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2 HAMBURG 52 · NOTKESTIEG 1

DIELECTRIC PROPERTIES OF KCl, KBr, and KI SINGLE CRYSTALS IN THE EXTREME ULTRAVIOLET UP TO 35 eV

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The reflectance of freshly cleaved single crystals of KCl, KBr, and KI has been measured for 15° angle of incidence at room temperature for photon energies between 5 and 35 eV, using the continuous spectrum of synchrotron radiation. For photon energies from 12 to 30 eV the optical constants, the dielectric constant, and the energy loss function were determined by reflectance measurements with parallel polarized light at several angles of incidence between 15° and 75°. A prominent doublet near 20 eV is found for all potassium halides. It is assigned to excitonic transitions from the K^+3p core level to the conduction band at Γ and X. Energy differences between some critical points at Γ and X are estimated by comparing the position of the fundamental doublet and the K^+3p doublet.

Die Reflektivität frisch gespaltener KCl-, KBr- und KJ-Einkristalle wurde bei 15° Einfallswinkel und Zimmertemperatur für Photonenenergien zwischen 5 und 35 eV gemessen. Als Lichtquelle diente das Kontinuum der Synchrotronstrahlung. Für Photonenenergien zwischen 12 und 30 eV wurden optische Konstanten, die Dielektrizitätskonstante und die Energieverlustfunktion aus Reflexionsmessungen mit parallel polarisiertem Licht bei mehreren Einfallswinkeln zwischen 15° und 75° bestimmt. Ein ausgeprägtes Dublett bei 20 eV findet man bei allen Kaliumhalogeniden. Es wird Exziton-Übergängen vom K^+3p Rumpfniveau zum Leitungsband bei Γ und X zugeordnet. Energiedifferenzen zwischen einigen kritischen Punkten bei Γ und X werden näherungsweise durch Vergleich der Lagen des Fundamentaldubletts und des K^+3p-Dubletts berechnet.

I. INTRODUCTION

The alkali halides show a rich spectrum of electronic excitation in the vacuum ultraviolet (vuv). Numerous investigations on single crystals and thin films have been performed at room temperature as well as at low temperatures for photon energies below 12 eV in order to study the fundamental absorption due to transitions from the halide valence band to the lower parts of the conduction band.[1] The resonances are interpreted as excitons or interband transitions at special points of high symmetry in the Brillouin zone. Though the resonances near the onset of absorption seem to be identified unambiguously, the assignments at higher energies are not yet certain.

For photon energies between 12 and 40 eV only few experiments have been undertaken at room temperature. Excitations from the first core states below the valence band now become energetically possible. For the study of alkali halide spectra in this range, only line sources have been used so far which are inconvenient when high spectral resolution is required as in the case of alkali halides. Synchrotron radiation offers a continuous spectrum of high intensity over the whole vuv-region which is ideally suited for such investigations.

In this work we have studied the reflectance spectra of the potassium halides KCl, KBr and KI between 5 and 35 eV at room temperature by means of the synchrotron radiation of the Deutsches Elektronen-Synchrotron.[2,3] We were mainly interested in the region beyond 20 eV where electronic transitions from

the K^+3p core level to the conduction begin to contribute to the absorption. The fundamental reflectance spectra of the potassium halides, beginning at about 6 eV, have been studied extensively by many authors.[1] Recent band calculations for KCl [4-7], KBr [8], and KI[9] have given new incentive for interpretation of the rich structure observed. When this work was initiated only a few investigations on single crystals had been undertaken at room temperature with line sources up to about 25 eV.[10-13] During the performance of this work Stephan and coworkers have published new data on KF [14], KCl [15], and KBr[16] single crystals up to 40 eV using a line source.

Above 12 eV we have derived the complex optical constant n+ik, and the dielectric constant $\varepsilon_1+i\varepsilon_2$ respectively, by the reflectance vs. angle of incidence method[17] from reflectance data in parallel polarized light. In all previous investigations the standard technique was to determine the dielectric constant by a Kramers-Kronig (KK)-analysis of the near normal incidence reflectance, a method first applied to the potassium halides by Philipp and Ehrenreich.[10] We have used the multiangle reflectance method since in contrast with the KK-analysis it was thus possible to obtain values independent of those determined at neighbouring photon energies together with an estimation of an absolute error.

II. EXPERIMENT, EVALUATION, AND RESULTS

The synchrotron radiation of the Deutsches Elektronen-Synchrotron[2,3] in Hamburg together with a normal incidence monochromator in a modified Wadsworth mount[18] provided the polarized vuv continuum for our reflectance measurements. The experiment was performed by use of a reflectometer[19] and a technique described earlier.[20] The degree of polarization of the incident light, $(J_{\parallel}-J_{\perp})/(J_{\parallel}+J_{\perp})$, was about 0.98. The single crystals freshly cleaved before mounting into the sample holder were provided by Karl Korth, Kiel, Germany. The pressure during the reflectance measurement was about 5×10^{-8} Torr. The reflectance was determined at room temperature for angles of incidence from 15° to 75° in steps of 7.5° for both parallel (p) and perpendicular (s) polarized light, with the normal of the sample lying on both sides of the incident beam for increased accuracy. The optical constants were calculated with a digital computer (IBM 360/75) by minimizing the mean square deviation between measured and calculated reflectance ratios.[20]

Figure 1 shows the reflectance spectra of KCl, KBr, and KI for 15° angle of incidence in p-polarized light at photon energies between 12 and 35 eV. In table 1 the position of the prominent features of the 15° reflectance spectra together with some commonly adopted interpretation are listed for energies from 6 to 35 eV. We have not reproduced the spectra below 12 eV because we did not determine absolute reflectance values in this region. The energetic position of special features, however, such as the first exciton peaks were obtained with an accuracy of about ± 10 Å (i.e. ca. ± 0.03 eV at

about 6 eV) throughout this part of the spectrum. Below 12 eV we used LiF and above 25 eV tellurium as a filter to avoid stray light or second order.

