MOLECULAR-PHOTOELECTRON ANGULAR DISTRIBUTIONS AS A PROBE OF DYNAMIC SYMMETRY BREAKING. Dan Dill, Scott Wallace, Jon Siegel, and J. L. Dehmer [Phys. Rev. Lett. 41, 1230 (1978)].

A review of the equations on which our asymmetry-parameter calculations were based has uncovered two phase errors. The first of these, tracing to Eq. (53) of our Ref. 8 [D. Dill and J. L. Dehmer, J. Chem. Phys. <u>61</u>, 692 (1974)], which should be

$$\frac{d\sigma}{d\hat{k}'} = 4\pi^2 \alpha \hbar \omega \sum_{i_t L L'} (2j_t + 1)^{-1} i^{i'-i} \exp[i(\sigma_i - \sigma_{i'})] D_{Lj_t}^{(-)} \times D_{L'j_t}^{(-)^{\bullet}} \Theta(j_t; 10, ll'; \theta'), (1)$$

was already corrected in our calculations. The second of these, tracing to Eq. (60) of the same paper (Ref. 8), which should be

$$D_{Lj_t}^{(*)} = \sum_{L'} c_{LL'}^{(*)*} D_{L'j_t}^{L}, \qquad (2)$$

is corrected here as indicated by the revision of Figs. 1 and 2.

This error affects only the asymmetry parameter β ; the integrated cross section σ shown in Fig. 1 is the same as before. The effect of hole localization remains: The delocalized-hole calculation yields an N₂ β intermediate between that of C and O in CO, whereas the localized-hole calculation yields an N₂ β resembling closely that for O rather than C in CO. Now, however, both calculations predict an oscillation in β across the shape resonance in the σ ionization channel.

The earlier calculations of our Ref. 4 [J. L. Dehmer and D. Dill, Phys. Rev. Lett. 35, 213 (1975)] and Ref. 5 [J. L. Dehmer and D. Dill, J. Chem. Phys. 65, 5327 (1976)] were based on the original Eqs. (53) and (60) of Ref. 8; since the errors in these equations cancel each other, the results and conclusions in Refs. 4 and 5 remain correct.



FIG. 1. Photoelectron asymmetry parameter β and integrated cross section σ for localized and delocalized treatments of K-shell photoionization of N₂.



FIG. 2. Photoelectron asymmetry parameters for hole-localized treatments of K-shell photoionization of CO and N_2 .