tetrahedron core[3] occurs, with inclusion of the rotating helions in the outer layer and strong interaction leading to rotating dihelions.

This work was supported in part by a grant from The Educational Foundation of America.

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Two-Electron, One-Photon *K* X-Ray Transition Energies

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Recently reported cooperative K x-ray transition energies for Fe and Ni are not consistent with predictions based on empirical satellite and hypersatellite energies or with Hartree-Fock calculations. Estimates of two-electron, one-photon K transition energies for elements in the C-Ni range are given.

There is growing interest in cooperative x-ray emission in which two electrons simultaneously fill two inner-shell vacancies, with the emission of a single photon. Relatively large probability for such emission in transitions to the L shell was predicted by Dow and Franceschetti.[1] This prompted an unsuccessful search of ion-excited K spectra from light elements (Be-Ne) for two-electron, one-photon lines.[2] Recently Wölfli *et al.*[3] reported evidence for cooperative transition lines in Fe and Ni, also excited by energetic ion-atom collisions. However, the observed energies are substantially smaller than predictions based on measured x-ray energies and *ab initio* calculations. We examine the discrepancies in this Comment.

The energy of a two-electron, one-photon transition can be simply related to the energies of satellite transitions. Consider an atom initially with two K-shell vacancies, a state denoted K^2. After cooperative $K\alpha$ transitions ($2p \rightarrow 1s$), there are two L-shell vacancies (denoted L^2). The same final state would be reached by two separate transitions, K^2-KL and KL-L^2. In short, using the symbol of a state to denote its energy,

$(K^2 - KL)$ Hypersatellite transition

$+\underline{(KL - L^2)}$ Satellite transition

$= (K^2 - L^2)$ Cooperative transition.

Because of this, we can estimate cooperative transition energies from observed hypersatellite[2] and satellite[4] transition energies. This procedure ignores the influence of additional vacancies in outer shells (M or higher). Although production of such vacancies can be likely in ion-atom collisions, their effect on transition energies is relatively small and can be ignored in this discussion.

K transition energies relative to the ordinary $K\alpha$ lines are given in Table I. We found[2] that a simple screening calculation fits both observed and Hartree-Fock (HF)[5] relative hypersatellite energies. With a screening constant S of 0.5, $\Delta E_S = (K^2 - KL) - K\alpha = (10.2\text{ eV})(Z - 0.25)$ for Z less than about 30. Wölfli *et al.*[3] used $S = \frac{1}{16}$, which is close to the neutral-atom value of 0.3,[6] and obtained $\Delta E_S = (10.2\text{ eV})(0.625\,Z - 0.098)$.[7] They compared energies computed from this equation (actually relative hypersatellite energies) with observed relative cooperative x-ray energies. The relative satellite energies, $(KL - L^2) - K\alpha$, are also given in the table. These are computed from a fit to the empirical values for $Z \leq 28$ in Ref. 4. The tabulated hypersatellite and satellite energies agree well with nonrelativistic HF calculations. For example, the absolute HF and ion-excited values of the hypersatellite line of Al agree to 0.3%.

Relative K cooperative energies are compared

TABLE I. K transition energies (eV) relative to the $K\alpha$ (K-L) energy. The two-electron, one-photon energy is denoted $K\alpha\alpha$ for two $2p \rightarrow 1s$ jumps.

Element	$(K^2$-KL)-Kα Hypersatellite[a]	(KL-L^2)-Kα Satellite[b]	Calculated[c]	K$\alpha\alpha$ - 2Kα Hartree-Fock[d]	Observed[e]
C	58.7	3.7	62.4		
N	68.9	4.4	73.3		
O	79.1	5.2	84.3		
F	89.3	6.0	95.3		
Ne	99.5	7.0	106	102 (5)	
Na	110	8.1	118		
Mg	120	9.3	129		
Al	130	10.5	140	136 (7)	
Si	140	11.9	152		
S	150	13.4	163		
P	161	15.0	176		
Cl	171	16.7	188		
Ar	181	18.5	200		
K	191	20.4	211		
Ca	202	22.4	224	219 (11)	
Sc	212	24.5	236		
Ti	222	26.7	249		
V	232	29.0	261		
Cr	242	31.4	273		
Mn	252	33.9	286		
Fe	263	36.5	300	294 (29)	150 (22)
Co	273	39.2	312		
Ni	283	42.0	325		168 (10)

[a] Computed from (10.2 eV)$(Z-0.25)$. These values differ somewhat from the experimental values given in Ref. 2 because of the fitting equations used here.

[b] Computed from $1.81+0.009\,26\,Z+0.0509\,Z^2$ eV.

[c] Sum of the preceding two columns.

[d] The parenthetical numbers are accuracy estimates (in eV) obtained from comparison of absolute calculated and measured hypersatellite and satellite energies.

[e] Wölfli *et al.* (Ref. 3). Their error estimates (in eV) are given in parentheses.

in the last three columns of the table. It can be seen that the sums of the hypersatellite and satellite energies agree well with the HF values as expected. The values of Wölfli *et al.*[3] for Fe and Ni are substantially smaller than the empirical values and HF calculations. The source of the differences is not yet clear. We have no basis for criticizing the experimental work of Wölfli *et al.*[3] Differences in outer-shell configurations in different experiments cannot account for the energy discrepancies. Measurements of K cooperative x-ray emission for other elements near energies indicated in the table should resolve the problem. Theoretical calculations of branching ratios, giving hypersatellite to cooperative intensity ratios, would also be valuable.

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