

## Ca AND Ti $K_{\alpha}$ HYPERSATELLITES INDUCED BY PROTONS

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Characteristic X-rays from thick Ca and Ti targets induced by 1.5 — 1.7 MeV protons were analysed with a combined Bragg and solid state spectrometer. The energies of hypersatellite lines relative to the  $K_{\alpha}$  lines were determined experimentally and also calculated using the specific scaled hydrogenic model. The ratios of double to single  $K$ -shell ionization cross sections were measured and calculated using the binary encounter approximation. Data determined experimentally and theoretically agree within experimental error.

### 1. Introduction

Hypersatellites were observed for the first time in a high resolution study of  $K$  X-ray spectra obtained from Ca targets bombarded by 30 MeV oxygen ions<sup>1)</sup>. Since then, many similar experiments have been done, mostly using heavy ion beams<sup>2-4)</sup>, but also electron<sup>5,6)</sup> and photon beams<sup>7)</sup>. The two principle mechanisms responsible for inner shell vacancy production in ion atom collisions are direct ionization and electron transfer<sup>8,9)</sup>, the latter being important for near symmetric collisions. The classical impulse or binary encounter approximation (BEA)<sup>10)</sup>, the semiclassical approximation (SCA)<sup>11)</sup> and the quantum-mechanical

plane wave Born approximation (PWBA)<sup>1,2)</sup> have all been used to describe the direct ionization process. The predicted cross sections can be compared with measured ones, particularly in experiments where electron transfer is negligible. Experiments with low  $Z$  projectiles (protons, alpha particles), for which direct ionization represents the principal mechanism responsible for inner shell ionization, are therefore most easily described. But ionization cross sections for these projectiles are low and such measurements are experimentally more demanding than those with heavier ions. Thus, hypersatellites induced by proton beams of 0.25 to 2.0 MeV have been studied only for the light elements Be, B and O<sup>1,3)</sup>.

In the present work we describe a study of the hypersatellite X-rays induced by protons from Ca and Ti. Simple scaled hydrogenic model (SSHM) calculations of hypersatellite energies were performed for these and also for other light and medium light elements for comparative purposes.

## 2. Experiment

1.5 – 1.7 MeV proton beams were produced by the 2 MeV Van de Graaff accelerator of the *J. Stefan* Institute. Thick and selfsupporting Ca and Ti targets were oriented in a vacuum chamber at 45° with respect to the proton beam. The typical beam current was about 0.5  $\mu$ A. The proton induced X-rays passed out through a 7.5  $\mu$ m thick kapton window in the vacuum chamber. They were analysed in the first order with Bragg spectrometer and then detected in a semiconductor X-ray detector, which followed the rotation of the spectrometer crystal. A helium atmosphere outside the vacuum chamber was used to minimize the absorption of X-rays. Li-F ( $2d = 0.4093$  nm) and quartz ( $2d = 0.61$  nm) crystals were used for the analysis of Ca and Ti X-rays, respectively. The signals from the X-ray detector were amplified and then analysed in a ND 6600 computer, which was used as a multichannel analyser. The energy resolution of the counting system was determined by the energy resolution of the Bragg spectrometer, which was 15 eV at an X-ray energy of 3.69 keV. The  $\gamma$ -ray background originating from the accelerator was reduced by shielding the semiconductor detector with lead. The high energy resolution semiconductor detector ( $\Delta E = 160$  eV at 5.9 keV) was used to select X-rays having their energy determined by the first order Bragg reflection from the background and only the counts in the corresponding energy peak were counted. The number of X-rays selected in this way per unit proton dose with respect to the Bragg scattering angle was measured.

From such spectra — examples are shown in Figs. 1 and 2 — the energies of the  $K_{\alpha H}$  hypersatellite lines were determined with respect to the  $K_{\alpha}$  lines:

$$\begin{aligned} \text{Ca} \quad E_{K_{\alpha H}} - E_{K_{\alpha}} &= 193 \pm 5 \text{ eV} \\ \text{Ti} \quad E_{K_{\alpha H}} - E_{K_{\alpha}} &= 222 \pm 4 \text{ eV.} \end{aligned}$$

A small peak also appeared in the measured spectra below the  $K_{\beta}$  line (Figs. 1 and 2). The energy shift with respect to the  $K_{\beta}$  line is somewhat greater than the ionization energy for the electrons in the  $M$ -shell. Therefore this line can be attri-

buted to the second-order radiative Auger effect in which another electron is emitted simultaneously with a photon when a transition of an electron from the  $M$ -shell to the  $K$ -shell takes place.

