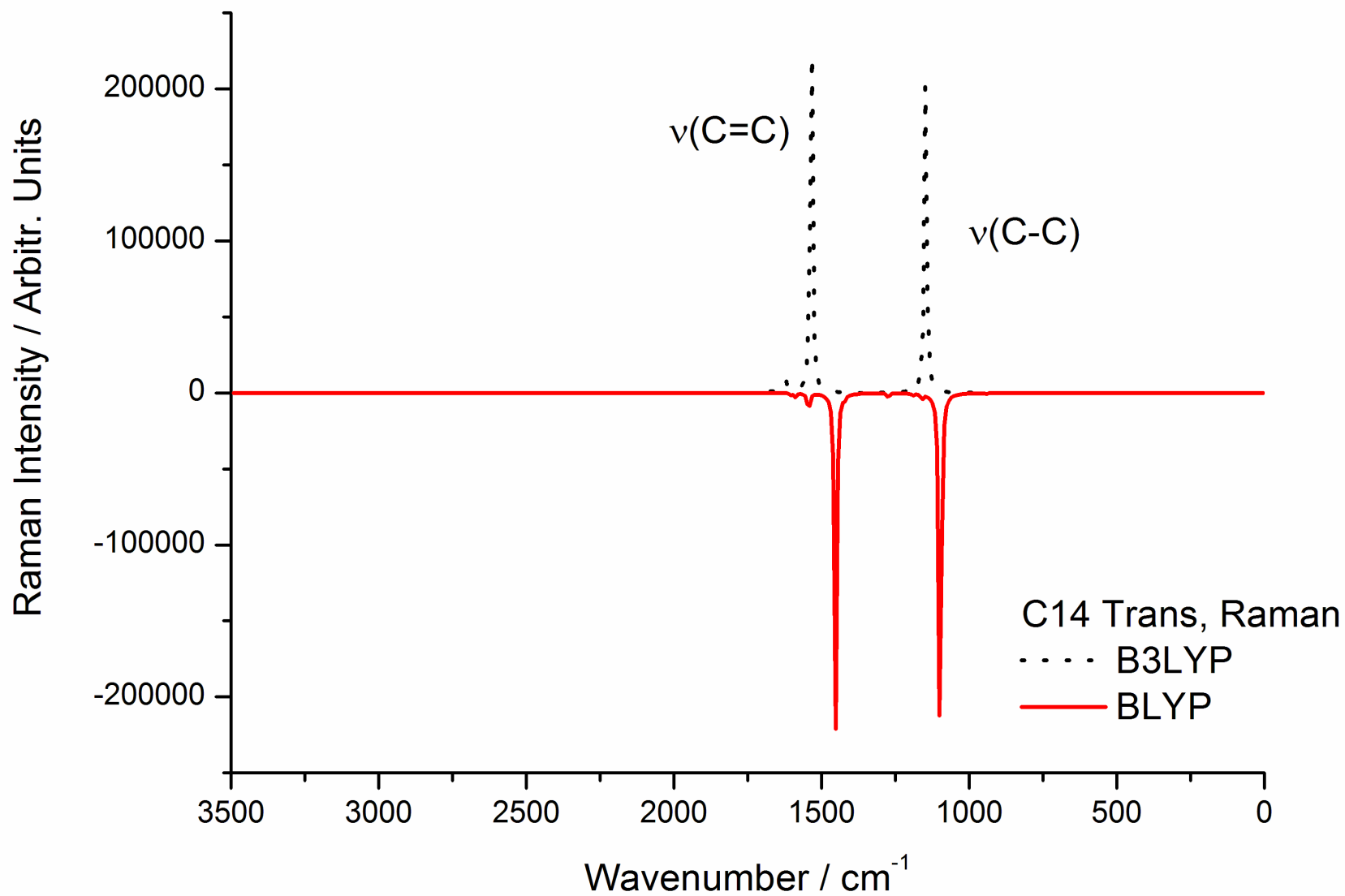
A

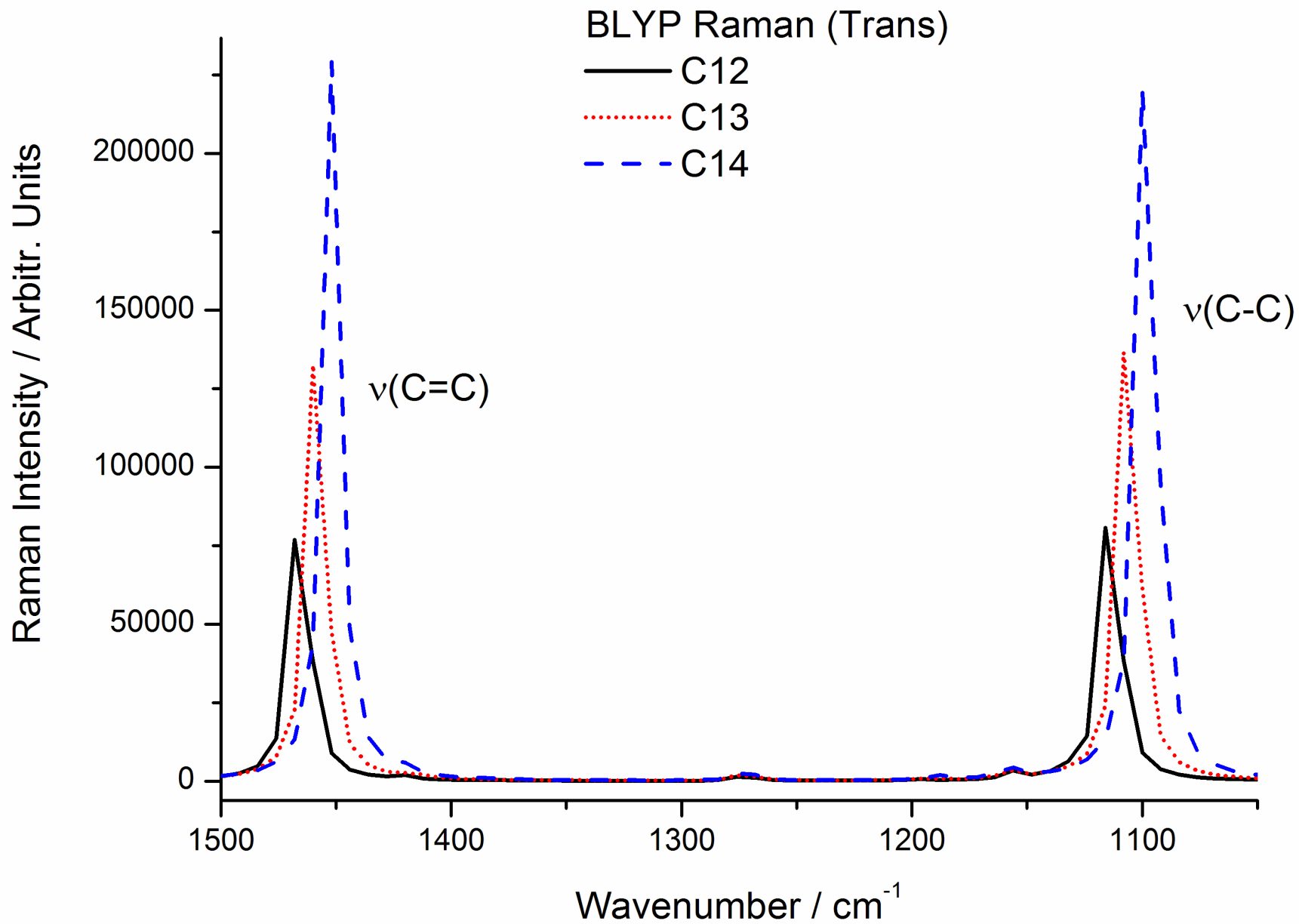
Theoretical IR spectra



B

Theoretical Raman spectra





Predicting the structure and vibrational frequencies of ethylene using harmonic and anharmonic approaches at the Kohn–Sham complete basis set limit