In fig. 2 the optical constants, the index of refraction n and the absorption coefficient k, are drawn for photon energies between 12 and 30 eV. The low reflectance above 30 eV did not allow to determine optical constants with reasonable accuracy up to 35 eV. The optical constants were calculated from p- as well as from s-measurements. As expected from Hunter's analysis,[17] the values obtained from p-measurements showed a much better convergence, therefore we took these values as the final results. We have calculated the optical constants for every two Å in wavelength, a value corresponding approximately to the band width of our monochromator (3 Å). An average absolute error for n and k, $\Delta n \sim \pm 0.02$ and $\Delta k \sim \pm 0.02$, was estimated by comparing the spectral behaviour of the measured reflectances and those recalculated with the best n- and k-values. For KI the error Δk was somewhat larger, namely $\sim \pm 0.04$. No errors have been reported, when the optical constants were determined by KK-analysis. In fig. 3 the dielectric constants $\varepsilon_1, \varepsilon_2$ and the energy loss function $|\mathrm{Im}\varepsilon^{-1}|$ are presented.

As expected n and k (fig. 2) and ε_1 and ε_2 (fig. 3) show the well known dispersion behaviour at each resonance energy. In a KK-analysis of reflectance data such a dispersion behaviour is a direct consequence of the dispersion integral while in our case the correct dispersion behaviour demonstrates the

accuracy of our measurements and of the analysis based upon the multiangle reflectance method.

Comparison between the broad maxima of the reflectance R, of the absorption coefficient k, ε_2 and $|\mathrm{Im}\varepsilon^{-1}|$ shows that if one considers the position of the reflectance peaks, the corresponding maxima of k and ε_2 are shifted by about 0.2 eV to smaller energies, the corresponding peaks of $|\mathrm{Im}\varepsilon^{-1}|$ by a maximum of 1 eV to higher energies. For the sharp reflectance doublet near 20 eV, however, the maxima of R, k, ε_2 and $|\mathrm{Im}\varepsilon^{-1}|$ lie much closer together.

The ε_2-spectrum, which is the primary one obtained by theory, gives the exact positions of the resonances. In section IV, however, where the location of resonances are discussed, we will use the reflectance spectra keeping in mind the differences between R, k, and ε_2. The reflectance can be compared directly with measurements of other authors, and we do not intend an accuracy better than about 0.1 eV in determining resonance energies.

III. COMPARISON WITH PREVIOUS RESULTS ABOVE 12 eV

The general spectral behaviour of the near normal reflectance found in this work agrees quite well with the results up to 25 eV of WNNM[11] on KCl, KBr, and KI and of RW[12] on KCl and with the results up to 40 eV obtained by Stephan and coworkers on KCl[15] and KBr[16]. Within the accuracy with which their figures could be read, the main peaks have the same position (cf. fig. 1 and table 1) and similar relative heights. The older data of PE[10] on KCl, KBr, and KI up to 25 eV agree well with our results for KCl only. In agreement with WNNM[11] and SR[15] we observed on KCl a maximum at 19.5 eV lying on the flank of the much stronger 20.1 eV peak. This weaker maximum has not been resolved by PE[10] and RW[12]. For KBr SGR[16] seem to have detected weak maxima at 22 and 24 eV which we could not observe. Around 22 eV we found only a saddle like decrease of the reflectance, similar to the results of WNNM[11]. The shoulder in the KI spectrum associated with the sharp peak at 20.2 eV (fig. 1) has not been seen before.

Differences in the absolute reflectance values may best be discussed for the most remarkable feature of the spectrum, that is the doublet near 20 eV observed for all potassium halides. For the second, somewhat greater peak of the KCl-doublet at 21.1 eV, WNNM[11] give a reflectance of 10 %, RW[12] 12 %, SR[15] 8.5 %, whereas we have obtained 10 % for p-polarized light and 15° angle of incidence. These differences may be explained by different surface conditions, by different angles of incidence, at which the so called near normal incidence measurements were

performed, or by different degrees of polarization. Additionally if no continuum source is available, an exact determination of the maximum reflectance may be difficult for sharp peaks since a large number of spectral lines is needed for this purpose. For the second peak of the KBr doublet at 21.3 eV, which is more significant than the first one at 19.9 eV, WNNM[11] obtained a reflectance of ∿7 %, SGR[16] ∿6 %, and we ∿8 %. For the KI doublet WNNM[11] measured about 4 %, and we 5 %. In the average our values agree better with those of WNNM[11] and RW[12] than with those of Stephan and coworkers.