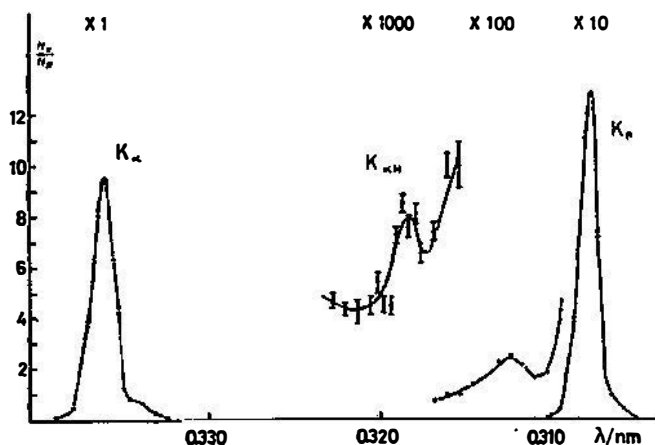


Fig. 1. X-ray spectrum from Ca between the  $K_{\alpha}$  and  $K_{\beta}$  lines at a proton energy  $E_p = 1.6$  MeV obtained by combined Bragg and semiconductor spectrometers.  $N_x$  is number of X-rays counted at proton dose  $N_p$ .

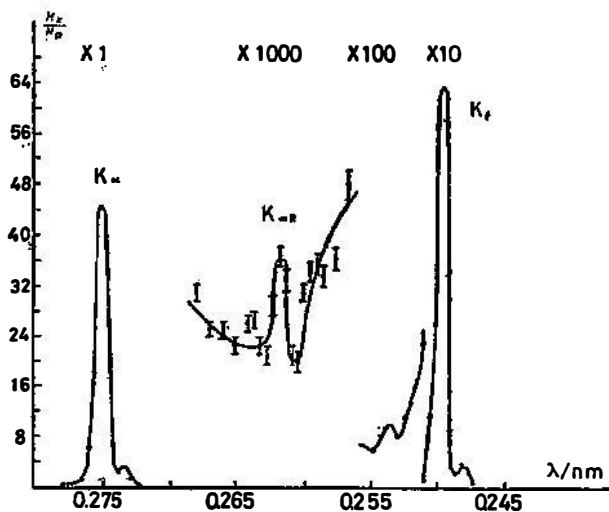


Fig. 2. X-ray spectrum from Ti at a proton energy  $E_p = 1.7$  MeV.

The ratio of the cross sections for production of the hypersatellite  $K_{\alpha H}$  to the characteristic  $K_{\alpha}$  X-ray for a particular element was determined taking into account

the corrections due to the beam-energy loss, as well as those due to the absorption of X-rays in the target material. The X-ray production cross section is then given by:

$$\sigma_x(E_p) = \frac{4\pi m_t}{\Omega \epsilon Q} ((dY/dE_p) \cdot (dE_p/dx) + \mu Y(E_p)).$$

Here  $m_t$  is atomic mass,  $\mu$  is the absorption coefficient for X-rays,  $(1/\rho)(dE_p/dx)$  is the stopping power of the target and  $\Omega \epsilon$  is the efficiency of the counting system.  $dY/dE_p$  is obtained by measuring the respective  $K_{\alpha H}$  or  $K_{\alpha}$  X-ray yields at two close proton energies  $E_p$ . In order to avoid errors in the determination of the efficiency  $\Omega \epsilon$ , only the ratios  $\sigma_{K_{\alpha H}}/\sigma_{K_{\alpha}}$  were determined. The results obtained from the measurements are shown in Table 2. Experimental error is mostly due to the error assigned to the measured values of  $dY/dE_p$ , which represent small differences of two measured X-ray yields at two close proton energies.

