Energy systematics of vanadium Kα x-ray satellites and hypersatellites

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Vanadium K x-ray spectra excited by 15 MeV/u Ne, Ar, Kr, Ag, and Ho ion collisions were described in last year's progress report [1]. Further analysis has been performed to investigate the dependence of the Kα satellite and hypersatellite energies on projectile atomic number and to compare them with the results of Dirac-Fock calculations.

Comparison of the vanadium x-ray energies measured with each target (V metal, VO, V_2O_4, and V_2O_5), excited by the same projectile indicated that chemical shifts must be quite small, as evidenced by the root-mean-square deviations obtained for each peak. However, the energy of a given peak steadily increases with the projectile atomic number. In the past, this latter effect has been attributed to outer-shell ionization.

The average energy shifts of the Kα satellite peaks relative to the average $K\alpha_{12}$ diagram energy (4949.7 eV) are compared for each projectile in Fig. 1. Here, it is shown that the energy shifts observed with the different projectiles range between the energy shifts predicted by average-of-configuration Dirac-Fock calculations using the Desclaux program [2] for the outer shell electrons all present (dashed

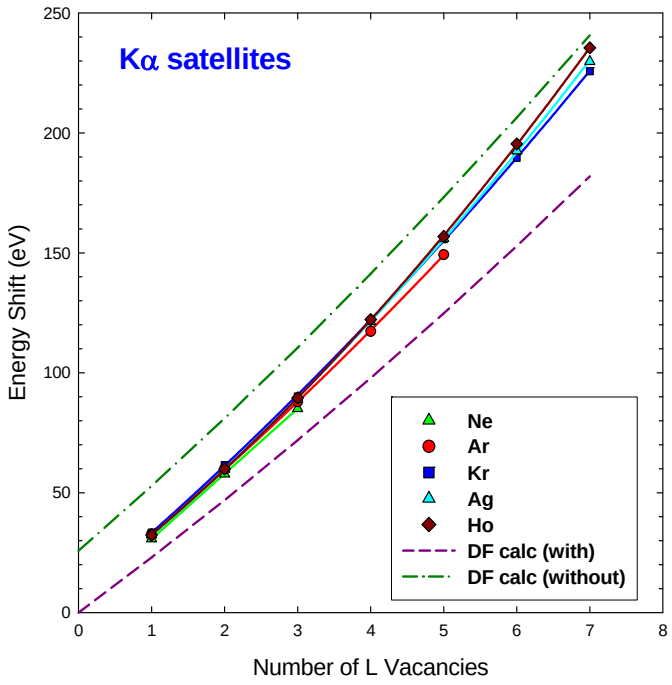

FIG. 1. The Kα satellite average energy shifts measured relative to the average $K\alpha_{1,2}$ diagram peak energy. The dashed (purple) and dot-dashed (green) curves show the average Dirac-Fock energy shifts calculated for a vanadium atom with all outer-shell electrons present and absent, respectively

purple curve) and all absent (dot-dashed green curve). The same kind of graph is shown for the average energy shifts of the Kα hypersatellite peaks relative to the average $K\alpha_{12}$ energy in Fig. 2. In the present work, the average Dirac-Fock energy shifts were obtained by averaging the calculated $K\alpha_1$ and $K\alpha_2$ transition energies;

$$\overline{E}(K\alpha_{1,2}) = \frac{E(K\alpha_1) + RE(K\alpha_2)}{1 + R} \quad , \tag{1}$$

where R is the $K\alpha_2/K\alpha_1$ intensity ratio. In the case of the satellites, the value of R is expected to be close to the statistical value of 0.5 because a large number of transitions is possible for electron configurations containing a single K plus additional L vacancies. The same holds true for the hypersatellites with n > 0. However, the K^2L^0 initial state configuration is a special case since, in the limit of LS-coupling, only transitions to the $^1P_1$ final state are allowed. Hence, the $K\alpha_2$ transition is expected to be heavily favored. In the present analysis, the average energy for the K^2L^0 hypersatellite was computed using a theoretical R value of 10.1, from the calculations of Costa et al. [3].

