Supplementary material

Conformational Analysis of *N*-Alkyl-*N*-[2-(diphenylphosphoryl)ethyl]amides of Diphenylphosphorylacetic acid: Dipole Moments, IR spectroscopy, DFT Study

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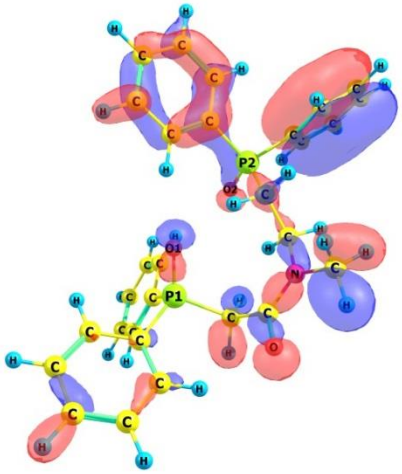

Figure S1. Visualization of the molecular orbital HOMO-29 (*E* = -10.617 eV) for **1c** (the interaction between the P=O bond and phenyl substituents is absent). The positive and negative wave functions are shown as blue and red areas, respectively. Isocontour value is 0.02 a.u.

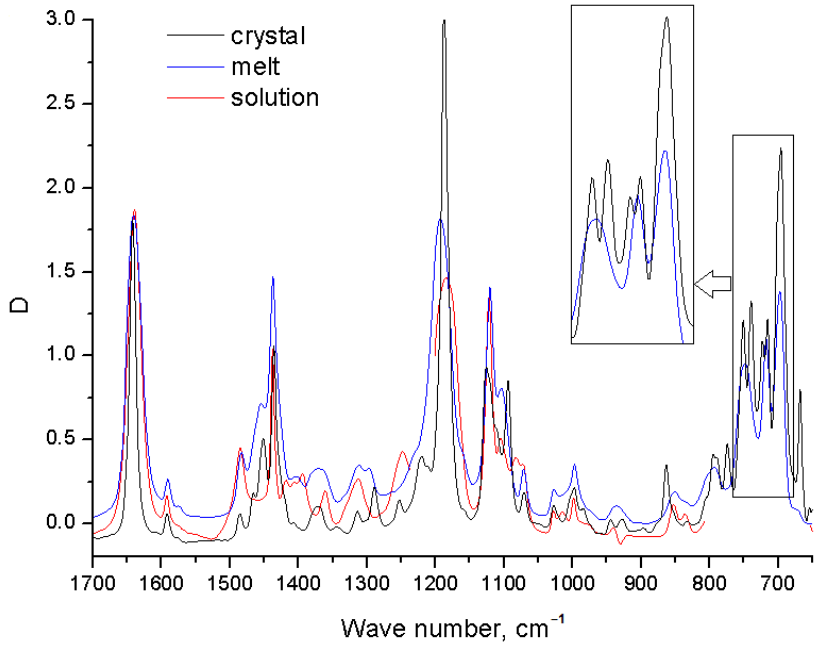

Figure S2. IR spectra of compound **2** in different aggregate states. D is the absorbance.

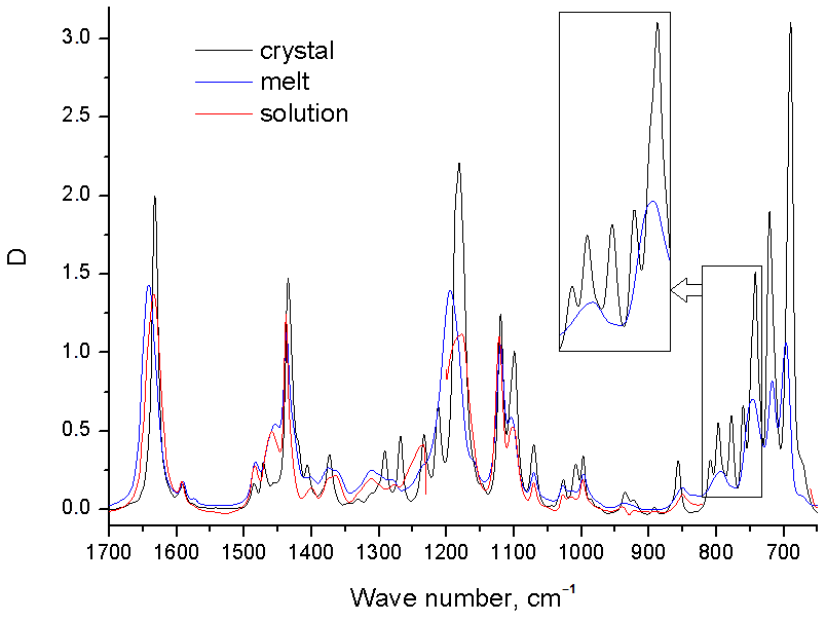

Figure S3. IR spectra of compound **3** in different aggregate states. D is the absorbance.