The spectral shape of the dielectric constants ε_1 and ε_2 calculated for KCl and KBr by KK-analysis is quite similar to that calculated in this work by the reflectance vs. angle of incidence method. The main difference between the data of Stephan and coworkers for KCl and KBr and ours is that our ε_1 is always smaller by about 0.3 whereas the ε_2 differ at most only by about 0.1. These differences are probably related to the smaller reflectance observed by Stephan and coworkers. Between 12 and 20 eV our results on KCl agree better with those of RW [12]. Above 20 eV their data are probably influenced by an incorrect extrapolation, since they did not measure up to 29 eV where another marked maximum was found in reflectance.

The spectral shape of the energy loss functions $|\mathrm{Im}\varepsilon^{-1}|$ derived from ε_1 and ε_2 (fig. 3) agrees quite well with that given by Stephan and coworkers for KCl and KBr and that obtained by Creuzburg[21] and Keil[22], who measured the energy loss of fast

electrons penetrating thin evaporated films (cf. table 2). Our values for $|Im\varepsilon^{-1}|$ are larger than those given by Stephan and coworkers by about 0.3 and 0.2 for KCl and KBr respectively, the main reason for which, is our smaller ε_1. The most reliable absolute values for $|Im\varepsilon^{-1}|$ of KCl and KBr obtained from optical experiments by different authors do not differ by more than 30 %, whereas the values obtained by energy loss experiments are about a factor of 2 larger. This discrepancy is not yet explained satisfactorily.

IV. INTERPRETATION

A first glance at the reflectance spectra (fig. 1) shows some similarities in the spectral structure of the sequence of the potassium halides KCl, KBr, and KI. After the region of the plasma energy (12 - 14 eV), associated with a steep decrease of reflectance and a corresponding maximum of $|Im\varepsilon^{-1}|$, some peaks follow probably still due to transitions from the valence band into the conduction band. At about 20 eV all spectra show a prominent reflectance doublet of much smaller half width than found for the neighbouring maxima. The energetic position, the small half width and the fact that the peak positions are nearly independent of the halogen ion, have led to the suggestion that we observe here [1] Γ- and X-excitons excited from the K^+3p core level. Above this doublet we find two or three other broader maxima of medium reflectance. At about 30 eV the reflectance decreases significantly, which is associated with a second prominent peak [1] in the $|Im\varepsilon^{-1}|$ spectrum. Beyond this region some weaker broad peaks can be found. Most of the structure above

20 eV may be assigned to transitions from the K^+3p level to the conduction band.

The doublet occurs for KCl at 20.1 / 21.4 eV, for KBr at 19.9 / 21.3 eV, and for KI at 20.2 / 21.2 eV. The spectral width of each line is about 0.4 eV, measured at 3/4 of the maximum reflectance. The doublet lines are somewhat broader than the width found in the first exciton lines where the fundamental absorption begins. In analogy with those excitons, the doublet may be assigned to excitonic transitions associated with $K^+3p \rightarrow \Gamma_6^+$ and $K^+3p \rightarrow X_7^+$. (cf. the band scheme for KI as calculated by OOI[9], fig. 4). The corresponding fundamental Γ, X-exciton doublet ($\Gamma_8^- \rightarrow \Gamma_6^+$, $X_7^- \rightarrow X_7^+$) lies at 7.68 / 9.59 eV for KCl, 6.58 / 8.61 eV for KBr and 5.61 / 6.67 eV for KI (cf. table 1). If one assumes equal binding energies for the Γ and X-exciton, the energy difference between X_7^+ and Γ_6^+ can be calculated as 1.3, 1.4, 1.0 eV for KCl, KBr, and KI resp., since the K^+3p level is assumed to be flat. Stephan and coworkers[15],[16] have deduced from their measurements 1.2 eV for KCl and 1.4 ev for KBr. The values obtained from band calculations are 1.22 eV[6] and 2.3 eV[7] for KCl, 2.2 for KBr[8], and 0.62 eV for KI[9] (compare table 3).

Combining the values of the position of the fundamental and K^+3p exciton doublet, one can calculate further under the same assumptions, the bending of the upper valence band, i.e. the energy difference $\Gamma_8^- - X_7^-$: 0.65, 0.28, and -0.13 eV for KCl, KBr, and KI respectively. Theoretical values from band calculations are 0.24 eV[4]; 0.16 eV[6], and 0.12 eV[7] for KCl, ~0.0 eV[8] for KBr, and 0.23 eV[9] for KI. In both cases the agreement between experi-

ment and band calculation is rather poor. The reason may be that the assumptions leading to the experimental numbers are oversimplified, or that the band calculations so far available are not accurate enough. Especially the negative value of Γ_8-X_7 for KI seem rather dubious, since it means that Γ is not the maximum of the valence band. One should also consider that an accuracy better than 0.1 eV cannot be reached in deriving energy differences from reflectance maxima, when resonances become broad (cf. end of Section II). Use of low temperature data may help to refine the experimental values for the characteristic energy differences.

