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Excitation of the Cs-5p Core Level in Cs Halides

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New electronic transitions from the Cs$^+$5p core level were found for all Cs halides by studying their reflection spectra for photon energies between 10 and 30 eV using synchrotron radiation.

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Core transitions of the Cs halides associated with the 5p level of the Cs^+ ion are expected to start at photon energies of about 13 eV. At 13.2 eV the first transition of the free Cs^+ ion is observed [1]. The optical transitions of the Cs halides have recently been studied between 10 and 25 eV by means of thin film absorption [2]. Since a line source has been used in this work and because of theoretical considerations, it was questionable whether the resolution was sufficient to resolve all spectral structure.

We have, therefore, measured the reflection spectra of all Cs halides using the synchrotron radiation of the Deutsches Elektronen-Synchrotron DESY. The measurements were performed at room temperature for 15° angle of incidence between 10 and 30 eV with a resolution of 2 Å over the entire energy range. The Cs halides were evaporated in situ onto glass slides at a pressure of 10^{-8} Torr. The experimental results are shown in Fig. 1.

In comparison to the absorption spectra [2] the reflection spectra show considerably more spectral details which are listed in Table 1. The most prominent feature, the pronounced peak at about 13.4 eV with a half-width of approximately 0.3 eV, was already known. It is found for all Cs halides at almost the same position. It is, therefore, attributed to the first excitonic transition from the Cs^+5p level. A spin orbit partner, associated with the first strong line, can be identified at about 15.1 eV. It is separated in energy by 1.7 eV in agreement with the spin orbit splitting of the 5p level of the free Cs^+ ion [1]. Above 17 eV two broad bands are observed. For CsCl, for instance, they are located around 19 and 24 eV. In general, corresponding peaks are shifted to smaller energies with an increasing atomic number of the halide (cf. Table 1). Beyond 25 eV, an energy which roughly coincides with the ionization limit of the singly ionized Cs atom (25.1 and 26.8 eV respectively), the reflectivity continuously decreases without significant structure.

As in the case of the Na^+2p [3] and K^+3p [4] excitation in alkali halides it should be possible to explain the observed Cs halide spectra in terms of excitons or interband transitions. Band structure calculations are published only for CsI [5, 6]. We have tried to assign the main peaks of the CsI spectrum to excitons at symmetry points in the Brillouin zone, but we could not obtain a conclusive correlation concerning energy positions of excitons.

A comparison with the free ion excitations, however, led to the suggestion that the first five marked peaks (or shoulders) between 13 and 17 eV could be attributed to the five lowest free ion transitions which are allowed in j-l-coupling, taking into account the selection rule $J=0 \rightarrow J=1$ for the total angular momentum. A tentative correspondence between the excitations of the solid and free ion is established in column 5 of Table 1. For this assignment one has to assume that the two s-transitions are approximately unaffected by the crystal field, while the three d transitions are shifted by about 1 eV to higher energies. A similar quintet-like structure has very recently been observed for all Rb halides between 16 and 19 eV, where the lowest transitions from the Rb^+4p level occur [7].

References

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Note added and proof:

H. Saito and R. Onaka (J.Phys.Soc. Japan 28, 1380 (1970)) have recently measured the absorption spectrum of CsI between 12 and 18 eV, which exhibits fine structure similar to that found in the reflection spectrum.

CsF	CsCl	CsBr	CsI	free Cs$^+$ transition	
	10.0	9.6	10.1		
12.4 s	11.3	11.2	10.9		
12.7	12.7	12.7 s			
13.6	13.3	13.3	13.2	6s [3/2]	13.4
			13.4 s		
14.3	14.3 s	14.3	14.0	5d [1/2]	13.2
	14.7	14.7	14.5	5d [3/2]	13.8
15.3	15.1	15.0	14.9	6s' [1/2]	15.2
			15.2 s		
17.5	16.7	16.6	16.4	5d' [3/2]	15.3
	17.9 s	17.7	17.0		
18.6	18.9	18.8 s	17.9		
20.0	19.8 s	19.6 s	19.3 s		
21.0 s			21.0		
		≈22.0 s	21.6		
23.5 s	23.2	23.2	23.0 s		
25.9	24.0 s		24.1 s		

Table 1: Position of the reflection maxima (in eV) for all Cs-halides (column 1 - 4, accuracy ± 0.05 eV for the sharp maxima). Shoulders are denoted by s. Tentative correlation with transition energies of the Cs$^+$ free ion: $5p^6$, $J=0 \rightarrow 5p^5\, n\ell\, [K]\, J=1$ according to reference 1 (column 5).