Aneta Buczek¹ · Teobald Kupka¹ · Malgorzata A. Broda¹ · Adriana Żyła^{1,2,3}

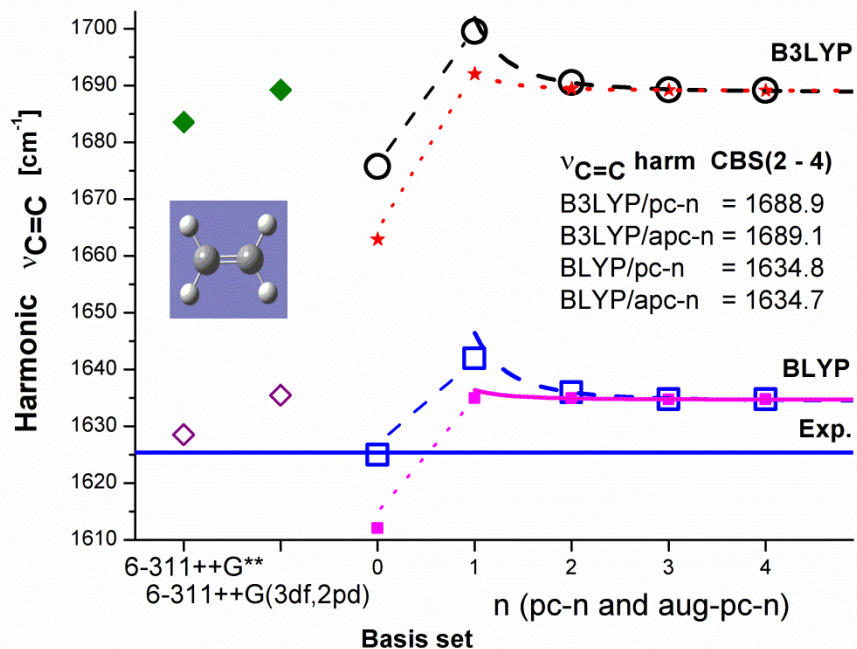


Fig. 1A

