THE JOURNAL OF PHYSICAL CHEMISTRY C

Addition/Correction

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Correction to "Vibrational Davydov Splittings and Collective Mode Polarizations in Oriented Organic Semiconductor Crystals"

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J. Phys. Chem. C **2012**, *116* (27), 14491−14503. DOI: 10.1021/jp304080g

In our paper, the GGA functional for the calculations of the free molecule was BP86-D2 instead of PBE-D2 as stated in the method part. Calculations with PBE-D2 show that the PFP-bond lengths shorten by approximately 0.001 Å and the vibrational frequencies increase uniformly by 3−10 cm^{-1}. The spectra are thus virtually identical (see Figure 1) and the conclusions are not affected by the small numerical differences.

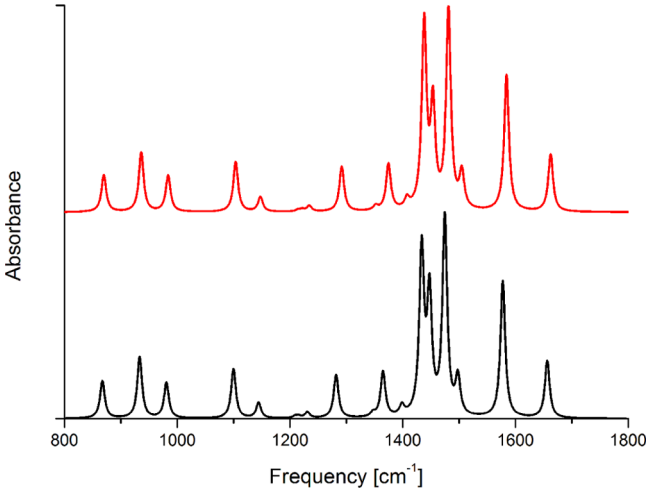

Figure 1. Comparison of simulated spectra for the PFP molecule using BP86-D2 (black) and PBE-D2 (red).

Published: October 10, 2012