Figure Caption

Fig. 1: Reflection spectra of evaporated Cs halides. The horizontal lines on the ordinate (linear scale) mark the level of zero reflectance for every substance.

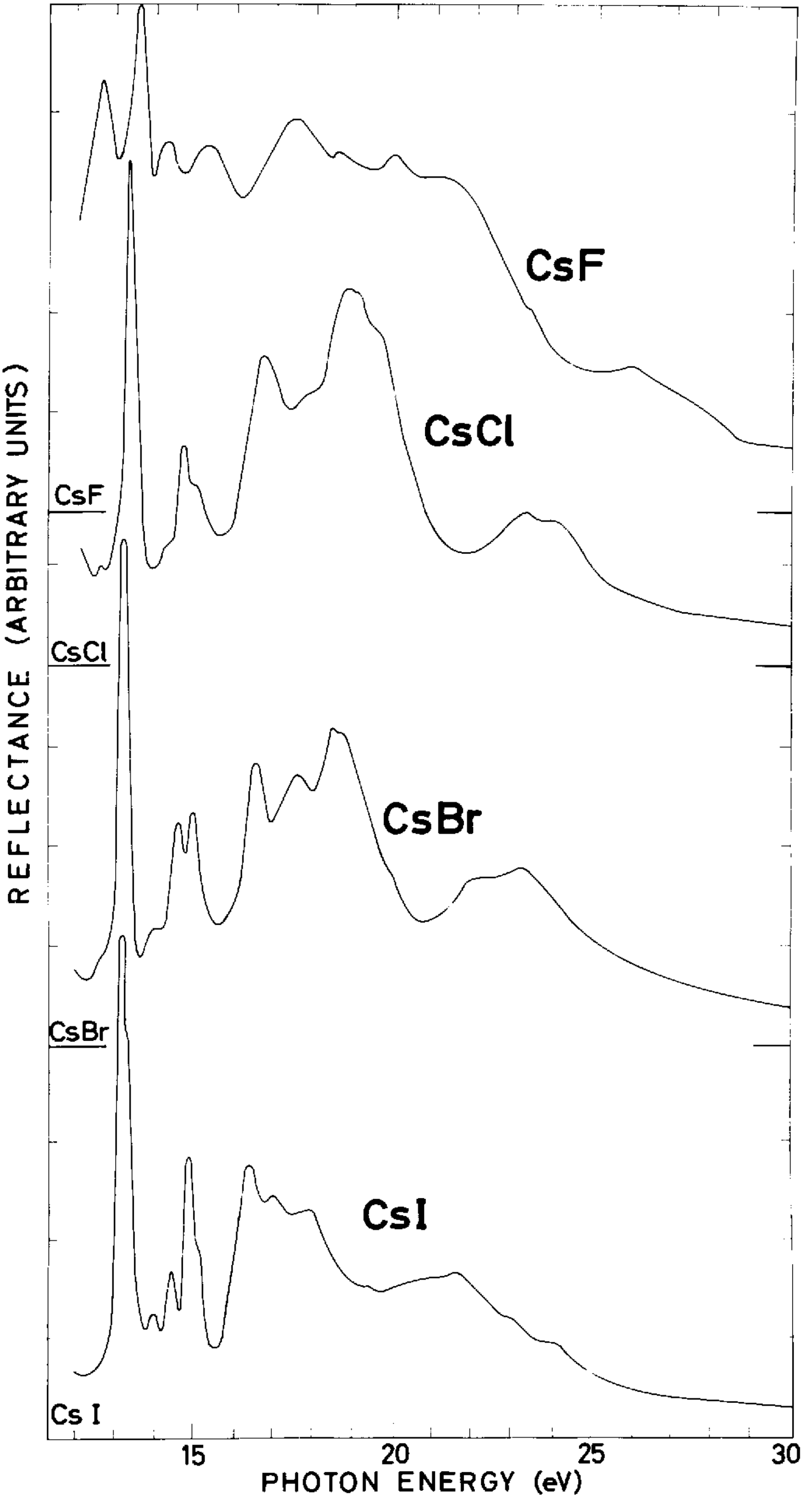
REFLECTANCE (ARBITRARY UNITS)
CsF
CsCl
CsBr
CsI
CsF
CsCl
CsBr
Cs I
15
20
25
30
PHOTON ENERGY (eV)

Fig. 1