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Electronic Absorption and Internal and External Vibrational Data of Atomic and Molecular Ions Doped in Alkali Halide Crystals

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Issued July 1974

Library of Congress Catalog Number: 74-600010

NSRDS-NBS 52

Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 52, 59 pages (July 1974)

CODEN: NSRDAP

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1974

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402
(Order by SD Catalog No. C13.48:52). Price 95 cents.
Stock Number 0303–01262

Foreword

The National Standard Reference Data System provides access to the quantitative data of physical science, critically evaluated and compiled for convenience and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, and responsibility to administer it was assigned to the National Bureau of Standards.

NSRDS receives advice and planning assistance from a Review Committee of the National Research Council of the National Academy of Sciences-National Academy of Engineering. A number of Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The System now includes a complex of data centers and other activities in academic institutions and other laboratories. Components of the NSRDS produce compilations of critically evaluated data, reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. The centers and projects also establish criteria for evaluation and compilation of data and recommend improvements in experimental techniques. They are normally associated with research in the relevant field.

The technical scope of NSRDS is indicated by the categories of projects active or being planned: nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, chemical kinetics, and colloid and surface properties.

Reliable data on the properties of matter and materials is a major foundation of scientific and technical progress. Such important activities as basic scientific research, industrial quality control, development of new materials for building and other technologies, measuring and correcting environmental pollution depend on quality reference data. In NSRDS, the Bureau's responsibility to support American science, industry, and commerce is vitally fulfilled.

Richard W. Roberts, *Director*

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Electronic Absorption and Internal and External Vibrational Data of Atomic and Molecular Ions Doped in Alkali Halide Crystals

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Spectral data for more than 70 atomic and molecular ions doped in alkali halide crystals are tabulated. The tables include electronic absorption data, listings of internal vibrational frequencies of doped complex ions, and tabulations of the frequencies of external modes. The data that appear in the tables were selected on the basis of the consistency among different authors, the types of instruments, and the temperature of measurement. In addition to the data, the tables include the spectroscopic assignments given by the authors in the references cited.

Key words: Atomic ions; doped alkali halide crystals; external vibrational modes; internal vibrational modes; molecular ions.

Introduction

When atomic and molecular impurity ions are doped in crystals, the optical (electronic) absorption spectrum of the ions will be modified. Because of the low symmetry of the environment (lower than spherical symmetry), the degeneracies of free ion levels can split and transitions between these split levels can take place. These transitions give rise to the so-called crystal field bands and can be interpreted on the basis of crystal field theory [1].[1] In addition, transitions involving the transfer of charge between the impurity ion and the surrounding ligands also can occur, giving rise to strong charge transfer absorption bands. If there is considerable overlap of the wave functions of the impurity ion and the ligands, further modifications of the spectra occur due to covalency effects, and the observed spectra can only be explained on the basis of ligand field theory and molecular orbital theory [2, 3]. Thus the study of optical absorption spectra gives information about the symmetry of the crystal field as well as the nature of the interaction between the impurity ion and the host lattice. The crystal field transitions are parity forbidden and they are phonon assisted. Temperature dependence of the optical spectrum gives the nature of the transitions.

Complex molecular ions, in addition to their electronic spectrum, give infrared and Raman spectra due to their internal vibrational modes [4, 5]. When such ions are doped in crystals, their vibrational frequencies shift depending upon the size of the host lattice sites and of the complex ion as well as the interaction between the ions [6]. Splitting of the degenerate vibrational modes may occur due to lowering of the symmetry of the ion whenever defects are present in the nearest or next nearest neighbour positions [7, 8]. These internal vibrational modes can sometimes show side bands due to combination with the external modes of impurity host lattice system [9, 10]. Therefore, a detailed study of the internal vibrational modes of molecular impurities gives useful information about the defect properties as well as the phonon spectrum of the host lattice.