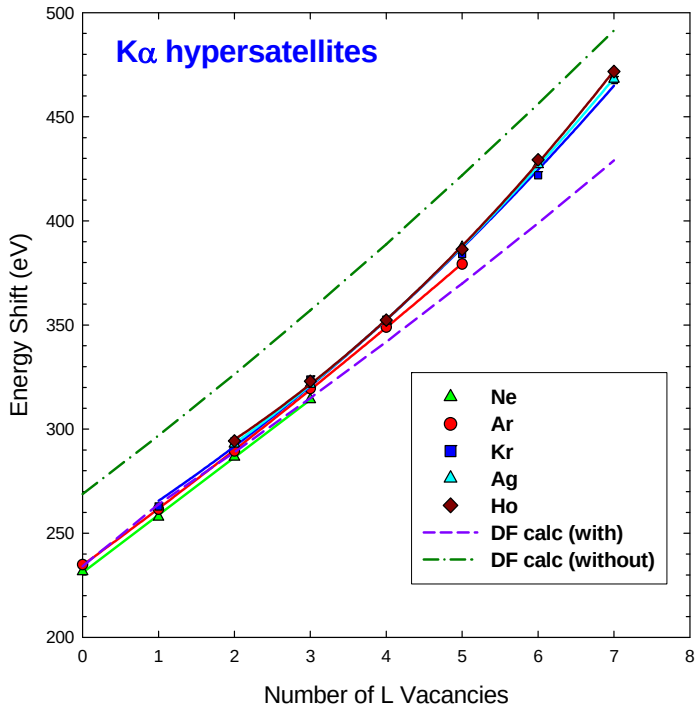

FIG. 2. The Kα hypersatellite average energy shifts measured relative to the average $K\alpha_{1,2}$ diagram peak energy. The dashed (purple) and dot-dashed (green) curves show the average Dirac-Fock energy shifts calculated for a vanadium atom with all outer-shell electrons present and absent, respectively.

It is reasonable to expect that the degree of outer-shell ionization should be related to the degree of inner-shell ionization, in which case the Kα satellite and hypersatellite energy shifts should correlate with p_L^x (the average fraction of L vacanies at the time of K x-ray emission). This was verified in Ref [4] for a variety of targets and projectiles. Plots of the satellite and hypersatellite energy shifts as a function of p_L^x using the current vanadium data are shown in Figs. 3 and 4, respectively. In the present work, the straight line least-squares fits displayed in these figures were extrapolated to predict the limiting energy shifts as p_L^x approaches zero. These energy shifts (ΔE_0) are presumed to be the energy shifts that would be observed if all outer-shell electrons were present. The calculated energy shifts for vanadium atoms with all outer-shell electrons present are shown by the diamond shaped points in Figs. 3 and 4. As may be seen from Fig. 3, the calculated energy shifts for the Kα satellites are systematically smaller (by 12 to 34%) than the experimental energy shifts. On the other hand, (as may be seen in Fig. 8) the agreement between the calculated (average-of-configuration Dirac-Fock) and experimental energy shifts is much better for the hypersatellites, with differences ranging from 2.8% to −1.0%.

