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Erratum

# Hyperpolarizabilities measured for interacting molecular pairs (Chem. Phys. Letters 215 (1993) 156)

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In the above work an incorrect expression was given for the dipole–induced-dipole (DID) contribution to the pair hyperpolarizability. As previously derived by Hunt [1], and recently pointed out by Buckingham et al. [2], the numerical coefficient of the $R^{-6}$ term of Eq. (3) should be 76/5 rather than 48, so Eq. (3) should read

$$\gamma(R)=\gamma[1+(76/5)(\alpha/4\pi\epsilon_0 R^3)^2] .$$

The error occurred because self-consistency was not enforced in the solution for the total induced dipole in terms of the externally applied field.

The thermal average of Eq. (3), given in Eq. (4), was used to estimate the DID contribution to the density dependence of the experimentally determined hyperpolarizability $\gamma(\rho)$ for several small molecules. Because of the error in Eq. (3) the magnitude of the calculated density dependence was overestimated, and some of the published results should be modified. The results for $b(\mathrm{AB})_{\mathrm{calc}}$ in Table 3 and the results for $b$ in Table 4 should all be reduced by a factor of 19/60. The density dependence of $\gamma(\rho)$ due to DID is now seen to be much smaller than that due to the local field corrections, and even when extrapolated to liquid density, the binary DID contribution is less than 15% of the individual molecule contribution. While the experimentally determined density dependence of $\gamma(\rho)$ is now seen to be about six times stronger than that due to the DID contribution alone, it still has the opposite sign, and is still consistent with the electron overlap contributions to $\gamma(R)$ seen in some semi-empirical calculations. The published experimental results and conclusions of this work are unchanged.

## References

[1] K.L.C. Hunt, Chem. Phys. Letters 70 (1980) 336.
[2] A.D. Buckingham, E.P. Concannon and I.D. Hands, J. Phys. Chem., in press.

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