

of exchange in individual partial cross sections, even away from the resonance.

We conclude that a detailed representation of short-range interactions, including exchange, is essential in order to obtain accurate momentum-transfer cross sections for highly polar molecules. The use of crude representations of short-range interactions does, however, yield results which are qualitatively correct in the absence of resonances, and hence we might hope that relatively simple, yet reliable, model potentials can be devised for more complicated systems. Measurement of electron affinities, and experimental observation of resonance behavior such as that predicted here for LiF, could prove very useful in this regard, because the accurate calculation of these quantities is a stringent test of model potentials.

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*Visiting staff member, Los Alamos Scientific Laboratory.

‡Staff member, Laboratory Astrophysics Division, National Bureau of Standards.

¹K. Takayanagi and Y. I. Itikawa, *Adv. At. Mol. Phys.* **6**, 105 (1970); W. P. Garrett, *Mol. Phys.* **24**, 465 (1972).

²R. C. Slater, M. G. Fickes, W. G. Becker, and R. C. Stern, *J. Chem. Phys.* **60**, 4692 (1974), and **61**, 2290 (1974); W. G. Becker, M. G. Fickes, R. C. Slater, and

R. C. Stern, *J. Chem. Phys.* **61**, 2283 (1974).

³M. R. H. Rudge, *J. Phys. B* **7**, 1323 (1974); K. Takayanagi, *Prog. Theor. Phys.* **52**, 337 (1974); F. T. Smith, D. L. Huestis, D. Mukherjee, and W. H. Miller, *Phys. Rev. Lett.* **35**, 1073 (1975); M. P. Maur and H. S. Desai, *J. Phys. B* **8**, 1959 (1975); A. S. Dickinson and D. Richards, *J. Phys. B* **8**, 2846 (1975); O. Ashihara, I. Shimamura, and K. Takayanagi, *J. Phys. Soc. Jpn.* **38**, 1732 (1975); K. Onda, *J. Phys. Soc. Jpn.* **40**, 1437 (1976); Y. Itikawa, *J. Phys. Soc. Jpn.* **41**, 619 (1976); M. R. H. Rudge, S. Trajmar, and W. Williams, *Phys. Rev. A* **13**, 2074 (1976); Y. Itikawa, to be published.

⁴A. D. McLean and M. Yoshimine, *IBM J. Res. Dev.* **12**, 206 (1968).

⁵M. E. Riley and D. G. Truhlar, *J. Chem. Phys.* **63**, 2102 (1975).

⁶S. Hara, *J. Phys. Soc. Jpn.* **22**, 710 (1967).

⁷A. C. Allison, *J. Phys. B* **8**, 325 (1975); Y. Itikawa, *J. Phys. Soc. Jpn.* **41**, 619 (1976).

⁸H. S. W. Massey, *Proc. Cambridge Philos. Soc.* **28**, 99 (1932); S. Altschuler, *Phys. Rev.* **107**, 114 (1957); O. H. Crawford, A. Dalgarno, and P. B. Hayes, *Mol. Phys.* **13**, 191 (1967).

⁹M. J. Seaton, *Proc. Phys. Soc.* **77**, 174 (1961), and **89**, 469 (1966).

¹⁰A. M. Arthurs and A. Dalgarno, *Proc. Roy. Soc. London, Ser. A* **256**, 540 (1960).

¹¹E. S. Chang and U. Fano, *Phys. Rev. A* **6**, 173 (1970).

¹²A. Temkin and K. V. Vasavada, *Phys. Rev.* **160**, 109 (1967).

¹³K. Takayanagi, *J. Phys. Soc. Jpn.* **21**, 507 (1966).

¹⁴W. P. Garrett, *Phys. Rev. A* **4**, 2229 (1971).

¹⁵K. D. Jordan and W. Luken, *J. Chem. Phys.* **64**, 2760 (1976).

¹⁶S. E. Novick, T. J. Mulloney, and W. C. Lineberger, private communication.

Asymmetry of Compton Lines

R. Hosemann, A. Müller, and D. Weick

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Teilinstitut für Strukturforschung, Berlin, Germany

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Because of the binding of the atomic electrons, the Compton line is asymmetric in shape and its center of gravity differs from the position to be expected for free electrons. Using a new Compton fluorescence method, this difference has been determined experimentally for a number of elements and primary wavelengths and it is compared with theoretical predictions. The agreement is satisfactory.