When impurity ions are introduced into a lattice, new modes are induced in the lattice giving rise to an absorption spectrum in the far infrared. If the impurity is monoatomic, only localized, resonant, or gap modes are induced, depending upon whether the new absorption appears above the optical band, in the acoustic continuum, or in the gap between the acoustic and optical branches, respectively [11]. Whether the impurity will induce a localized, resonant, or gap mode will depend upon the relative mass of the impurity ion with respect to the ion it replaces, as well as the force constant between the impurity and the host lattice ions. If, on the other hand, the impurity is molecular, in addition to these modes, librational as well as tunneling modes are also induced [7, 12]. These new modes can give rise to far infrared absorption and Raman scattering, and show strong resonant scattering of phonons in thermal conductivity. Impurity also breaks down the

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[1] Figures in brackets indicate literature references on page 2.

translational symmetry of the lattice, and vibrations at all points in the Brillouin zone become infrared and/or Raman active depending upon the symmetry of the mode. Thus impurity induced infrared and Raman spectra can be used to map the phonon spectrum of the host lattice.

Alkali halide crystals doped with more than 70 different impurity ions have been investigated from the above-mentioned points of view [13]. This is because of the ease with which pure and well-characterized alkali halide crystals can be grown, as well as to their almost perfect ionic nature, precise knowledge of the location of the ions and the neighbouring defect in the lattice, etc. The cubic symmetry of the crystal field and the exact knowledge of the symmetry of the field due to defects in the vicinity of the impurity ion, make alkali halides excellent hosts to study and to interpret the optical and other defect sensitive properties of ions.

In alkali halide crystals most of the impurities enter substitutionally at the cation or anion site depending upon whether the impurity is cationic or anionic, respectively. In the case of a few large complex impurity ions such as $Co(CN)_6$, $Fe(CN)_6$, etc., the impurity replaces a complex group of seven lattice sites MX_6 (M–alkali ion and X–halide ion). If the impurity is aliovalent, extra charge is compensated by the creation of vacancies or by intentionally doped or background charge compensating impurity ions. The symmetry of the environment about the $Co(CN)_6$ group is determined by the location of the charge compensating entity.

Impurity doped alkali halides find many modern technological applications. Tl^+ doped NaI is a well known scintillator and is extensively used in γ-ray scintillation counters. Color centers in alkali halides are being used successfully as memory devices. Recently it has been shown that the paraelectric property of Li^+ in KCl can be used as a thermometer to measure extremely low temperatures.

With the wide academic interest and potential technological applications of impurity centers in alkali halides, the availability of comprehensive optical data of different centers in alkali halide crystals is extremely valuable. The amount of literature on the optical properties of impurity centers in alkali halides has grown so much in the last ten years that it is extremely difficult for one to keep track of the development. It is therefore desirable to gather all the optical data in one place for all the impurity centers doped in alkali halides so that this can serve as a ready reference.

The following tables on the optical properties have been prepared by critically going through more than 500 papers listed in [13] and other relevant papers published before 1964. The references are given for those papers from which the actual data reported is taken. If more than one paper exists on the same impurity ion, the data are evaluated on the basis of the experimental procedures used, the resolution and accuracy of the instruments employed for measurements, consistency of the data between different authors, and quality of the samples on which measurements were made. Assignments given for the absorption bands in the table are those reported in the references.

The reference data are divided into three parts. In Part I the electronic absorption bands are tabulated. Here the peak positions are given in nanometers (nm). The data given in eV in the paper are converted to nm using the relation 1 eV = 1239.0 nm. Wherever possible the temperature of measurement is also indicated for each band.

Since the available data on halfwidth/oscillator strength of the absorption bands are meager and not consistent among different authors, we have not included them.

The data on the internal vibrational frequencies of complex ions doped in alkali halide crystals are given in Part II.[2] Here the frequencies are given in wavenumbers (cm^{-1}) and the ions are arranged in the order of increasing number of atoms in the complex ions.

In Part III the frequencies of the external modes are presented. Here again the frequencies are in wavenumbers (cm^{-1}). The data are presented first for monoatomic impurities and then for the molecular ions.

References are given at the end of each table.

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[2] In keeping with commonly accepted conventions in molecular spectroscopy, certain energies have been expressed in their wavenumber (cm^{-1}) equivalents. The actual energy can be obtained by multiplying the cm^{-1} equivalent by *hc*.

