ADDITIONS AND CORRECTIONS

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Page 4115. Equation 5 for the molecular orientation analysis should be corrected in the following way:

$$\varphi = \tan^{-1} \left(\sqrt{2 \frac{I_{\rm IP}}{I_{\rm OP}}} \right)$$

The infrared absorption-intensity ratio in the equation represents the ratio of the absorption index (k) in the in-plane and out-of-plane directions. The absorption index of a direction is proportional to the probability of vibrational transition per unit of time, which is also proportional to $\langle \phi_{\rm f} | \mu_j E_j | \phi_i \rangle^2$ where μ_j and E_j are the dipole moment and electric field in the j direction, respectively, and $\phi_{\rm f}$ and ϕ_i are the wave functions of the initial and final vibrational states via the interaction with the dipole moment, respectively. When we discuss the orientation of a dipole, therefore, the square root of the ratio of absorbance intensities must be calculated before applying the inverse tangent function. This is also mentioned in a different way by Chollet et al.¹

References and Notes

(1) Chollet, P.-A.; Messier, J.; Rosillio, C. J. Chem Phys. 1976, 64, 1042

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