### 3. Comparison of experimental and theoretical results

The energies of hypersatellite lines were calculated by the specific scaled hydrogenic atomic model<sup>14-16</sup> which uses the virial  $w = \sum r_i \nabla_i W_p$  as the model potential energy operator. According to this simple atomic model, total atomic energies with arbitrary electron configuration can be easily calculated, using a simple and short iterative procedure. The X-ray energies are then given as the differences of the full energies of atoms before and after X-ray emission. The atomic energy is given by the expression:

$$W = - \sum_i Z_i^2 / (2n_i^2)$$

where  $n_i$  is the main quantum number and  $Z_i$  is the effective charge of the  $i$ -th electron. Effective charges are expressed in terms of internal and external screening parameters of  $i$ -th electron, respectively

$$Z_i = Z - \sum_{s < i} f_{is} - \sum_{t > i} g_{it}.$$

Here the  $t$ -th electron is more or equally bound and the  $s$ -th electron is less bound than the  $i$ -th electron. Procedures for calculating these parameters are given in Ref. 14. An HP 9825 A desk-top computer was used for all the necessary calculations.

The calculated energy differences  $E_{K_{\alpha H}} - E_{K_{\alpha}}$  are presented in Table 1. They are compared with the experimental data, as well as with the results of Hartree-Fock (*HF*) and Hartree-Fock-Slater (*HFS*) calculations. Numerical results obtained with this simple model agree well with the experimental data and also with those performed by *HF* calculations, but disagree with those obtained with the *HFS* model.

TABLE 1.

element	$(E_{K\sigma H} - E_{K\alpha})/eV$			
	experiment	SSHM	HF	HFS
Cu	$303 \pm 3$	296		
Ni	$292 \pm 3$	285		220
Fe	$268 \pm 2$	264		205
Mn	$272 \pm 20$	253	252	200
Ti	$222 \pm 4$	221		
Ca	$194 \pm 4$	200	202	157
Al	$124 \pm 5$	127	126	
Ne	$105 \pm 29$	96	96	
F	$83 \pm 18$	87	87	
O	$77 \pm 11$	78	78	
N	$68 \pm 6$	69	69	
C	$55 \pm 3$	61	60	
B	$48 \pm 1.5$	52	52	
Be	$37 \pm 0.5$	44		

The energies of hypersatellite lines with respect to the  $K_{\alpha}$  lines. Experimental values for Ca and Ti are from this work, others are taken from Ref. 5. The values denoted by *SSHM* are calculated by the specific scaled hydrogenic model (see text). The values obtained by *HF* and *HFS* models given in the last two columns are taken from Ref. 5.

If the fluorescence yields for atoms with one or two vacancies in the  $K$  shell are assumed to be equal, the ratios of the X-ray excitation cross sections are equal to the ratios of the ionization cross section. The ionization cross sections were calculated using the binary encounter approximation<sup>10)</sup>. The cross section for removing  $n_K$  electrons from the  $K$ -shell is given by equation<sup>17)</sup>:

$$\sigma_{nK} = \int_0^{\infty} 2 \pi b \binom{2}{n_K} P_K^{nK}(b) db.$$

Here  $b$  is the impact parameter and  $P_K(b)$  is the probability for removing an electron from the  $K$ -shell with a projectile having an impact parameter  $b$  if there is only one electron in the  $K$ -shell. In the *BEA* calculation  $P_K(b)$  is easily calculated using the expression:

$$P_K(b) = 2 \int_0^{\infty} \sigma(v_p, v_e(r_e)) \varrho_K(r_e) dz.$$

Here  $\varrho_K(r_e)$  is the probability density of the  $K$ -shell electron at radius  $r_e$ . The cross section  $\sigma(v_p, v_e(r_e))$  for removing the electron at  $r_e$  from the atom with a proton having a velocity  $v_p$  is given by the following expressions<sup>18)</sup>:

a) if  $U_i < 2m_e v_p (v_p - v_e)$ , then:

$$\sigma(v_p, v_e(r_e)) = \frac{2\pi e^4}{m_e v_p^2} (1/U_i + (m_e v_e^2)/(3U_i^2) - 1/(2m_e (v_p^2 - v_e^2))).$$

b)  $2m_e v_p (v_p - v_e) < U_i < 2m_e v_p (v_p + v_e)$

$$\sigma(v_p, v_e(r_e)) = \frac{\pi e^4}{m_e v_p^2} (1/(2m_e v_e (v_e + v_p)) + 1/U_i + m_e (2v_p^2 + v_e^2 - (2U_i/m_e + v_e^2)^{3/2})/(3v_e U_i^2)).$$

c)  $U_i \geq 2m_e v_p (v_p + v_e)$

$$\sigma(v_p, v_e(r_e)) = 0$$

where  $U_i$  is the ionization energy and  $m_e$  is mass of the electron.