PART I.

Electronic Absorption of Impurity Centers Doped in Alkali Halide Crystals

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TABLE 1. *Optical absorption bands (in nm) of copper centers in alkali halides*

Center	NaCl	KCl	KBr	KI	Assignment	References
Cu^{2+}	---	---	---	[d]366	---	[1]
	---	---	[d]300	---	---	[1]
	---	[d]248	---	---	---	[1]
	---	[b]243	---	---	---	[2]
Cu^{+}	[c]372	---	---	---	---	[3]
	---	---	[c]305	---	---	[4]
	[c]282	[b]284	[c]292	278	---	[2, 5]
	[c]257	[c]261	[c]263	262	---	[1, 4, 5]
	[c]214	[c]202	[c]210	[d]229	---	[1, 4]
	---	[c]194	[c]199	---	---	[4, 6]
	[c]185	[c]186	---	---	---	[6]
Cu^{0}	[c]550	---	---	---	---	[7]
	[c]496	[d]457	[d]480	[d]556	---	[1, 7]
	[c]460	---	---	---	---	[7]
	---	---	---	[d]283	---	[1]
	---	[d]246	[d]247	[d]251	---	[1]
	---	[d]242	[d]243	---	---	[1]
	---	[d]235	[d]240	---	---	[1]
	---	[d]233	[d]236	---	---	[1]
	---	[c]232	[c]233	---	---	[1]
	---	[c]229	[c]230	---	---	[1]
	---	[c]225	---	---	---	[1]
Colloidal Cu	[a]574	[c]568	[c]575	575	---	[1, 8]
	413	---	---	---	---	[8]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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TABLE 2. *Optical absorption bands (in nm) of silver centers in alkali halides*

Center	NaCl	NaBr	KCl	KBr	KI	RbCl	RbBr	CsCl	CsBr	CsI	Assignment	References
Ag^{2+}	---	---	[b]800	[d]1137	---	---	---	---	---	---	---	[1, 2]
	---	---	[b]630	---	---	---	---	---	---	---	---	[1]
	---	---	[b]560	[d]539	---	---	---	---	---	---	---	[1, 2]
	---	---	[b]460	---	---	---	---	---	---	---	---	[1]
	---	---	---	[d]409	---	---	---	---	---	---	---	[2]
	---	[a]356	[b]338	---	[d]350	---	---	---	---	---	---	[1, 2]
Ag^{+}	[d]225	[a]242	[a]244	[a]241	[d]276	---	---	---	---	---	Ag^{+} pairs	[3, 5]
	---	---	[d]230	---	---	---	---	---	---	---	---	[3, 5]
	---	[a]229	---	---	---	---	---	---	---	---	---	[4]

TABLE 2. *Optical absorption bands (in nm) of silver centers in alkali halides*—Continued