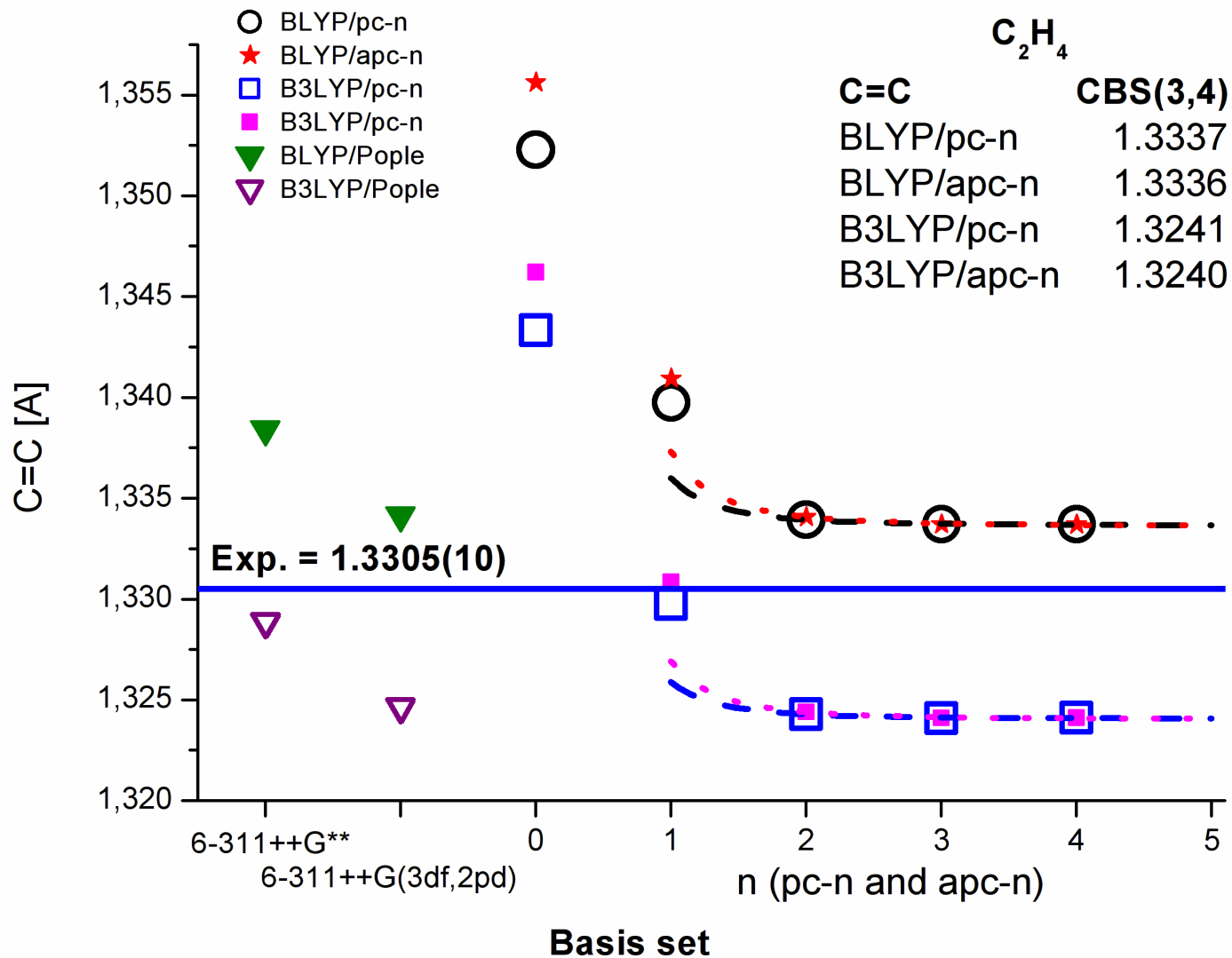


Fig. 1B

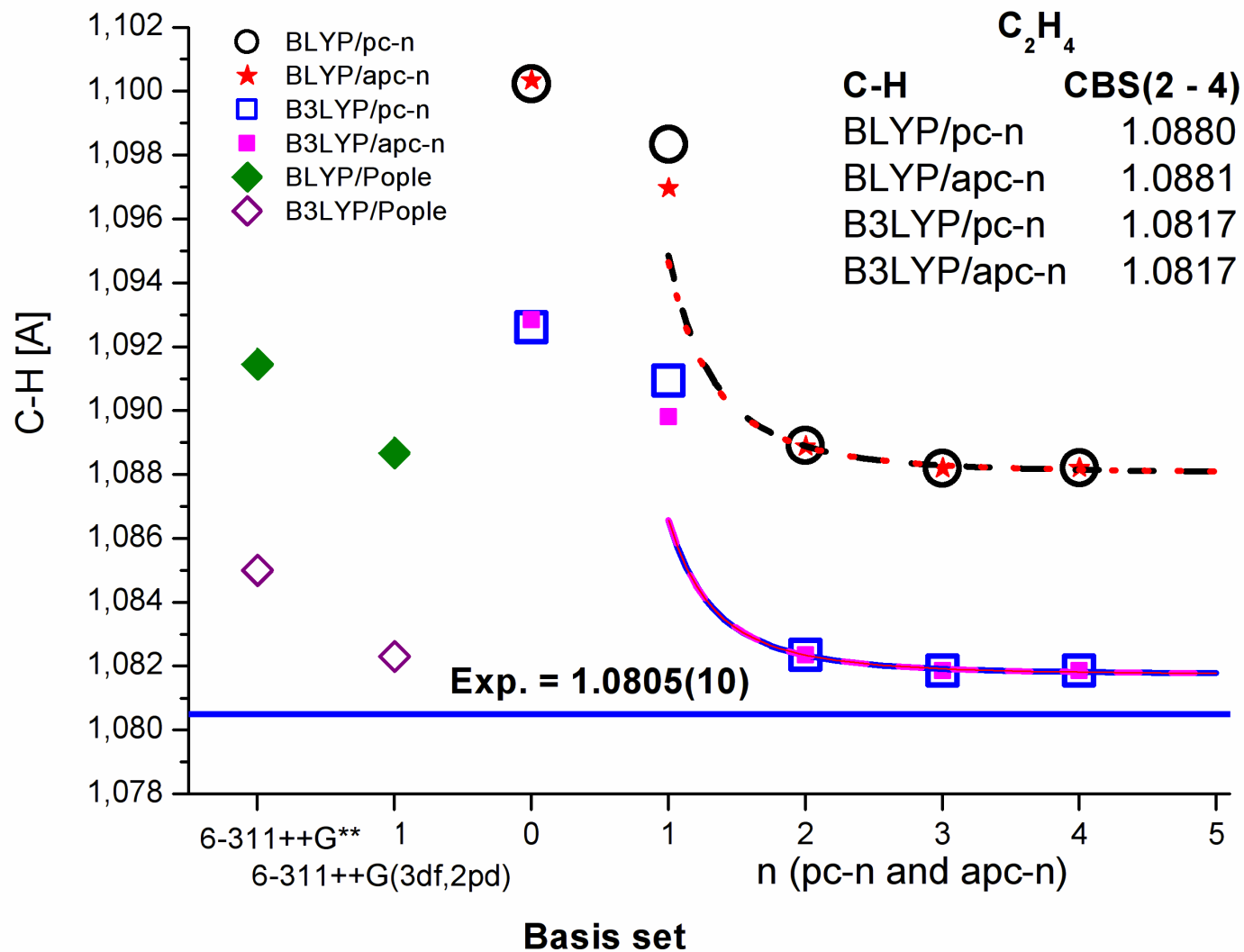


Fig. 1C

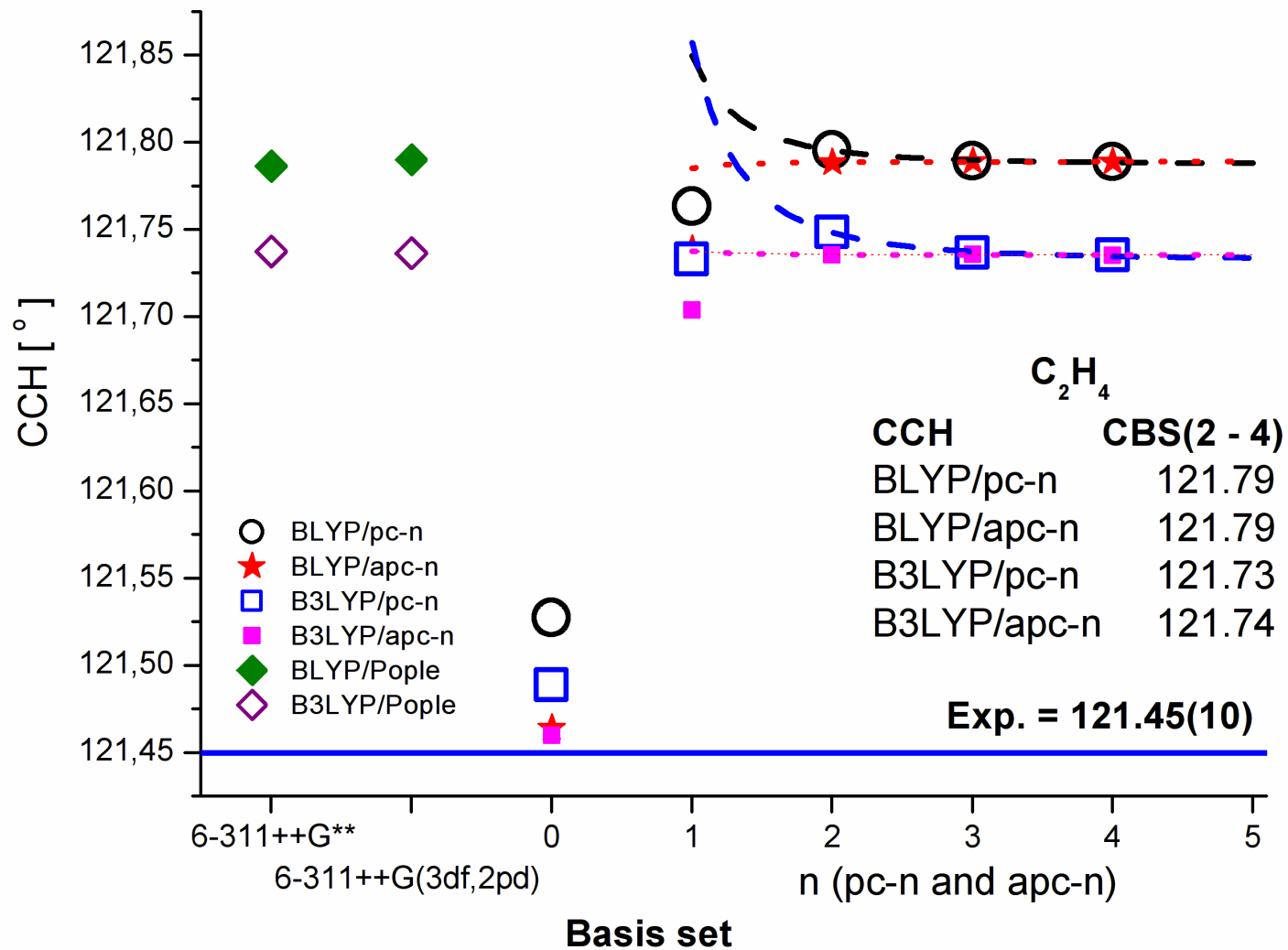