If we assume equal binding energies for the excitons originating from the valence band and the K^+3p core level at the point Γ in the Brillouin zone, we obtain for the energy distance from Γ_8^- (halogen ion level) to Γ_8^-, Γ_6^- (K^+3p) $\sim$12.4, 13.3, and 14.6 eV for KCl, KBr, and KI respectively. Band calculations yield $\sim$13.0 for KCl[4] and 15.0 for KI [9].

On the low energy side of the Γ-exciton of KCl (20.1 eV) and KI (20.2 eV) shoulders with a difference of 0.6 and 0.3 eV to the main peak can be seen. The smaller difference for KI with a value of 0.3 eV suggests that we observe here the spin orbit splitting of the K^+3p level (cf. fig. 4), which has been detected so far only for KBr[22] in energy loss experiments at liquid nitrogen temperature. The spin orbit splitting for the free K^+ ion is 0.27 eV. The distance of the KCl-shoulder is too large to be attributed to a spin orbit splitting. Observation on

mixed KCl-KBr crystals[11] indicate that this peak can be assigned to transitions from the valence band, since the corresponding peak for KBr is shifted to smaller energies. Low temperature experiments may help to resolve spin orbit splitting in all doublets.

Although transitions from the valence band and the K^+3p core level are governed by the same selection rules for angular momentum (both initial states are p-like) we were not able to establish an unequivocal correspondence between the less prominent peaks of the fundamental region and those of the core excitation region as has been tried for KF [14]. Obviously one could not expect to find a one to one correspondence for all peaks. The valence band formed by the anion p-electrons shows a strong wave vector dependence and a spin orbit splitting, whereas the K^+3p core level is completely flat and its spin orbit splitting is only about 0.3 eV. Furthermore the wavefunctions for the valence band and the K^+3p band are probably too different to yield comparable matrix elements for transitions at the same point in the Brillouin zone. We have tried to attribute some peaks beyond the doublet at 20 eV to singularities in the conduction band calculated by A.B. Kunz[7,8] and OOI[9], but all assignments we made did not seem very convincing because of ambiguity or lack of agreement in energy.

For KCl and KBr Stephan and coworkers have discussed recently the onset of excitation of two electrons by one photon at an energy which is the sum of the band gap differences Γ_8^- (halogen) $\rightarrow \Gamma_6^+$ and $K^+3p \rightarrow \Gamma_6^+$. They expect this process at about 28.5 for

KCl[15] and 27.8 eV for KBr [16]. We do not find any remarkable steps of absorption (k or ε_2) but only an absorption peak at this energy so that we are not sure that such a process takes place. In the sodium chlorides where such a process was first suggested[23] the situation is somewhat different since a significant step in the absorption coefficient has been found at about the expected energy when the Na^+2p core excitations were studied experimentally.[24] Theoretical investigations on double excitations give contradictory results for the probability of such a process.[25,26]

V. SUMMARY

We have studied the reflectance spectra of KCl, KBr, and KI single crystals at room temperature with the continuum of synchrotron radiation for photon energies between 6 and 35 eV. Above 12 eV we derived from measurements with parallel polarized light the optical constants, the dielectric constants and the energy loss function by means of the reflectance vs. angle of incidence method. An absolute error for n and k could be estimated. We compared our results to those obtained recently on KCl and KBr by the use of line sources and Kramers-Kronig-techniques. So far as the shape of the electronic spectra of KCl and KBr is concerned, our results agree quite well with those measurements except for details which are probably more easily resolved with a continuous source. Larger differences were found for the absolute magnitude of R, n, k, ε_1 ε_2 and $|\mathrm{Im}\varepsilon^{-1}|$.

The most prominent feature of all reflectance spectra is the strong doublet at about 20 eV which is assigned to a Γ_6^+- and a X_7^+-exciton, the initial state being the K^+3p core level. The

first member of the KI doublet shows a shoulder 0.3 eV apart from the main maximum which is probably due to the spin orbit splitting of the K^+3p level. Beyond the doublet some weaker characteristic peaks are found up to 30 eV. The reflectance then begins to decrease markedly. Transitions from the K^+3p core level to the conduction band seem responsible for the spectral behaviour above 20 eV.

The energy differences $X_7^+ - \Gamma_6^+$ (conduction band), and $\Gamma_8^- - X_7^-$ (valence band), as well as the separation between the top of the valence band and the K^+3p core level were estimated from the position of the reflectance maxima of the fundamental and the corresponding K^+3p exciton doublet. Hereby equal binding energies for all excitons were assumed. The values obtained were compared to those from band calculations. For a more accurate interpretation, further theoretical investigations on band structure of the potassium halides and exciton binding energies, as well as measurements at low temperatures in the extreme ultraviolet are necessary.

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Figure captions

Fig. 1 Reflectance spectra of KCl, KBr, and KI single crystals at 15^{o} angle of incidence for parallel polarized light at room temperature. The arrow indicates the plasma energy, where $|\mathrm{Im}\varepsilon^{-1}|$ has its most prominent peak.

Fig. 2 Index of refraction n and absorption coefficient k for KCl, KBr, and KI derived with the reflectance vs. angle of incidence method. Full line k, dashed line n.

Fig. 3 The dielectric functions ε_1, ε_2 and $|\mathrm{Im}\varepsilon^{-1}|$. Full line ε_2, dashed line ε_1, dotted line $|\mathrm{Im}\varepsilon^{-1}|$.