Center	NaCl	NaBr	KCl	KBr	KI	RbCl	RbBr	CsCl	CsBr	CsI	Assignment	References
	---	[a]222	---	---	---	---	---	---	---	---	---	[4]
	[d]214	---	[d]225	[d]238	[d]253	[d]223	[d]243	---	---	---	---	[3. 5]
	[d]210	---	[d]219	[d]233	---	---	---	---	---	---	---	[3. 5]
	---	---	---	[d]225	---	---	---	---	---	---	---	[3. 5]
	[d]194	---	[d]209	[d]212	[d]244	---	---	---	---	---	---	[3. 5]
	---	---	---	---	---	[d]218	[d]222	---	---	---	---	[5]
	---	---	---	---	---	[d]212	[d]218	---	---	---	---	[5]
	[d]188	---	[d]200	---	---	---	---	---	---	---	---	[3]
	---	---	[d]191	---	---	[d]198	[d]208	---	---	---	---	[3. 5]
	[b]163	---	[b]173	[c]199	238	---	---	---	---	---	---	[5. 6. 7]
Ag^0	[a]385	[a]450	[a]425	[a]494	[a]494	---	---	---	---	---	Interstitial Ag atom.	[2. 4. 8]
	---	---	[c]420	[c]445	[c]470	[c]410	---	---	---	---	---	[9]
	---	---	[b]197	---	---	---	---	---	---	---	---	[1]
Ag^-	---	---	[b]435	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	---	---	[b]403	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	[b]330	---	[c]399	[d]413.8	[d]431	---	---	---	---	[d]446.5	$^1A_{1g} \rightarrow {}^3T_{1u}$ (A)	[11. 12. 13. 14]
	---	---	[b]390	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	---	---	[b]330	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	[b]310	---	[d]381.5	[d]396	[d]415.8	---	---	---	---	[d]432.8	$^1A_{1g} \rightarrow {}^3T_{2u}$ or ^3E_u (B)	[11. 12. 14]
	[b]275	---	[c]285	[d]296.5	[d]311	---	---	[d]301.5	[d]308.5	[d]328.8	$^1A_{1g} \rightarrow {}^1T_{1u}$ (C)	[10. 14]
	---	---	[b]283	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	---	---	[b]278	---	---	---	---	---	---	---	$(Ag^-)^2$	[10]
	---	---	[b]267	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	---	---	[b]263	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]
	---	---	[b]228	---	---	---	---	---	---	---	$(Ag^-)_2$	[10]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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Table 3. *Optical absorption bands (in nm) of gold centers in alkali halides*

Center	NaCl	KCl	KBr	KI	Assignment	References
$AuCl_4^-$	---	[a] 320	---	---	$^1A_{1g} \rightarrow {}^1A_{2u}$	[1]
	---	[a] 226	---	---	$^1A_{1g} \rightarrow {}^1E_u$	[1]
Au^0	---	[a] 271	---	---	---	[1]
Au^-	[d] 294	[d] 304	[d] 311	[d] 321.5	$^1A_{1g} \rightarrow {}^3T_{1u}$ (A)	[2]
	[d] 272.5	[d] 284	[d] 293.3	[d] 310.0	$^1A_{1g} \rightarrow {}^3T_{2u}$ or ^3E_u (B)	[2]
	[d] 220.7	[d] 228.3	[d] 235.6	[d] 245.5	$^1A_{1g} \rightarrow {}^1T_{1u}$ (C)	[2]
	[d] 195.6	[d] 202.5	[d] 209.2	[d] 219.0	(D_1)	[2]
	[b] 172	[d] 175.5	---	---	(D_2)	]3]
Au Colloids	---	[a] 555	---	---	---	[4]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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Table 4. *Optical absorption bands (in nm) of magnesium ions in alkali halides*

Center	LiF	KCl	Assignment	References
Mg^{2+}	---	[a] 320	---	[1]
	[a] 308	---	---	[2]
	[b] 216	[a] 272	---	[1, 2, 3]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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Table 5. *Optical absorption bands (in nm) of calcium centers in alkali halides*

Center	NaCl	KCl	KBr	Assignment	References
Ca^{2+}	[b] 469	[b] 596	[b] 697	Z_2	[1]
	---	[b] 588	---	Z_1	[2]
	[b] 398	[b] 488	[b] 554	Z_3	[1]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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Table 6. *Optical absorption bands (in nm) of strontium centers in alkali halides*

Center	NaCl	NaBr	KCl	KBr	KI	RbCl	Assignment	References
Sr^{2+}	---	---	[b] 834	---	---	---	Z_4	[1]
	[b] 514	[b] 560	[b] 635	[b] 713	[b] 840	---	Z_2	[2, 3]
	[b] 565	[b] 550	[b] 595, 617	[b] 658	---	[b] 664	Z_1	[2, 3, 4]
	[b] 398	---	[b] 494	[b] 556	---	---	Z_3	[2, 3]
	---	---	[b] 450	[b] 510	---	---	S	[5]
	---	---	---	[b] 198	---	---	---	[5]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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Table 7. *Optical absorption bands (in nm) of barium centers in alkali halides*

Center	KCl	KBr	Assignment	References
Ba^{2+}	[b] 812	[b] 845	Z_2	[1]
	[b] 636	[b] 713	Z_2	[1]
	[b] 599	---	Z_1	[2]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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Table 8. *Optical absorption bands (in nm) of zinc centers in alkali halides*