Fig. 2A

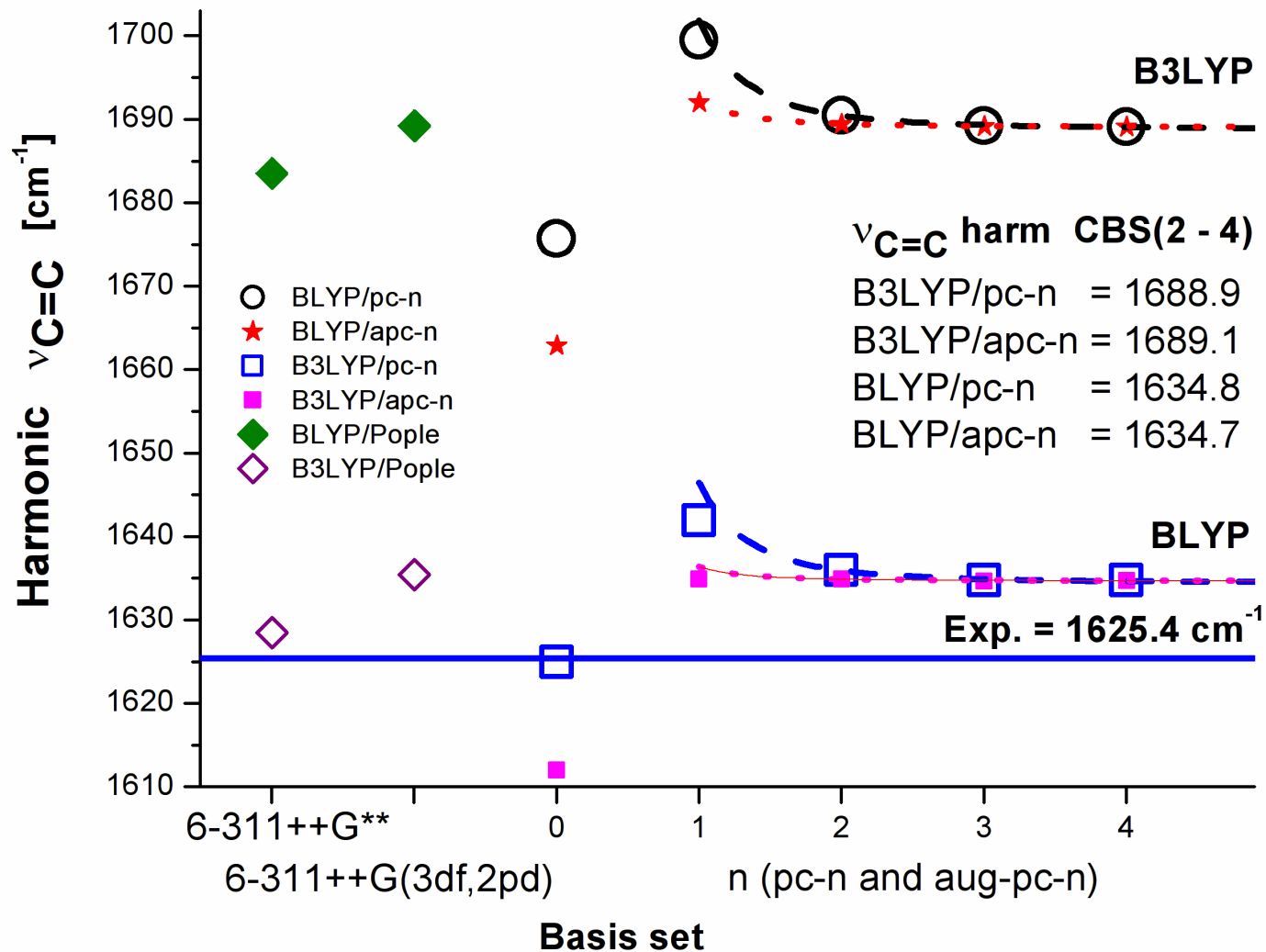


Fig. 2B

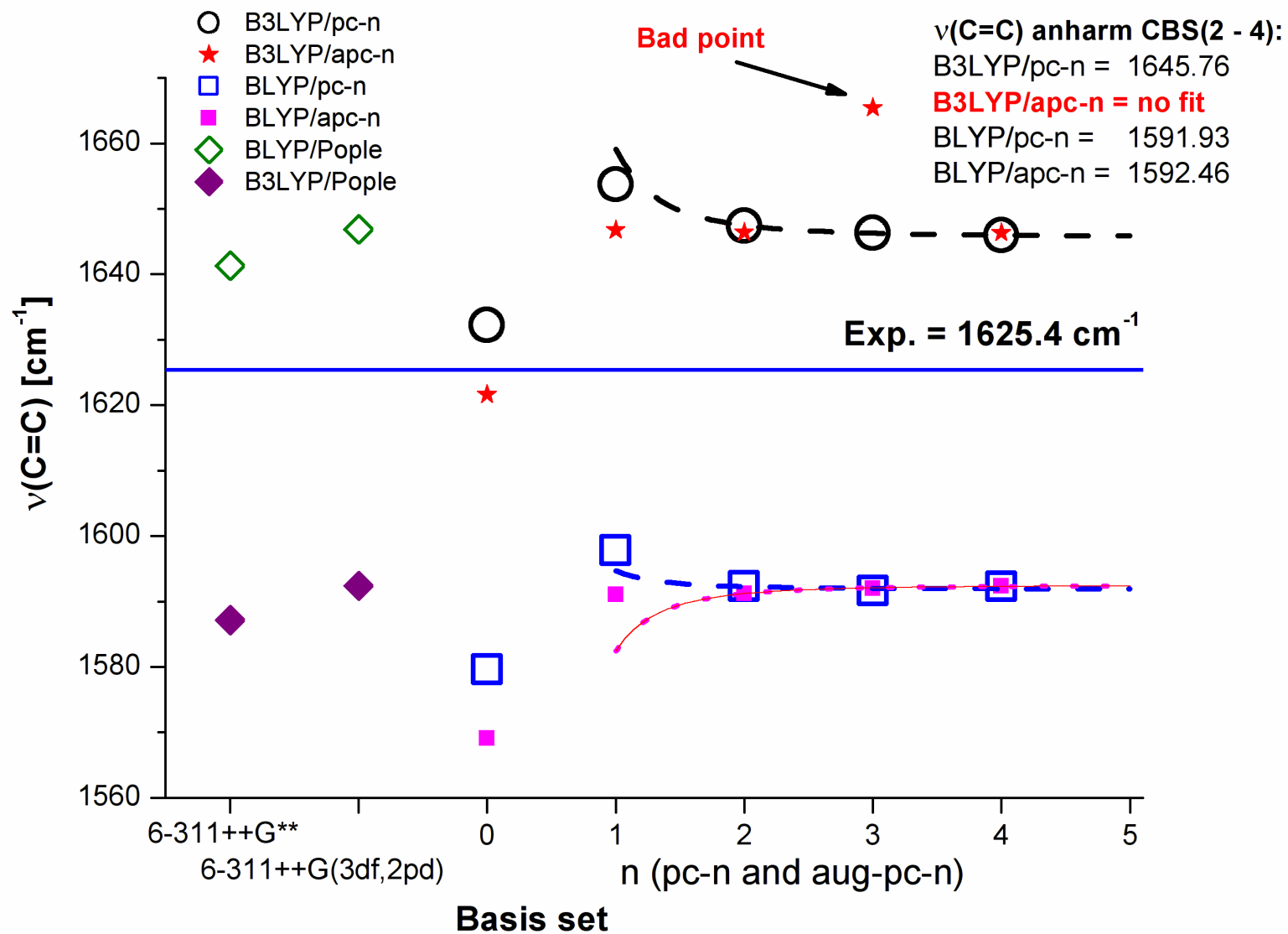
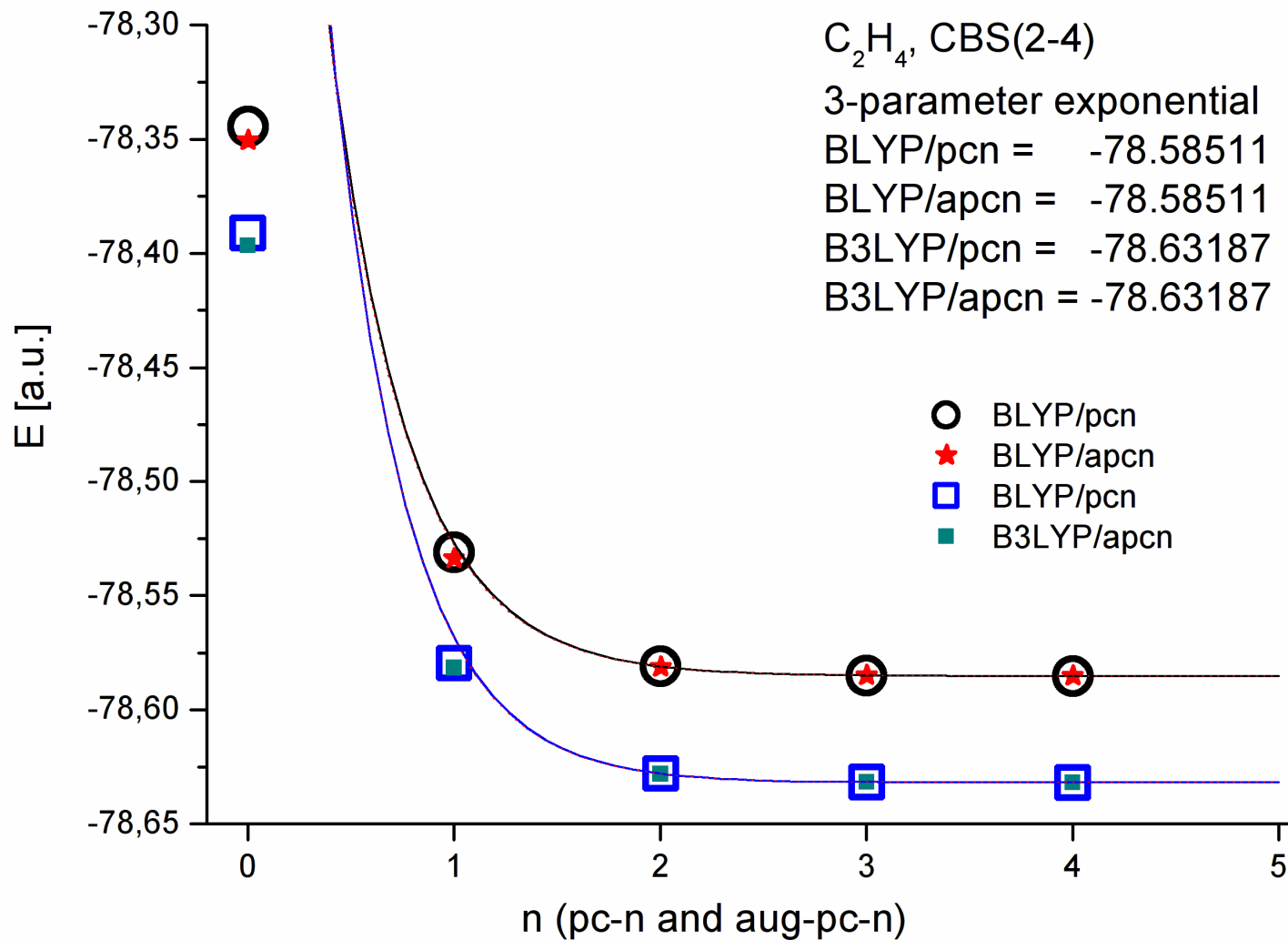