Equations for α and γ calculations (Guggenheim-Smith equation):

$$\alpha = \frac{\varepsilon_i - \varepsilon_0}{\omega_i}$$

$$\gamma = \frac{n_i^2 - n_0^2}{\omega_i}$$

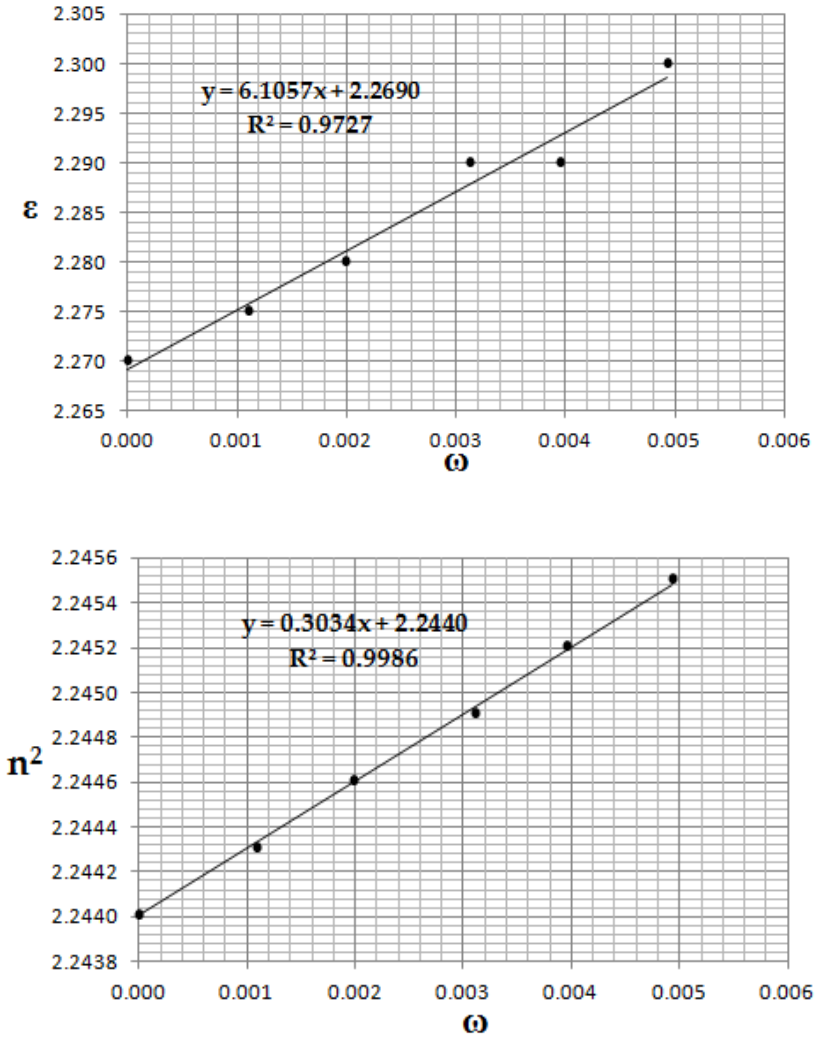

Figure S4. The ε_i–w_i and n_i^2–w_i plots for compound **1**.