Center	NaCl	KCl	KBr	KI	Assignment	References
Zn^{2+}	[a]273	[a]272	---	---	---	[1, 2]
	[a]256	---	[a]212	[a]245	---	[1, 3]
	[a]189	[a]200	[a]202	---	---	[4]
Zn^{1+}	---	[a]245	[a]275	[a]330	---	[2, 3, 4]
Zn^{0}	---	[a]350	[a]370	[a]440	---	[3, 5]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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TABLE 9. *Optical absorption bands (in nm) of cadmium centers in alkali halides*

Center	NaCl	NaBr	KCl	KBr	KI	Assignment	References
Cd^{2+}	---	---	---	---	b292	$(Cd^{2+})_2$	[1]
	---	---	a278	a280	b275	---	[1, 2]
	---	---	---	a250	---	---	[1]
	---	---	---	a263	---	$(Cd^{2+})_2$	[1]
	---	---	---	a227	---	$(Cd^{2+})_2$	[1]
	---	---	---	a212	b235	---	[1, 2]
	a190	---	a190	a202	---	---	[2, 3]
Cd^{1+}	a310	a300	a310	a340–310	a355	---	[1, 4, 5]
	---	---	---	a300	---	$(Cd^{+})_2$	[1]
	---	---	---	a280	---	---	[1]
Cd^0	---	---	---	a365	a510	---	[2, 5]
Cd Colloids	a270	a275	a275	a300	a310	---	[2, 4]

aRoom temperature.
bLiquid air/nitrogen temperature.
cLiquid helium temperature.
dTemperature between 4.2 and 77 K.

References

[1] Ben-Dor, L., Glasner, A., and Zolotov, S., J. Solid State Chem. **4**, 4 (1972).
[2] Jain, S. C., and Radhakrishna, S., Phys. Rev. **172**, 972 (1968).
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[5] Radhakrishna, S., J. Phys. Soc. Japan **26**, 1204 (1969).

TABLE 10. *Optical absorption bands (in nm) of mercury centers in alkali halides*

Center	KCl	KBr	KI	Assignment	References
Hg^{2+}	a265	---	---	$(Hg^{2+})_2$	[1]
	a245	b300	a347	---	[1, 2]
	---	b275	a290	---	[1]
	---	---	a275	---	[1]
Hg^{1+}	a410	---	a455	---	[1]
	---	b315	---	$(Hg^{1+})_2$	[1]
	a290	b260	a280	---	[1]
	---	---	a260	---	[1]
Hg°	a345	---	a425	---	[1]
$Hg^{2+}:OH^-$	a195	---	---	---	[2]
HgO	a215	---	---	---	[2]

aRoom temperature.
bLiquid air/nitrogen temperature.
cLiquid helium temperature.
dTemperature between 4.2 and 77 K.

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[1] Ben-Dor, L., Glasner, A., and Zolotov, S., J. Solid State Chem. **2**, 549 (1970).
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TABLE 11. *Optical absorption bands (in nm) of gallium centers in alkali halides.*