Fig. 3A

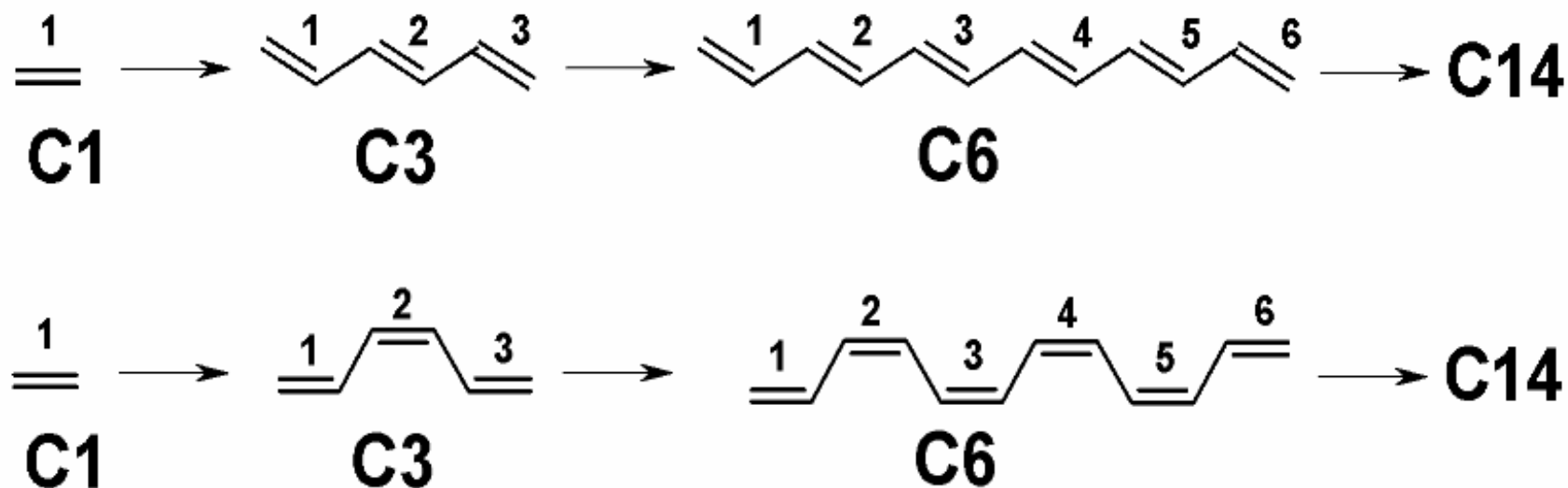


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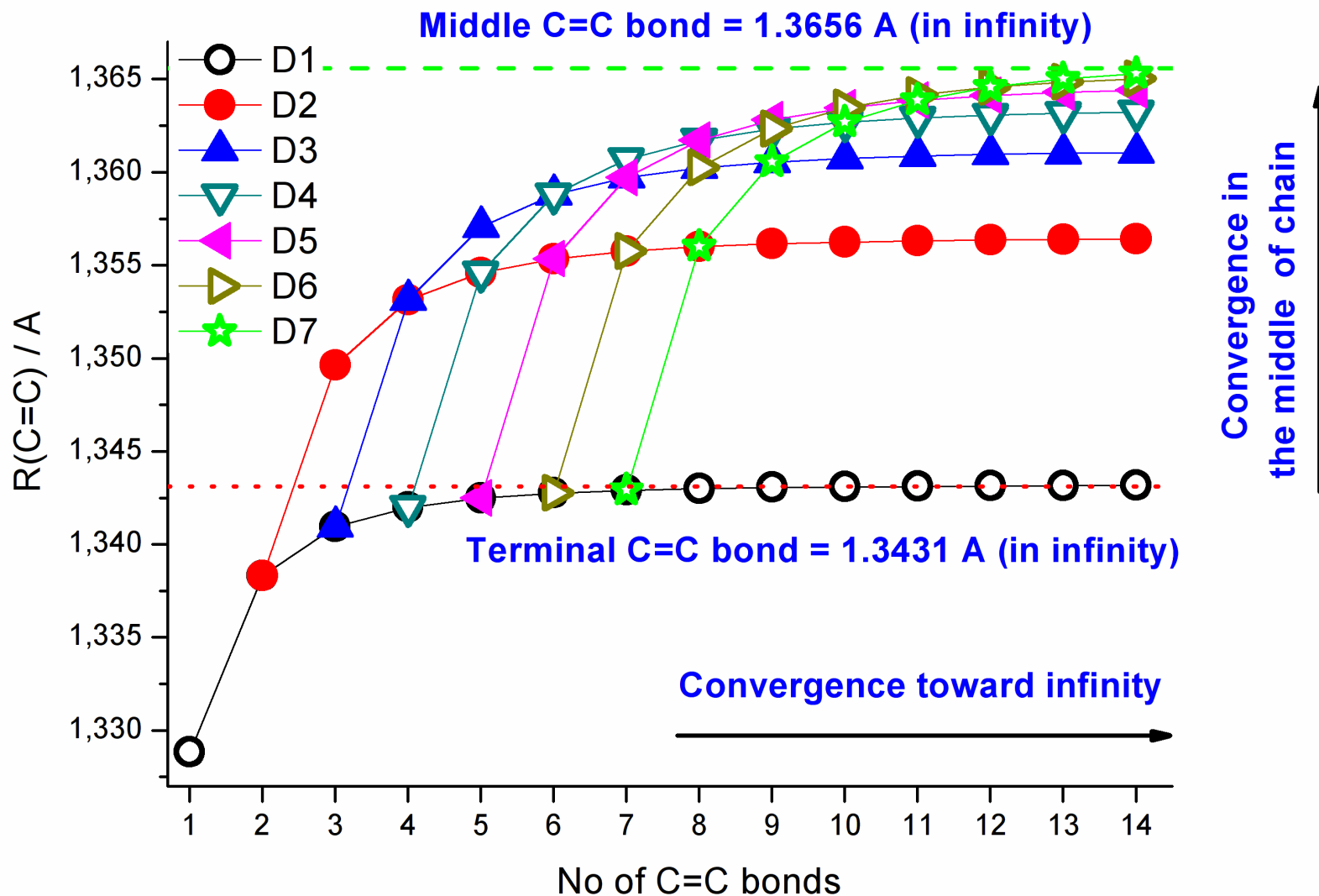
DFT studies on structural and vibrational properties of polyenes

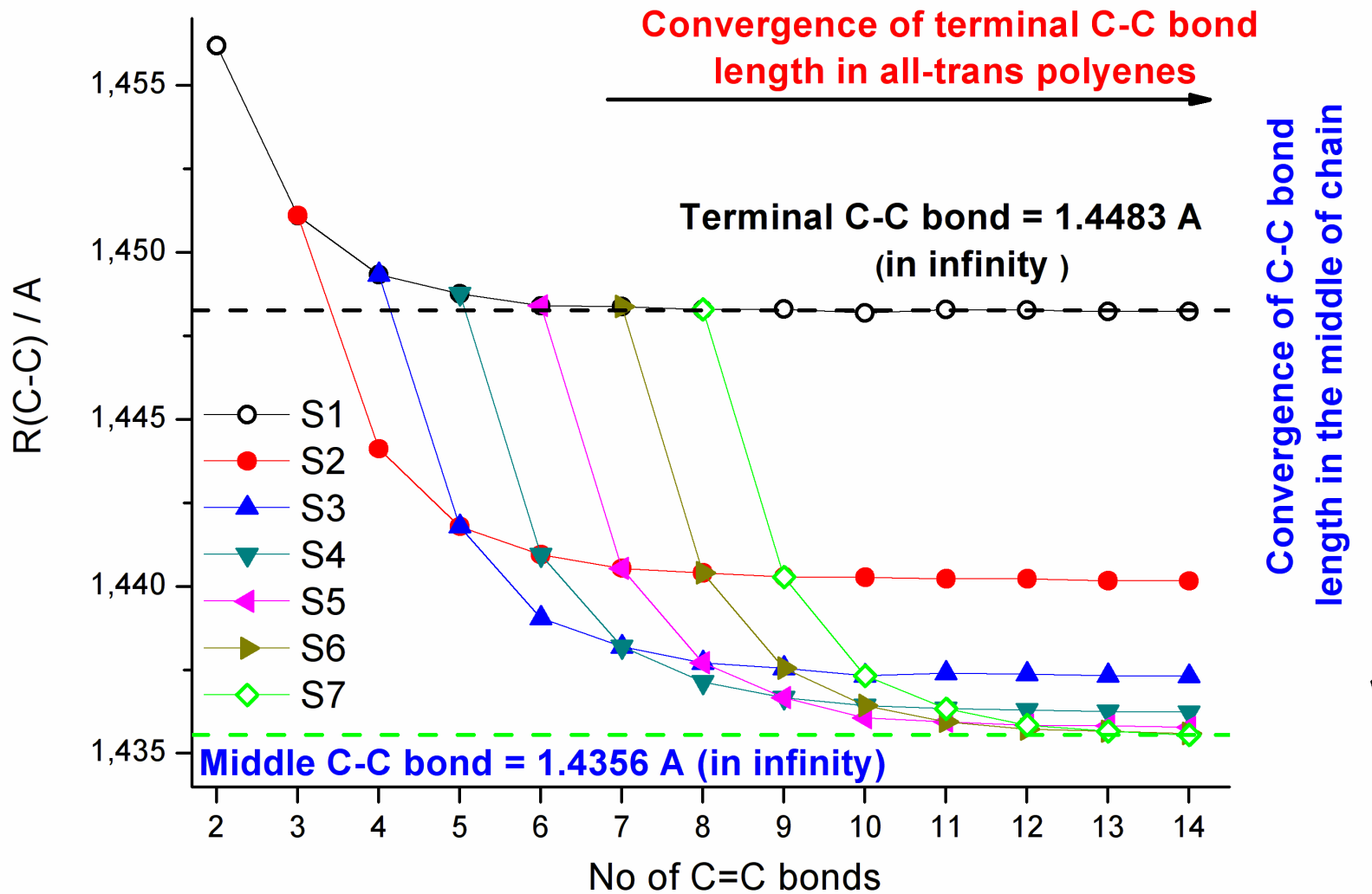
Teobald Kupka*, Aneta Buczek*, Małgorzata A. Broda, Michał Stachów, Przemysław Tarnowski

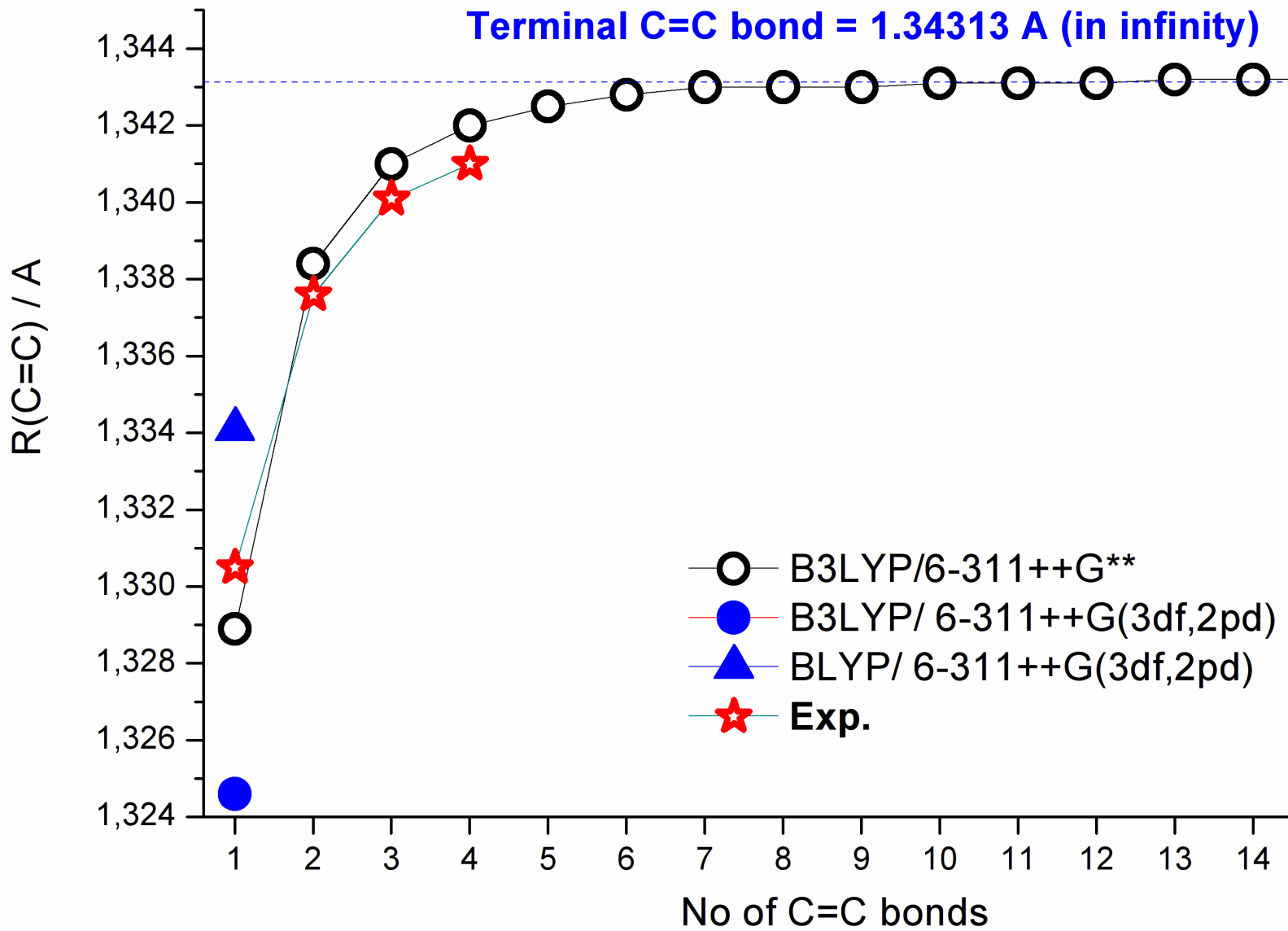
Faculty of Chemistry, University of Opole, 48, Oleska Street, 45-052 Opole, Poland

