$\rightarrow K^{-1}L^{-n-1}$) *and* satellites ($K^{-1}L^{-n} \rightarrow L^{-n-1}$). These additional L vacancies have then no influence on the energy difference ΔE between the two-electron, one-photon transition and twice the value of the *measured* $K\alpha$ energy.

In conclusion, one can say that the energy value of the line observed by Wölfli *et al.* is in good accord with his proposed explanation. However, it should be considered that in most cases of heavy-ion bombardment, numerous additional M vacancies are observed during K^{-2} ionization[8] and that the discussed line observed in a SiLi detector should be broadened or shifted. These multiple additional M vacancies can also allow various $K^{-2}M^{-n} \rightarrow L_{ij}^{-2}M^{-n}$ two-electron, one-photon transitions.

Note added.—A similar conclusion about the assignment of the transition observed by Wölfli was also obtained by Hoogkaner *et al.*[10] and by Åberg, Jamison, and Richard,[11] these later authors having done a Hartree-Fock calculation for the considered elements which is in good accord with our present results.

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[1]D. J. Nagel, P. G. Burkhalter, A. R. Knudson, and K. W. Hill, Phys. Rev. Lett. 36, 164 (1976).

[2]W. Wölfli, Ch. Stoller, G. Bonani, M. Suter, and M. Stöckli, Phys. Rev. Lett. 35, 656 (1975).

[3]J. P. Briand, A. Touati, M. Frilley, P. Chevallier, A. Johnson, J. P. Rozet, M. Tavernier, S. Shafroth, and M. O. Krause, to be published.

[4]Y. Cauchois and H. Hulubei, *X-Ray Table* (Hermann & Cie, Paris, 1947).

[5]O. Hörnfeldt, Ark. Fys. 23, 235 (1962).

[6]K. Siegbahn *et al.*, *ESCA: Atomic, Molecular and Solid State Structure Studied by Means of Electron Spectroscopy* (Almqvist and Wiksell, Stockholm, Sweden, 1967).

[7]C. L. Cocke, B. Curnutte, J. R. MacDonald, and R. Randall, Phys. Rev. A 9, 57 (1974).

[8]P. Richard, W. Hodge, and G. F. Moore, Phys. Rev. Lett. 29, 393 (1972).

[9]D. K. Olsen and C. F. Moore, Phys. Rev. Lett. 33, 194 (1974).

[10]T. P. Hoogkaner, P. Woerlee, F. W. Saris, and M. Gavrila, to be published.

[11]T. Åberg, K. A. Jamison, and P. Richard, Phys. Rev. Lett. 37, 63 (1976) (this issue).

Calculation of Two-Electron, One-Photon K–X-Ray Transition Energies

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It is shown that recently reported two-electron, one-photon K–x-ray transition energies for collision-excited Fe and Ni ions can be described on the basis of Hartree-Fock calculations, provided that multiple ionic excitation and selection rules for $E1$ transitions are taken into account.

Investigations of x-ray spectra from heavy-ion–atom collisions have revealed unusual x-ray lines attributed to cases in which two K-shell vacancies in a single ion are filled simultaneously by two electrons with the emission of a single photon. Wölfli *et al.*[1] reported energies of such transitions with an accuracy of better than approximately ± 20 eV for Fe and Ni ions with transition energies near 13 and 15 keV, respectively. Recently, Nagel *et al.*[2] claimed that these transition energies reported in Ref. 1 are inconsistent with predictions based on empirical satellite and hypersatellite energies or with Hartree-Fock calculations. They conclude that the values of Wölfli *et al.*[1] for Fe and Ni are too low by ~150 eV. It is the purpose of this Comment to demonstrate that the assessment of Nagel *et al.*[2] cannot be supported mainly because the selection rules for radiative dipole transitions were not properly taken into account. Experimental transition energies can be reproduced in a consistent manner when $E1$ selection rules, electronic binding energies, and ionization states are duly considered.

Atomic binding energies are readily calculated with existing relativistic Hartree-Fock programs.[3] In the cases of present interest, it is sufficient to

TABLE I. Calculated Hartree-Fock transition energies for various initial and final electronic configurations in Ni. Experimental values are from Ref. 1.