Fig. 4 Sketch of a part of the band structure of KI as calculated by OOI[9]. Only the lowest part of the conduction band is drawn.

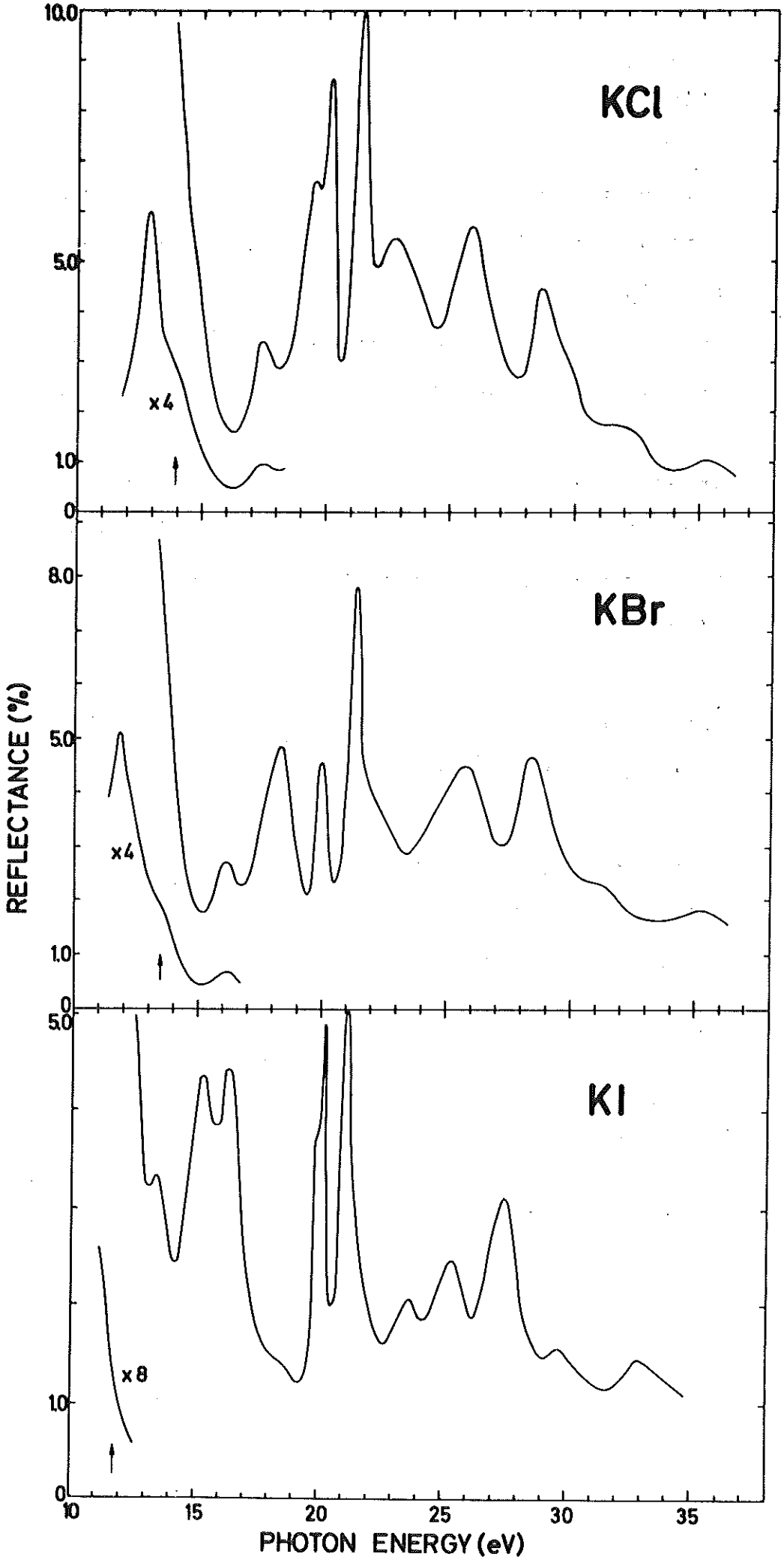
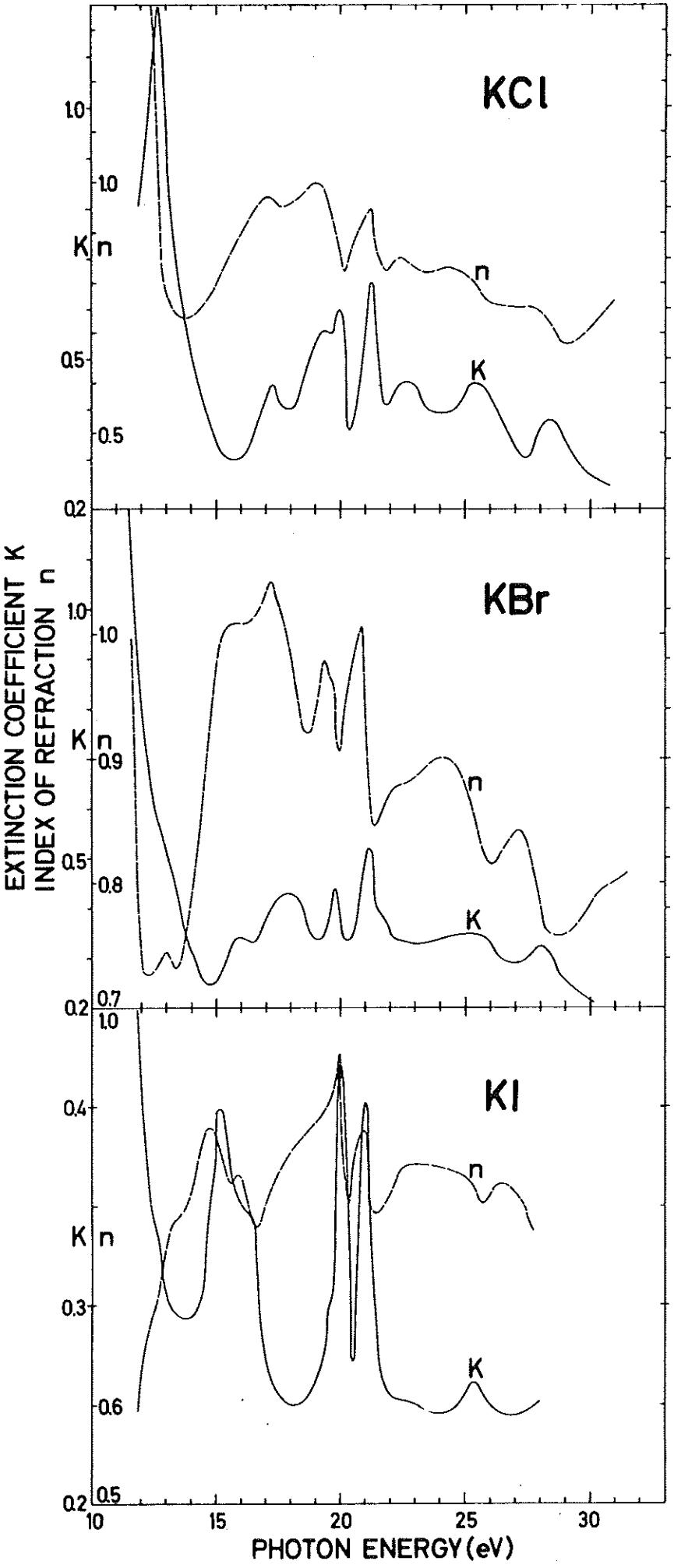