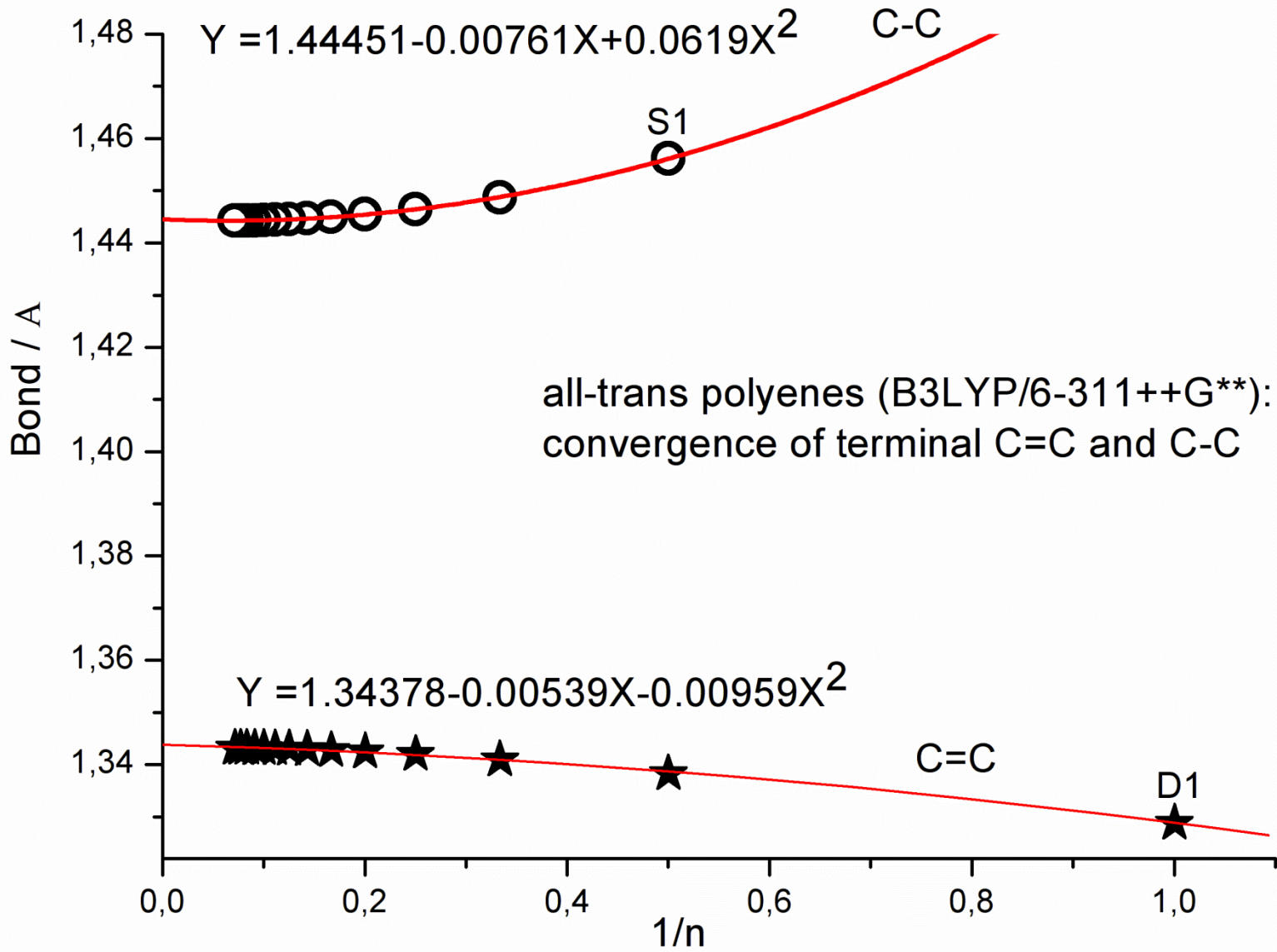


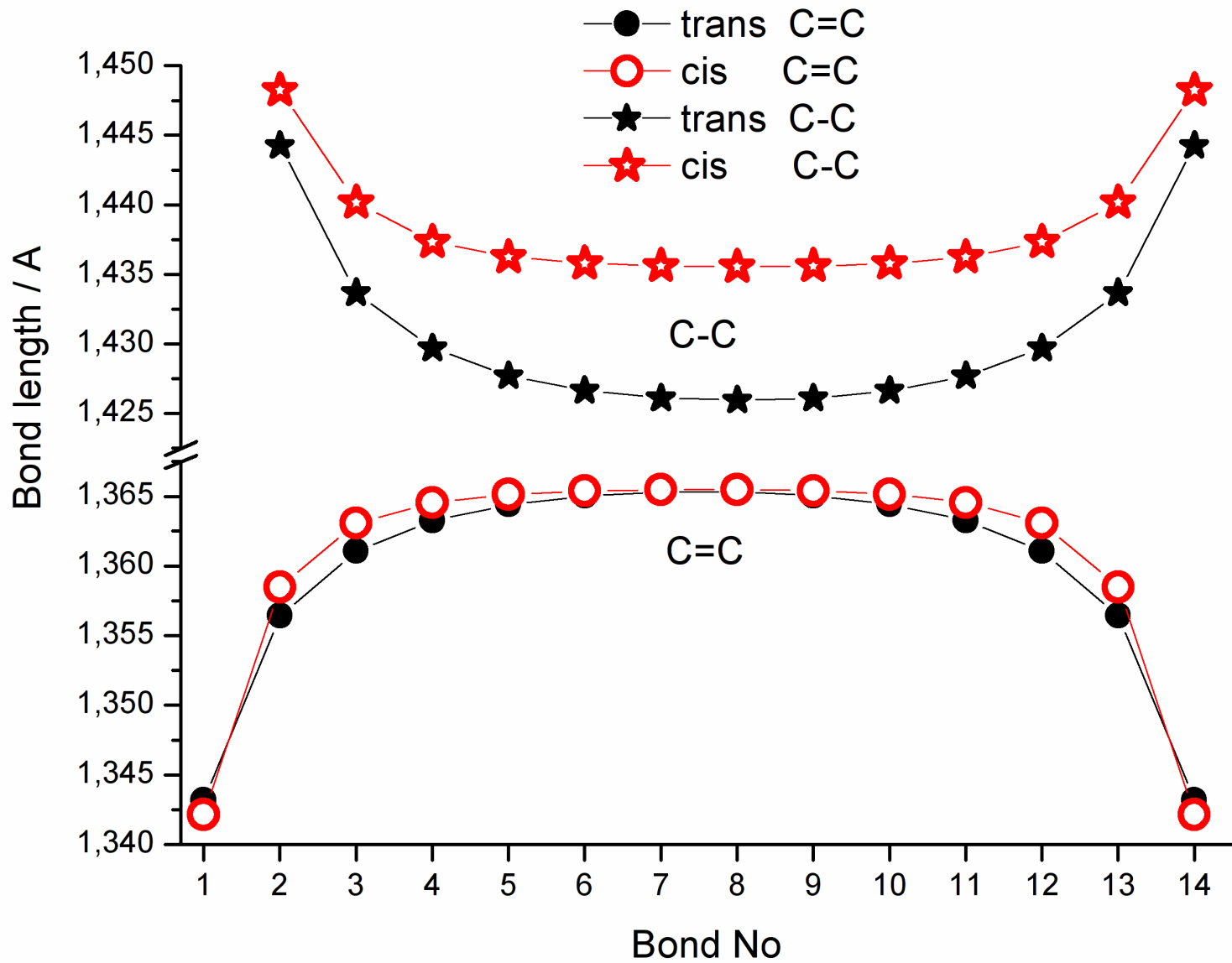
A



B

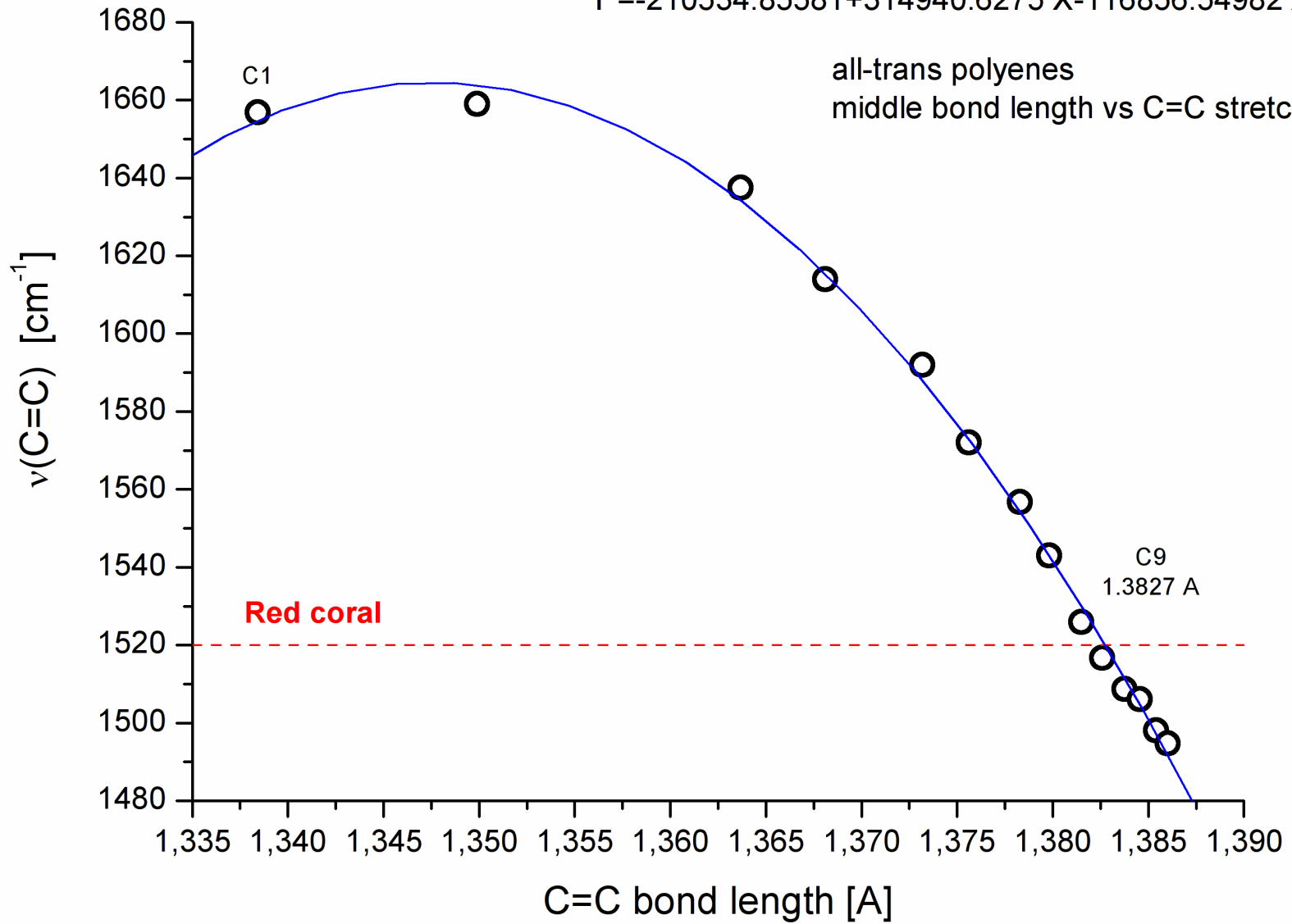


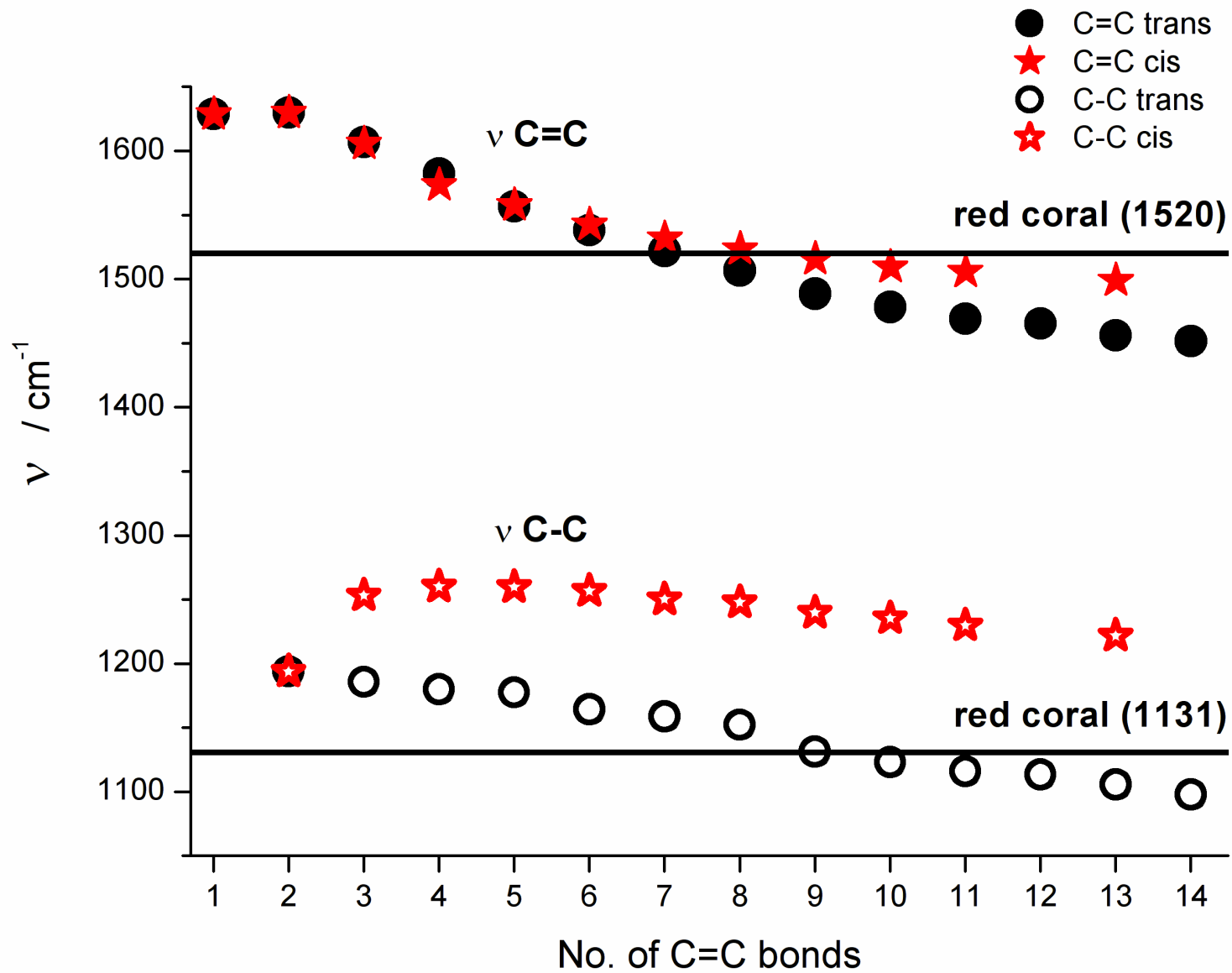