Center	NaCl	KCl	KBr	KI	CsBr	CsI	Assignment	References
Ga^{1+}	---	---	---	[c]307	---	---	$(Ga^{1+})_2$	[1]
	---	---	---	[b]287	[b]288	[b]310	$^1A_{1g}\rightarrow{}^3T_{1u}(A)$	[1, 2, 3]
	[b]272	[b]261	[b]272	---	---	---	$^1A_{1g}\rightarrow{}^3T_{1u}(A_1)$	[1, 2]
	[b]265	[b]255	[b]265	---	---	---	$^1A_{1g}\rightarrow{}^3T_{1u}(A_2)$	[1, 2]
	[b]257	[b]247	[b]257	---	[b]269	[b]290	$^1A_{1g}\rightarrow{}^3E_u$ or $^3T_{2u}(B)$	[1, 2, 3]
	[c]241	[c]228	[c]245	[c]275	---	---	$(Ga^{1+})_2$	[1]
	[b]216	---	---	---	[b]229	[b]253	$^1A_{1g}\rightarrow{}^1T_{1u}(C)$	[4, 5]
	---	[c]218	[c]228	[c]254	---	---	$^1A_{1g}\rightarrow{}^1T_{1u}(C_1)$	[4]
	---	[c]214	[c]225	[c]251	---	---	$^1A_{1g}\rightarrow{}^1T_{1u}(C_2)$	[4]
	---	[c]210	[c]222	[c]247	---	---	$^1A_{1g}\rightarrow{}^1T_{1u}(C_3)$	[4]
	[b]158	[b]166	[b]188	---	---	---	(D′)	[2]
$Ga^\circ-Ga^\circ$	---	---	---	---	[b]427	[b]400	---	[5]
$Ga^\circ-Ga^{1+}$	---	---	---	---	---	[a]517–563	---	[5]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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TABLE 12. *Optical absorption bands (in nm) of indium centers in alkali halides*

Center	NaCl	KF	KCl	KBr	KI	RbCl	CsBr	Assignment	References
In^{1+}	---	---	---	---	[c]330	---	---	$(In^{1+})_2$	[1]
	---	---	[b]284	---	[c]312	---	---	$^1A_{1g}\rightarrow{}^3T_{1u}(A)$	[2, 3]
	[b]302	[a]284	[b]290	[c]297	[a]325	---	[c]284	$^1A_{1g}\rightarrow{}^3T_{1u}(A_1)$	[3, 4, 5, 7]
	[b]295	[a]265	[b]282	[c]293	[a]309	---	[c]281	$^1A_{1g}\rightarrow{}^3T_{1u}(A_2)$	[3, 4, 5, 7]
	[b]276	[a]246	[b]265	[c]280	[a]291	---	[c]267	$^1A_{1g}\rightarrow{}^3E_u$ or $^3T_{2u}(B)$	[3, 4, 7]
	---	---	[c]248	[c]266	[c]292	---	---	$(In^{1+})_2$	[1]
	[c]238	[a]213	[b]228	[b]243	[c]264	---	---	$^1A_{1g}\rightarrow{}^1T_{1u}(C)$	[1, 3, 4, 6]
	[c]247	---	[b]234	---	[b]269	[c]231	[c]238	$^1A_{1g}\rightarrow{}^1T_{1u}(C_1)$	[6, 7]
	[c]239	---	[b]229	---	[b]265	[c]227	[c]235	$^1A_{1g}\rightarrow{}^1T_{1u}(C_2)$	[6, 7]
	[c]232	---	[b]225	---	[b]262	[c]224	[c]232	$^1A_{1g}\rightarrow{}^1T_{1u}(C_3)$	[6, 7]
	[b]164	[a]133	[b]167	[b]187	[a]230	[b]176	[c]220	(D)	[3, 4, 7, 8]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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TABLE 13. *Optical absorption bands (in nm) of germanium centers in alkali halides*

Center	NaCl	KCl	KBr	Assignment	References
Ge^{2+}	[b] 264	[b] 264	[b] 274	$^1A_{1g} \rightarrow {}^3T_{1u}(A)$	[1]
	---	[b] 294	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_1)$	[2]
	---	[b] 262	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_2)$	[2]
	[b] 222	[b] 222	[b] 226	$^1A_{1g} \rightarrow {}^1T_{1u}(C)$	[1]
	---	[b] 230	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_1)$	[2]
	---	[b] 219	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_2)$	[2]
	---	[b] 212	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_3)$	[2]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77K.