TABLE 2.

element	$E_p$ MeV	$\sigma_{K\alpha II}/\sigma_{K\alpha}$	
		measured	BEA
Ca	1.65	$(4.1 \pm 3) \cdot 10^{-4}$	$5.28 \cdot 10^{-4}$
Ti	1.6	$(4.0 \pm 2) \cdot 10^{-4}$	$3.55 \cdot 10^{-4}$

The measured ratios of the double to the single  $K$ -shell ionization for Ca and Ti (first column) and those calculated using the BEA method (second column).

In Table 2 the calculated ratios of the respective cross sections with those determined experimentally are compared. Calculated values agree with experimental ones within experimental error. It is also worth comparing these results with those obtained on Ca atoms ionized with oxygen ions<sup>2,17</sup>). There, the experimental value of ratio is three times lower than the calculated one. So, as expected, because in the BEA we take into account only the direct ionization process and neglect polarization effects, the method is more accurate for the description of the ionization process produced by low  $Z$  projectiles.

#### References

- 1) P. Richard, W. Hodge and C. F. Moore, Phys. Rev. Lett. **29** (1972) 393;
- 2) D. K. Olsen and C. F. Moore, Phys. Rev. Lett. **33** (1974) 194;
- 3) Y. Awaya, T. Katou, H. Kumagai, T. Tonuma, Y. Tendow, K. Izumo, A. Hashizume, T. Takahashi, T. Hamada, Phys. Lett. **75 A** (1980) 478;
- 4) J. Hall, P. Richard, T. J. Gray, K. Jones, B. Johnson and D. Gregory, Phys. Lett. **90 A** (1982) 129;
- 5) J. P. Briand, A. Touati, M. Frilley, P. Chevallier, A. Johnson, J. P. Rozet, M. Tavernier, S. Shafroth and M. O. Krause, J. Phys. B: Atom. Molec. Phys. **9** (1976) 1055;

- 6) S. I. Salem: Phys. Rev. A **21** (1980) 858;
- 7) O. Keski-Rahkonen, J. Saijonmaa, M. Suvanen and A. Servomaa, Phys. Scr. **16** (1977) 105;
- 8) J. Hall, P. Richard, T. J. Gray, C. D. Lin, K. Jones, B. Johnson and D. Gregory: Phys. Rev. A **24** (1981) 2416;
- 9) J. Hall, P. Richard, T. J. Gray, J. Newcomb, P. Pepmiller, C. D. Lin, K. Jones, B. Johnson, D. Gregory: Phys. Rev. A **28** (1983) 99;
- 10) M. Gryzinski, Phys. Rev. **138** A (1965) 336;
- 11) J. Bang and J. M. Hansteen, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. **31** (1959);
- 12) E. Merzbacher and H. W. Lewis, *Handbuch der Physik*, edited by S. Flugge, **34**, 166, Berlin, Göttingen, Heidelberg: Springer 1958;
- 13) K. Kawatsura, K. Ozawa, F. Fujimoto and M. Terasawa, Phys. Lett. **64** A (1977) 282;
- 14) M. Kregar, Physica Scripta **29** (1984) 438;
- 15) M. Kregar, Physica C **113** (1982) 249;
- 16) M. Kregar, Fizika **14** (1982) 327;
- 17) J. H. McGuire and P. Richard. Phys. Rev. A **8** (1973) 1374;
- 18) L. Vriens. Proceed. Phys. Soc. **90** (1967) 935.

## S PROTONI INDUCIRANI HIPERSATELITI V Ca IN Ti

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S kombiniranim Braggovim in Ge-Li rentgenskim spektrometrom so bile določene energije hipersatelitskih rentgenskih črt  $K_{\alpha H}$  in izmerjeno razmerje presekov za dvojno in enojno vzbujanje lupine  $K$  v Ca in Ti s 1,5–1,7 MeV protoni. S specifičnim atomskim modelom so bile izračunane energije hipersatelitskih rentgenskih črt. Razmerje presekov je bilo izračunano s semiklasičnim modelom. Teoretični in eksperimentalni rezultati se ujemajo v okviru eksperimentalnih napak.