KCl
KBr
KI
x4
x4
x8
REFLECTANCE (%)
PHOTON ENERGY (eV)
10.0
5.0
1.0
0
8.0
5.0
1.0
0
5.0
1.0
0
10
15
20
25
30
35

Fig. 1


KCl
KBr
KI
n
K
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INDEX OF REFRACTION n
PHOTON ENERGY (eV)
10
15
20
25
30

Fig. 2

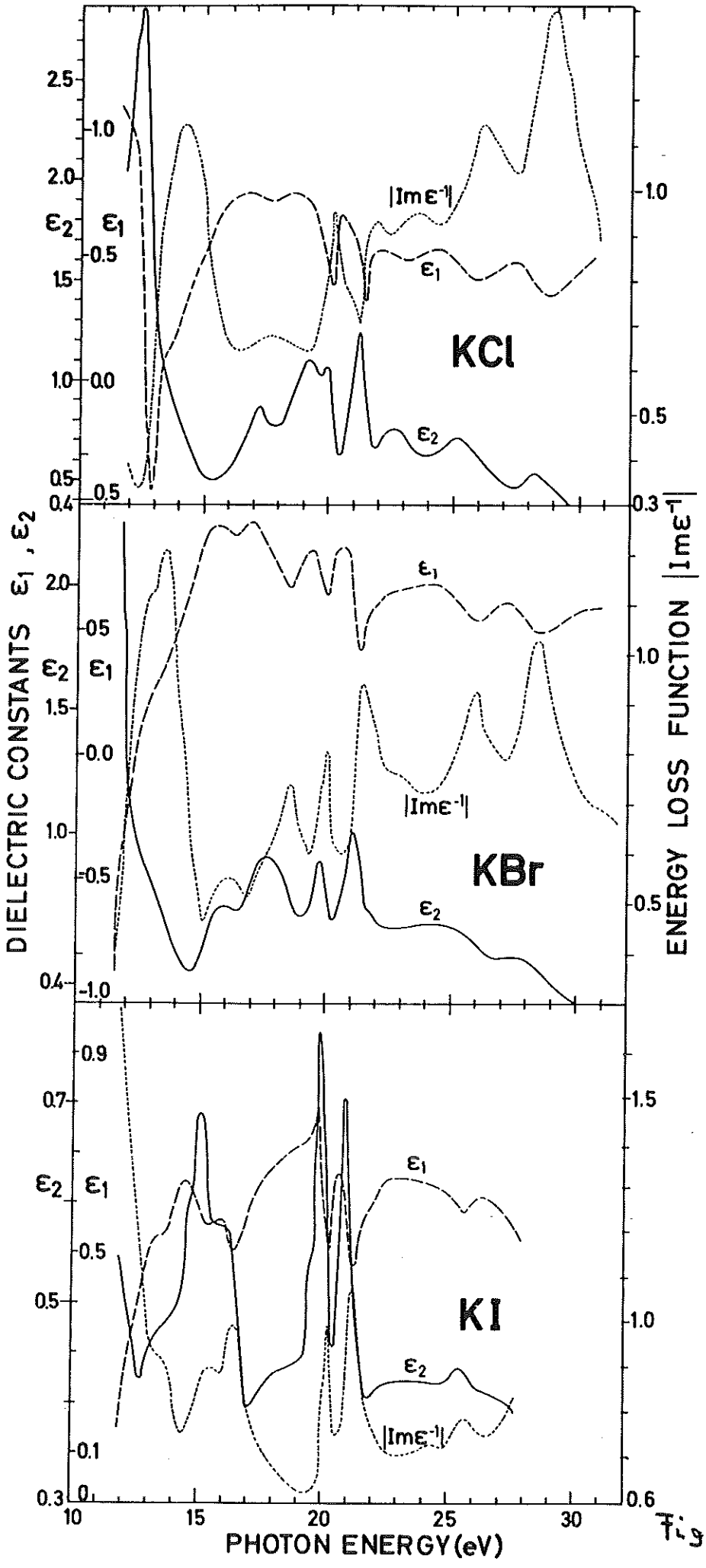
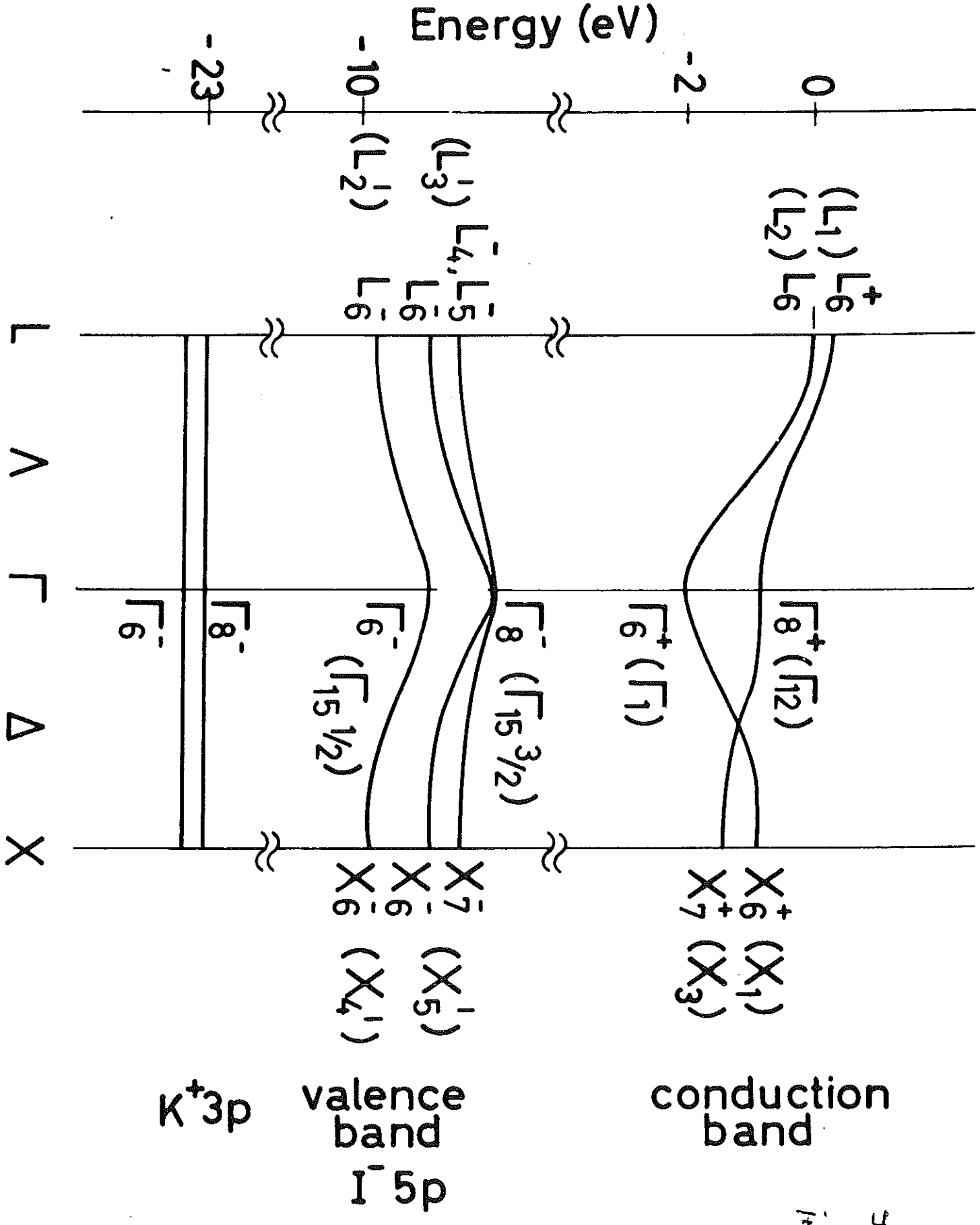

KCl
KBr
KI
ε_1
ε_2
$|Im\varepsilon^{-1}|$
DIELECTRIC CONSTANTS ε_1, ε_2
ENERGY LOSS FUNCTION $|Im\varepsilon^{-1}|$
PHOTON ENERGY (eV)
10
15
20
25
30