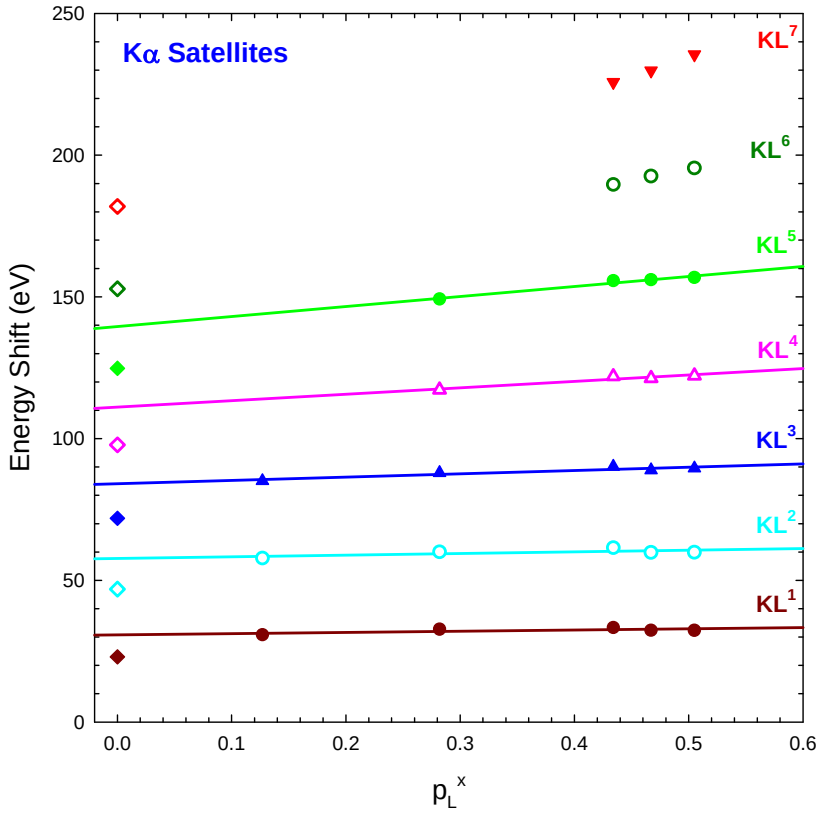

FIG. 3. The Kα satellite average energy shifts as a function of p_L^x. The results of straight line least-squares fits are shown by the solid lines and the average Dirac-Fock energy shifts calculated for vanadium atoms with all outer shell electrons present are shown by the diamond shaped data points at $p_L^x = 0$.

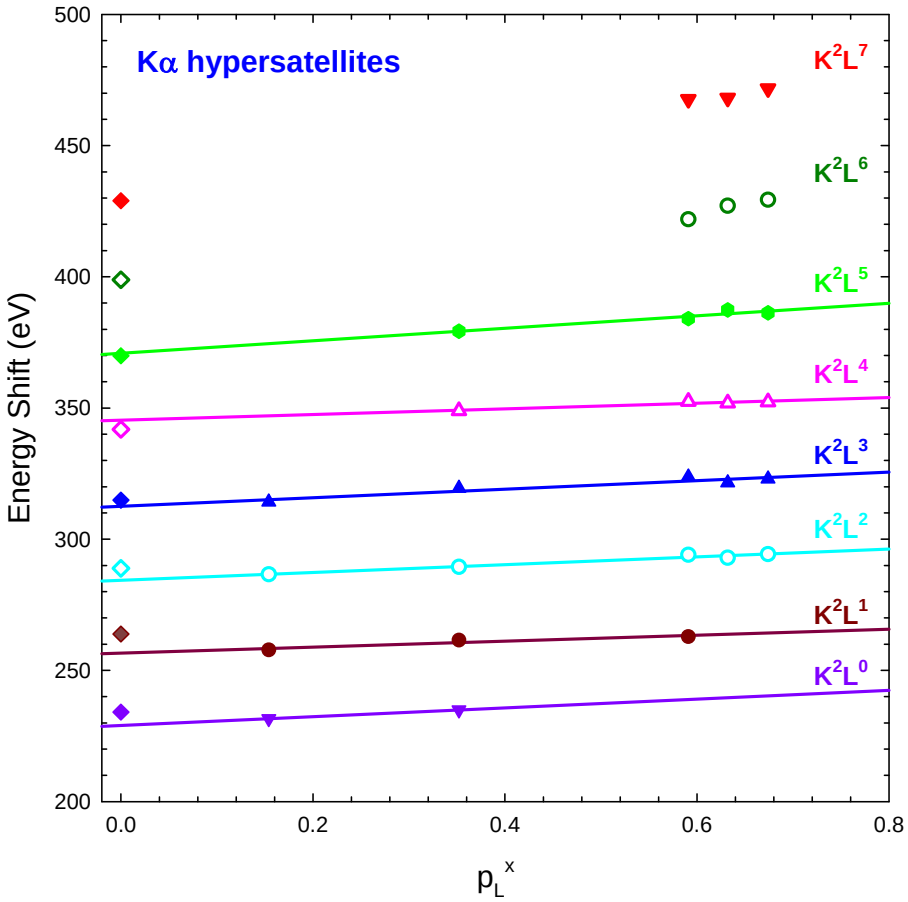

FIG. 4. The Kα hypersatellite average energy shifts as a function of p_L^x. The results of straight line least-squares fits are shown by the solid lines and the average Dirac-Fock energy shifts calculated for vanadium atoms with all outer shell electrons present are shown by the diamond shaped data points at $p_L^x = 0$.

The $K^2\alpha L^0$ hypersatellite is of particular interest since several authors have performed calculations for this case that take into account the Breit interaction [3, 5] and include radiative corrections from the most recent QED calculations [3]. The experimental value of the $K^2\alpha L^0$ hypersatellite energy shift is 229.0 ± 1.2 eV, which is in good agreement with the theoretical value of 228.0 eV[3].

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