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TABLE 14. *Optical absorption bands (in nm) of bismuth centers in alkali halides*

Center	KCl	KBr	KI	Assignment	References
Bi^{3+}	[b] 324	---	[a] 460	$^1A_{1g} \rightarrow {}^3T_{1u}(A)$	[1, 2, 3]
	---	[b] 369	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_1)$	[3]
	---	[b] 359	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_2)$	[3]
	[b] 244	---	---	$^1A_{1g} \rightarrow {}^3E_u$ or $^3T_{2u}(B)$	[3]
	[b] 220	---	[a] 255	$^1A_{1g} \rightarrow {}^1T_{1u}(C)$	[1, 2]
	[b] 212	[b] 233	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_1)$	[3]
	[b] 207	[b] 224	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_2)$	[3]
	[b] 201	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_3)$	[3]
	[b] 194	[b] 211	---	D′	[3]
Bi^{2+}	[a] 335	---	---	---	[4]
BiO^+	[b] 324	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A)$	[3]
	[b] 217	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_1)$	[3]
	[b] 207	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_2)$	[3]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77K.

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TABLE 15. *Optical absorption bands (in nm) of thallium centers in alkali halides*

Center	NaCl	NaBr	NaI	KCl	KBr	KI	RbCl	RbBr	RbI	CsCl	CsBr	CsI	Assignment	References
Tl^{1-}	---	---	[c] 306	---	---	[c] 292	---	---	---	---	---	---	$(Tl^{1+})_2$	[1]
	---	---	[c] 303	---	---	[c] 289	---	---	---	---	---	---	$(Tl^{1+})_2$	[1]
	---	---	---	---	---	---	---	---	---	---	---	[c] 290	---	[2]
	---	---	---	---	---	---	---	---	---	---	---	[c] 276	---	[2]
	---	---	---	---	---	---	---	---	---	---	---	[c] 257	---	[2]
	[b] 253	[b] 268	[b] 291	[b] 245.8	[b] 258	[b] 281	[b] 242	[b] 258	[c] 280.5	[a] 247	[c] 256	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A)$	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
	---	---	---	---	---	---	---	---	---	---	---	[c] 246	---	[2]
	---	---	---	[d] 247.3	---	---	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_1)$	[3, 4]
	---	---	---	[d] 246.4	---	---	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A, A_2)$	[3]
	---	---	---	[d] 245.8	---	---	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_2)$	[3, 4]
	---	---	---	[d] 243.6	---	---	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_3)$	[3, 4]
	---	---	[c] 263	---	---	[c] 250	---	---	---	---	---	---	B′	[1]
	---	---	[d] 260	---	---	---	---	---	---	---	---	---	B'_1	[11]
	---	---	[d] 257	---	---	---	---	---	---	---	---	---	B'_2	[11]
	---	---	---	---	---	---	---	---	---	---	---	[c] 238	---	[2]
	---	---	[c] 258	---	---	[c] 249	---	---	---	---	---	---	C′	[1]
	[b] 214	[b] 228	[b] 250	[b] 208	[b] 221	[b] 243.1	[b] 205	[b] 220	[b] 243	---	[c] 242	---	$^1A_{1g} \rightarrow {}^3T_{2u}$ or $^3E_u(B)$	[1, 2, 3, 4, 5, 7, 9, 11]
	[b] 199	[b] 218	[b] 238	[c] 194	[b] 208	[b] 232	[b] 197	[b] 208	[b] 234	[a] 196	[c] 225	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C)$	[3, 4, 7, 8, 9, 11]
	---	---	---	[c] 196.3	---	[c] 234	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_1)$	[3, 4, 5]
	---	---	---	[c] 194.4	---	[c] 232.8	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_2)$	[3, 4, 5]
	---	---	---	[c] 192.8	---	[c] 232	---	---	---	---	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_3)$	[3, 4, 5]
	[b] 161	[b] 188	[b] 224	[b] 169	[b] 190	[c] 223.9	[b] 174	[b] 198	[b] 226	---	---	---	D	[5, 7, 10]
Tl^0	---	---	---	[c] 1470	[c] 1580	[c] 1695	---	---	---	---	---	---	$^2P_{1/2} \rightarrow {}^2P_{3/2}$	[12]
	---	---	---	[c] 1300	[c] 1430	[c] 1550	---	---	---	---	---	---	$^2P_{1/2} \rightarrow {}^2P_{3/2}$	[12]
	---	---	---	[b] 640	---	---	---	---	---	---	---	---	---	[13]
	---	---	---	[b] 380	---	---	---	---	---	---	---	---	---	[13]
	---	---	---	[b] 300	---	---	---	---	---	---	---	---	---	[13]
	---	---	---	[b] 250	---	---	---	---	---	---	---	---	---	[13]
Tl^{2+}	---	---	---	[b] 364	---	---	---	---	---	---	---	---	---	[13]
	---	---	---	[b] 294	---	---	---	---	---	---	---	---	---	[13]
	---	---	---	[b] 262	---	---	---	---	---	---	---	---	---	[13]
	---	---	---	[b] 220	---	---	---	---	---	---	---	---	---	[13]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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Table 16. *Optical absorption bands (in nm) of tin centers in alkali halides*