Fig. 3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-10
-2
0
L
Δ
Γ
Δ
X
(L_2^-)
(L_3^-)
L_6^-
L_4^-, L_5^-
L_6^-
(L_1) L_6^+
(L_2) L_6^-
Γ_6^-
Γ_8^-
Γ_6^- $(\Gamma_{15}\,1/2)$
Γ_8^- $(\Gamma_{15}\,3/2)$
$\Gamma_6^+(\Gamma_1)$
$\Gamma_8^+(\Gamma_2)$
X_6^- (X_4^-)
X_6^- (X_5^-)
X_7^-
X_7^+ (X_3)
X_6^+ (X_1)
K^+3p
valence band
I^-5p
conduction band

Fig. 4

Table 1

Position of the maxima of the 15° reflectance spectra from the onset of excitonic absorption up to 35 eV photon energy including interpretation as Γ or X-exciton

KCl			KBr			KI		
7.68±0.03 eV	max.	$\Gamma_{15}(3/2, 1/2)\rightarrow\Gamma_1$	6.58±0.03 eV	max.	$\Gamma_{15}(3/2)\rightarrow\Gamma_1$	5.61±0.03 eV	max.	$\Gamma_{15}(3/2)\rightarrow\Gamma_1$
8.30 - 8.80	shoulder	exciton series with edge $\Gamma_{15}\rightarrow\Gamma_1$	7.13±0.03	max.	$\Gamma_{15}(1/2)\rightarrow\Gamma_1$	~6.05	shoulder	exciton series with edge $\Gamma_{15}(3/2)\rightarrow\Gamma_1$
9.59±0.03	max.	$X_5', X_4'\rightarrow X_3$	7.75	weak shoulder		6.67 0.03	max.	$X_5'\rightarrow X_3$
10.5	shoulder		8.61±0.03	max.	$X_5'\rightarrow X_3$	7.11	max.	$\Gamma_{15}(1/2)\rightarrow\Gamma_1$
12.78±0.05	max.		10.20	shoulder		7.8 / 8.4	weak double max.	
13.8	shoulder		11.81±0.05	max.		9.65	max.	
17.35±0.05	max.		13.20	shoulder		11.10	max.	
19.5 ±0.05	weak max.		16.10±0.05	max.		11.81	shoulder	
20.10±0.05	max.	$K^+3p\rightarrow\Gamma_1$	18.25	max		13.5	max.	
21.40±0.05	max.	$K^+3p\rightarrow X_3$	19.93±0.05	max.	$K^+3p\rightarrow\Gamma_1$	15.3	max.	
22.65±0.05	max.		21.30±0.05	max.	$K^+3p\rightarrow X_3$	16.35	max.	
23.6	weak shoulder		22.50	shoulder		~18.5	shoulder	
25.8 ±0.1	max.		25.90±0.1	max.		20.0	shoulder	
28.7 ±0.1	max.		28.30±0.1	max.		20.2±0.05	max.	$K^+3p\rightarrow\Gamma_1$
29.9	weak shoulder		30.90	shoulder		21.20±0.05	max.	$K^+3p\rightarrow X_3$
31.6 ±0.1	weak max.		35.0 ±0.1	weak max.		23.8 ±0.1	max.	
35.4 ±0.1	weak max.					25.3 ±0.1	max.	
						27.4 ±0.1	max.	
						29.6 ±0.1	weak max.	
						33.0 ±0.1	max.	

Table 2

Position of the maxima of $|\mathrm{Im}\varepsilon^{-1}|$ between 12 and 30 eV compared to those obtained by energy loss experiments by Creuzburg[21] and Keil[22]. Pl indicates the plasma energy.

KCl		KBr			KI	
this work	Creuzburg	this work	Creuzburg/Keil		this work	Creuzburg
∿13.5	∿13.5	13.0	13.2	13.0	13.6	13.8
14.1 Pl	14.1	13.6 Pl	13.5	13.52	15.5	15.45
17.6	17.5	16.1	16.2	16.3	16.45	16.45
20.2	20.2	18.6	18.55	18.56		∿18.6
21.8	21.6	20.05	20.00	20.03	20.1	20.20
23.5	23.6	21.5	21.50	21.45	21.25	21.30
26.1	26.2	∿23.0		∿22.8	24.2	23.7
28.9	28.9	26.0	25.7	26.2	25.7	
		28.4	28.4	28.4		

Table 3

Energy differences in eV estimated from reflectance data at room temperature (exp.) compared to values obtained by band calculations (th.).

	$X_7^+ - \Gamma_6^+$		$\Gamma_8^- - X_7^-$		Γ_8^- (valence band) $- \Gamma_8^-, \Gamma_6^-$ (K^+3p)	
	exp.	th.	exp.	th.	exp.	th.
KCl	1.3	1.22 [6]	0.65	0.24 [4]	12.4	13.0 [4]
		2.3 [7]		0.16 [6]		
				0.12 [7]		
KBr	1.4	2.2 [8]	0.28	∿0.0 [8]	13.3	
KI	1.0	0.62 [9]	-0.13	0.23 [9]	14.6	15.0 [9]