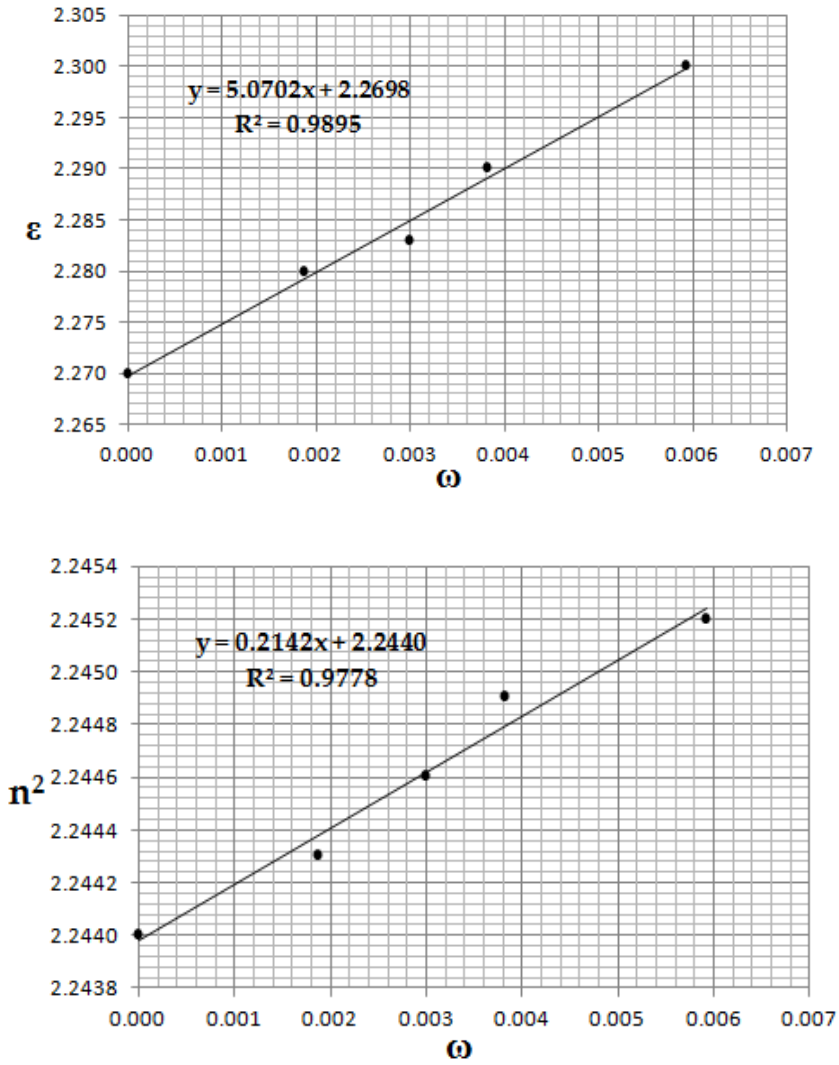

Figure S5. The ε_i–w_i and n_i^2–w_i plots for compound **2**.

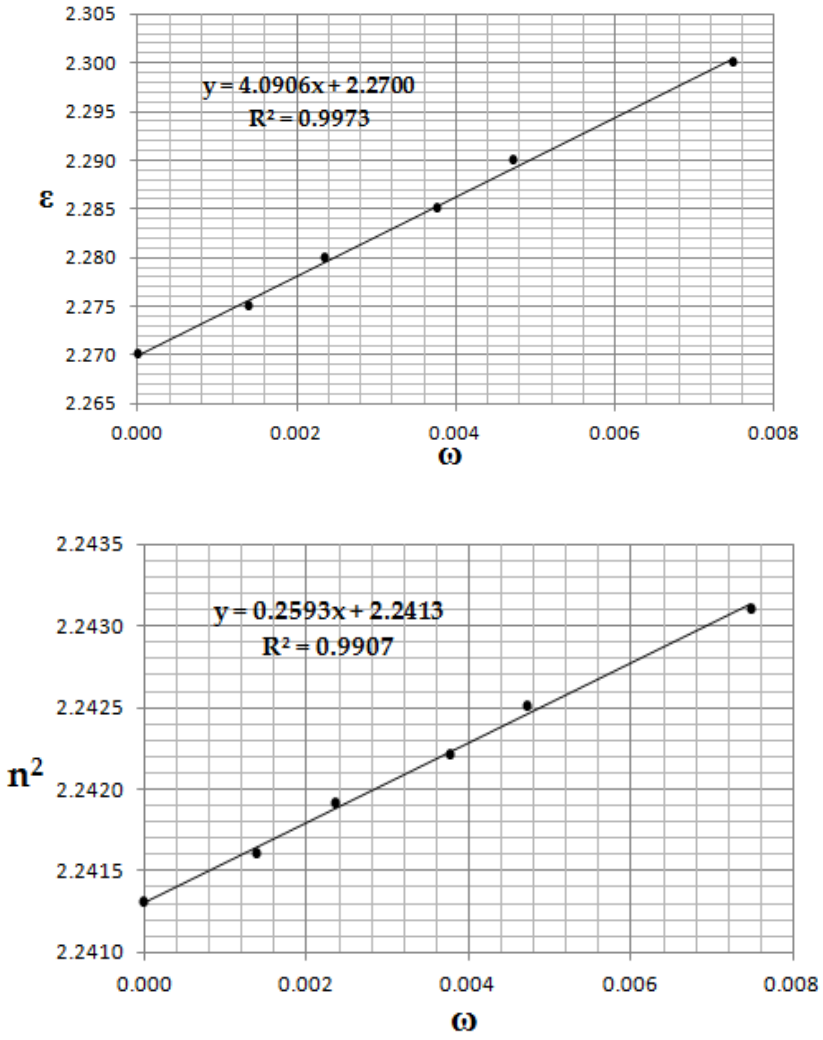

Figure S6. The ε_i–w_i and n_i^2–w_i plots for compound **3**.