Shell occupancy 1s	2s	2p	3s	3p	Transition energy (keV) HFS	Expt.	
						7.530	
1	2	6	2	}	7.516		$K\alpha$
2	2	5	2	}			
1	2	5	2	5 }	7.523		$K\alpha$
2	2	4	2	5 }			
1	2	5	2	4 }	7.528		$K\alpha$
2	2	4	2	4 }			
1	2	5	2	3 }	7.533		$K\alpha$
2	2	4	2	3 }			
1	2	5	2	2 }	7.539		$K\alpha$
2	2	4	2	2 }			
1	2	5	2	}	7.553		$K\alpha$
2	2	4	2	}			
						15.228	
0	2	5	2	3 }	15.217		$K\alpha\alpha$
2	1	4	2	3 }			
0	2	5	2	}	15.262		$K\alpha\alpha$
2	1	4	2	}			
0	2	5	2	3 }	15.336		$K\alpha\alpha$ $\Delta l = 2$
2	2	3	2	3 }			
						16.174	
0	2	5	2	3 }	16.179		$K\alpha\beta$
2	1	5	2	2 }			
0	2	5	2	3 }	16.270		$K\alpha\beta$
2	2	4	1	3 }			
0	2	5	2	3 }	16.144		$K\alpha\beta$ $\Delta l = 0$
2	1	5	1	3 }			

use a simplified relativistic Hartree-Fock-Slater (HFS) program[4] which allows calculation of transition energies with an accuracy of better than ~10 eV for $Z = 28$, whereby the HFS results overestimate the correct values.

An important problem is to determine the average degree of shell ionization in excited heavy ions which results from heavy-ion collisions. We proceed as follows: For various electronic configurations ordinary $K\alpha$ energies are calculated and compared with the experimental value. Though this procedure is not unique, it allows us to pin down the relevant inner-shell configurations with sufficient accuracy. For 40-MeV Ni-Ni collisions[1] creation of a 1s vacancy is usually accompanied by one additional L-shell and many M-shell vacancies (Table I). Such a configuration and the resulting line shift of ~50 eV relative to the diagram $K\alpha_1$ line are in good agreement with results obtained from other collision systems.[5] We neglect further complications due to collisional rearrangement processes in outer shells.

The two-electron, one-photon line is then obtained from configurations which are assumed to be identical to the ones above except that two K holes are present. The resulting $K\alpha\alpha$ and $K\alpha\beta$ transition energies agree excellently with the experimental values (Table I), provided that the selection rules for $E1$ transitions are observed. In the $K\alpha\alpha$ case, for example, one $2s$ and one $2p$ electron must jump; transitions of two $2s$ or two $2p$ electrons give transition energies which are, because of $2s$-$2p$ energy splitting, too high or too low, respectively, by ~120 eV.

We conclude that our calculations of the $K\alpha\alpha$ and $K\alpha\beta$ transition energies reproduce experimentally obtained values for Ni (and for Fe, not shown in Table I) and are in accord with the two-electron, one-photon interpretation of the observed transitions. Finally, we note that attention should also be given to the results by Afrosimov *et al.*[6] who identified the Auger analog in transitions of the type *LL-MMM*; i.e., two holes are simultaneously filled by two electrons and the entire released energy is carried away by a single third electron rather than by a photon.

[1]W. Wölfli, Ch. Stoller, G. Bonani, M. Suter, and M. Stöckli, Phys. Rev. Lett. 35, 656 (1975).

[2]D. J. Nagel, P. G. Burkhalter, A. R. Knudson, and K. W. Hill, Phys. Rev. Lett. 36, 174 (1976).

[3]J. P. Desclaux, Comp. Phys. Commun. 9, 31 (1975).

[4]J. P. Desclaux, private communication.

[5]H.-D. Betz, J. P. Delvaille, K. Kalata, H. W. Schnopper, A. R. Sohval, K. W. Jones, and H. E. Wegner, in *Proceedings of the International Conference on Inner Shell Ionization Phenomena and Future Applications, Atlanta, Georgia, 1972,* edited by R. N. Fink, J. T. Manson, I. M. Palms, and R. V. Rao, CONF-720404 (U. S. Atomic Energy Commission, Oak Ridge, Tenn., 1973), p. 1374.

[6]V. V. Afrosimov, Yu. S. Gordeev, A. N. Zinov'ev, D. Kh. Rasulov, and A. P. Shergin, Pis'ma Zh. Eksp. Teor. Fiz. 21, 535 (1975) [JETP Lett. 21, 249 (1975)].