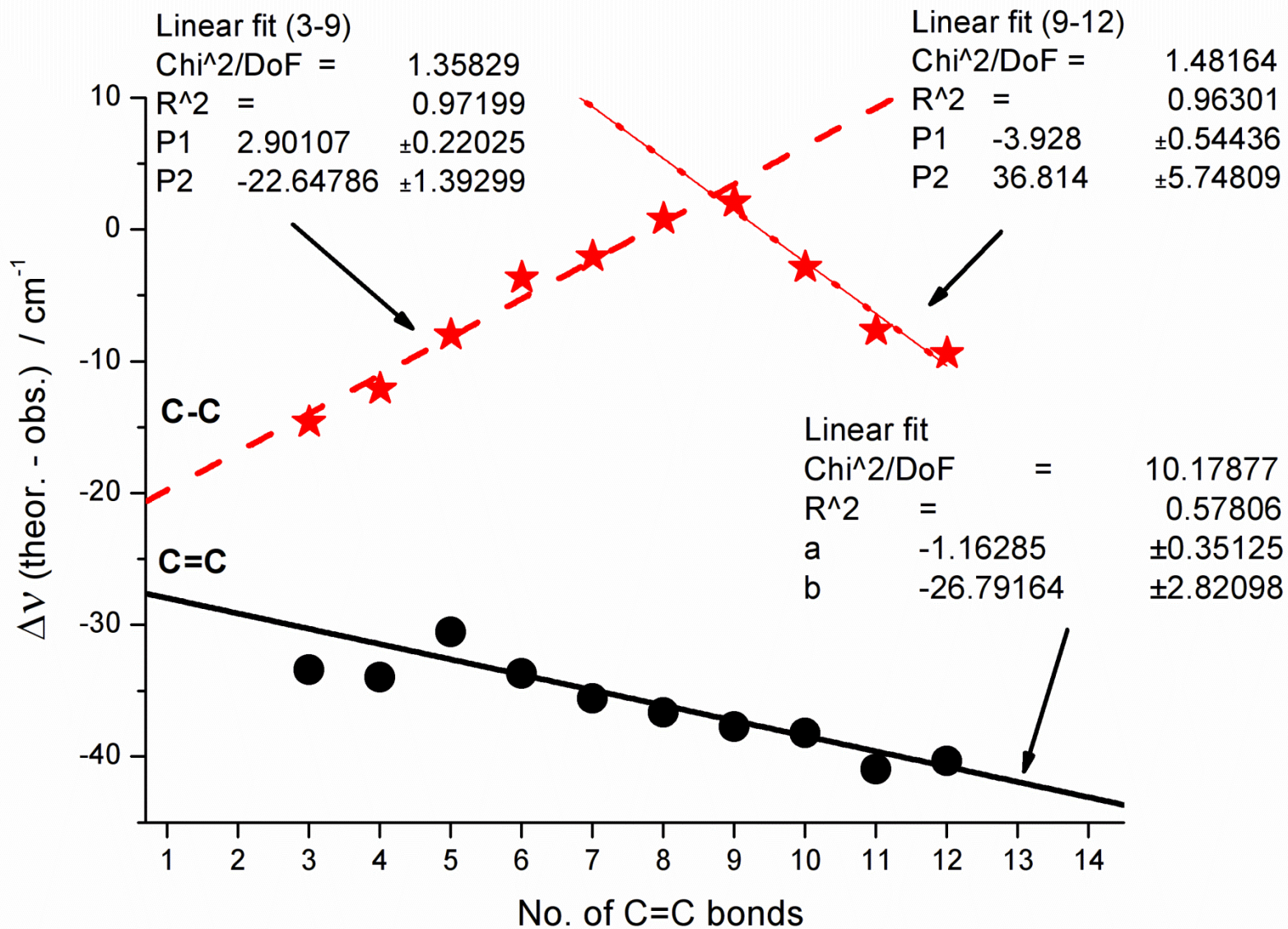


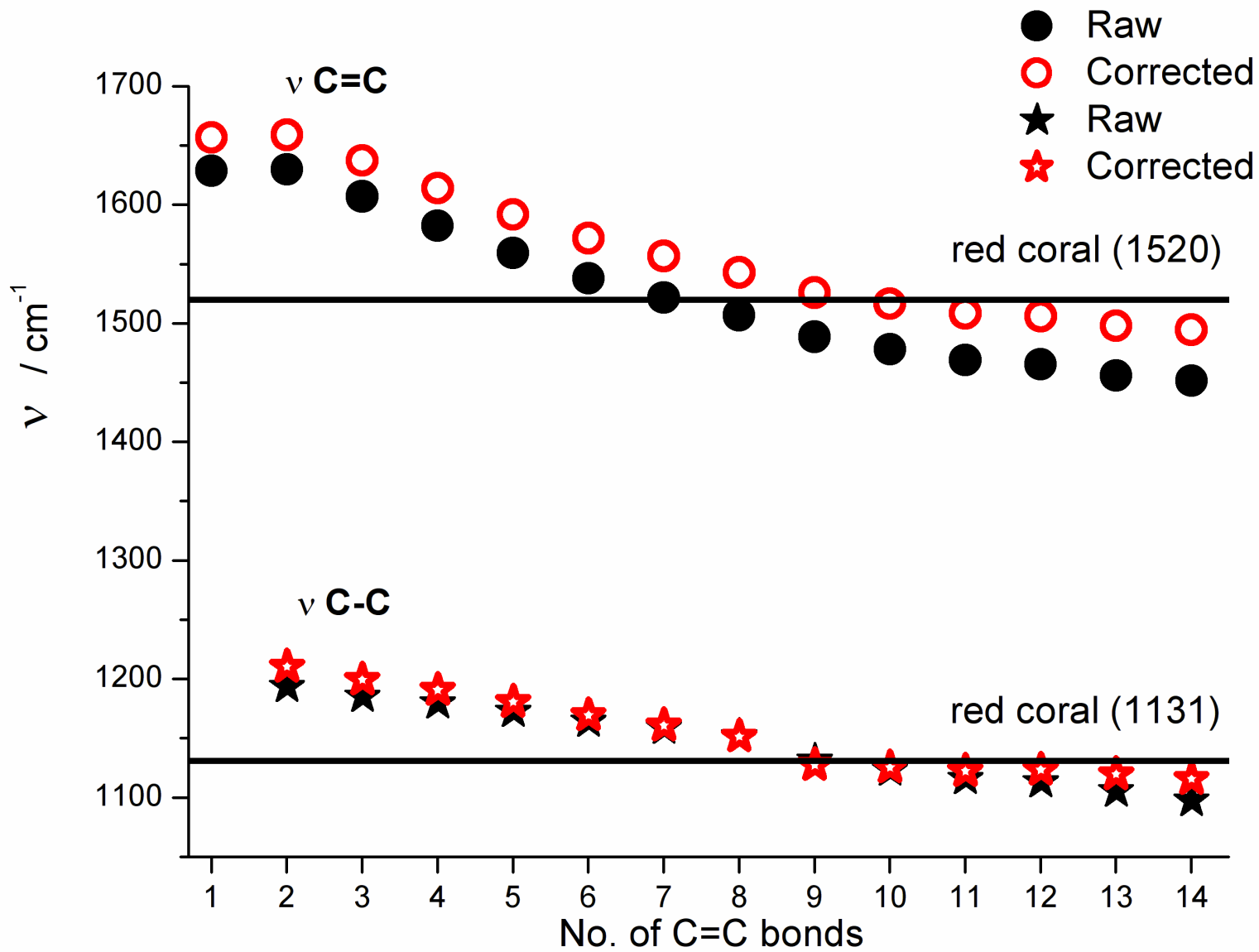
$$Y = -210534.85581 + 314940.6275 X - 116856.54982 X^2$$