The spectral intensity distribution of the Compton line can be calculated by matrix elements f_{ij} including excited states. Bloch¹ investigated hydrogenic wave functions and found that their Compton lines are asymmetric and shifted. It has been shown recently² that the Waller formula can be evaluated with the help of the Thomas-Fermi approximation and leads also to any asym-

metric line profile. The shift of its center of gravity is larger by a factor $Z/(Z-F)$ compared with the Compton shift $2\lambda_c \sin^2 \varphi/2$. This means a shift of the center to negative values in the momentum scale q . F is well known from the Waller-Hartree formula and depends solely on the ground states. This result is generally valid and independent of the Thomas-Fermi model. The

TABLE I. Shift factor $Z/(Z-F)$ measured with the Compton-fluorescence method.

Fluorescent radiation	$(\sin\varphi/2)/\lambda_0$		Al	Ti	Fe	Cu
Zr $K\alpha$	1.18 \AA^{-1}	Theor.	1.180 ± 0.015	1.295 ± 0.010
$\lambda_0 = 0.785 \text{ \AA}$	$(\varphi = 127^\circ)$	Expt.	1.17 ± 0.03	1.26 ± 0.03
Mo $K\alpha$	1.26 \AA^{-1}	Theor.	1.160 ± 0.015	1.265 ± 0.010	1.305 ± 0.015	...
$\lambda_0 = 0.71 \text{ \AA}$	$(\varphi = 127^\circ)$	Expt.	1.17 ± 0.03	1.25 ± 0.03	1.29 ± 0.03	...
Ag $K\alpha$	1.60 \AA^{-1}	Theor.	1.110 ± 0.015	1.18 ± 0.01	1.210 ± 0.015	1.230 ± 0.015
$\lambda_0 = 0.56 \text{ \AA}$	$(\varphi = 127^\circ)$	Expt.	1.11 ± 0.03	1.14 ± 0.03	1.19 ± 0.04	1.24 ± 0.04

influence of the excited states is canceled out by integrating over the whole Compton profile.

The experimental verification of this shift is practically impossible using the conventional x-ray method because of the difficulties in separating the wavelength-dependent background. By a refined technique using convolution methods, it was found that the shift factor is larger than unity.³ For a quantitative comparison with the theoretical prediction, the accuracy, however, still was too low. These difficulties were removed almost entirely with the help of a new experimental technique in which fluorescence radiation is used as the primary beam which is totally free from the disturbing white spectrum.⁴ The advantage of this new technique is the very low

and well-defined background compared to the conventional x-ray method and a sufficiently strong radiation. The principle is briefly illustrated in Fig. 1. The monochromatic radiation from the fluorescence shield Sh has nearly the same intensity as the $K\alpha$ line from the x-ray tube, because the whole spectrum of the tube comes into action to produce the fluorescence radiation. $K\beta$ is removed by a filter F .

The experimental results are listed in Table I together with theoretical values based on calculations of Cromer and Mann.⁵ The quite satisfying agreement permits the conclusion that the theoretical prediction is essentially correct and we are thus able to use the measurement of the shift factor as a criterion for the validity of approximations in atomic and molecular wave functions.

There is no doubt that these new theoretical and experimental results are of interest also for a more accurate determination of electron momentum density distributions.

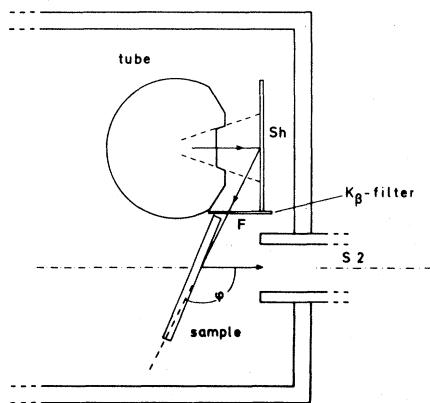


FIG. 1. The arrangement of x-ray-fluorescence Compton profile measurements. Sh, fluorescence shield; S2, entrance soller slit of the crystal analyzer.

¹F. Bloch, Phys. Rev. **46**, 674 (1934).

²D. Weick, Ann. Phys. (N.Y.) **25**, 2, 143 (1970).

³D. Esslinger, dissertation, Freie Universität, Berlin, 1972 (unpublished).

⁴D. Esslinger, R. Hosemann, A. Müller, and D. Weick, J. Appl. Phys. **45**, 4100 (1974).

⁵D. T. Cromer and I. B. Mann, J. Chem. Phys. **47**, 1892 (1967); D. T. Cromer, J. Chem. Phys. **50**, 4857 (1969).