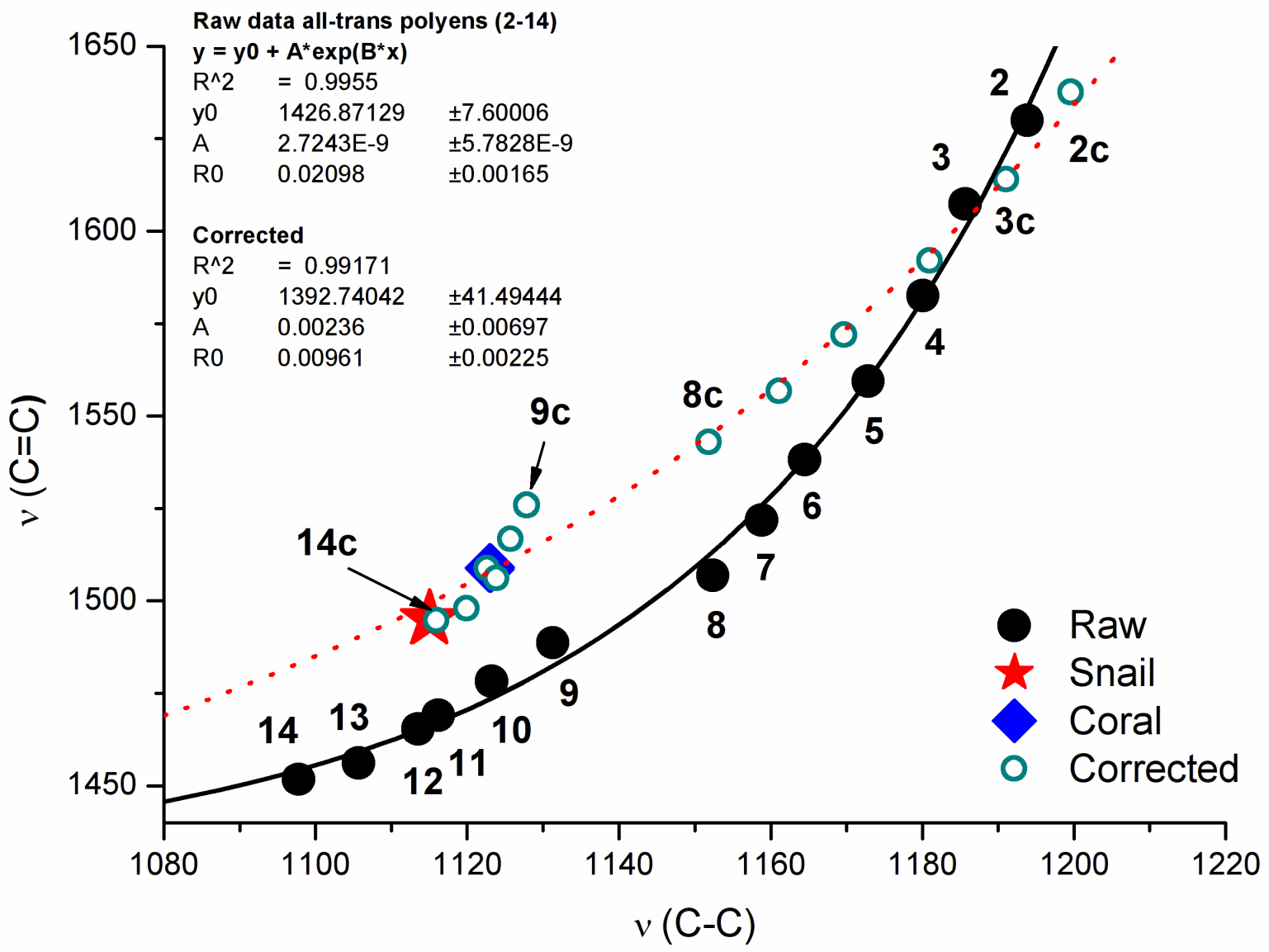
all-trans polyenes
middle bond length vs C=C stretch





B





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