Center	NaCl	KCl	KBr	KI	RbCl	RbBr	RbI	Assignment	References
Sn^{2+}	[b] 294	[b] 288	[b] 312	---	---	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_1)$	[1]
	[b] 285	[b] 279	[b] 305	---	---	---	---	$^1A_{1g} \rightarrow {}^3T_{1u}(A_2)$	[1]
	[b] 259	[b] 250	[b] 275	---	---	---	---	$^1A_{1g} \rightarrow {}^3E_u$ or $^3T_{2u}(B)$	[1]
	[b] 239	[b] 237	[b] 260	[b] 300	[b] 239	[b] 264	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_1)$	[1, 2]
	---	---	---	---	---	---	[b] 292	---	[2]
	[b] 233	[b] 231	[b] 254	[b] 296	[b] 233	[b] 256	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C_2)$	[1, 2]
	[b] 225	[b] 224	[b] 247	[b] 287	[b] 225	[b] 248	[b] 279	$^1A_{1g} \rightarrow {}^1T_{1u}(C_3)$	[1, 2]
	[b] 168	[b] 173	[b] 201	[b] 236	[b] 179	[b] 200	[b] 235	D′	[1, 2]
	[b] 160	[b] 165	[b] 190	[b] 222	[b] 173	[b] 194	[b] 224	D	[1, 2]
Sn^-	[b] 387	[b] 420	---	---	---	---	---	T	[3]
	---	[b] 371	---	---	---	---	---	T	[3]
	[b] 294	[b] 317	---	---	---	---	---	T	[3]
	[b] 265	[b] 279	---	---	---	---	---	T	[3]
	[b] 236	[b] 252	---	---	---	---	---	T	[3]
	[b] 223	[b] 238	---	---	---	---	---	T	[3]
	[b] 207	[b] 221	---	---	---	---	---	T	[3]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

References

[1] Fukuda, A., Science of Light **13**, 64 (1964).
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[3] Velicescu, B., and Topa, V., Int. Conf. on Color Centers in Ionic Crystals, Reading U.K., 1971, Abs. No. D62.

Table 17. *Optical absorption bands (in nm) of lead centers in alkali halides*

Center	NaCl	NaI	KCl	KBr	KI	RbCl	RbBr	RbI	CsCl	CsBr	CsI	Assignment	References
Pb^{2+}	---	---	---	---	---	---	[a] 363	---	---	---	---	---	[1]
	---	---	---	[b] 324	---	---	---	---	---	---	---	$(Pb^{2+})_2(A)$	[2]
	[b] 271	---	[b] 270	[b] 297	[b] 353	[b] 270	[b] 302	[b] 358	[a] 278	[a] 310	[a] 373	$^1A_{1g} \rightarrow {}^3T_{1u}(A)$	[1, 2, 3, 4, 5, 6]
	---	---	---	---	---	---	---	[a] 330	---	---	---	---	[1]
	[b] 209	---	[b] 211	[b] 272	[b] 308	---	---	---	[b] 232	[b] 251	[b] 281	$^1A_{1g} \rightarrow {}^3E_u$ or $^3T_{2u}(B)$	[2, 3, 4, 6]
	---	---	---	---	---	---	[a] 274	---	---	---	---	---	[1]
	---	---	---	[b] 267	[b] 297	---	---	---	---	---	---	$(Pb^{2+})_2(C')$	[2]
	---	---	---	---	---	---	[a] 258	---	---	---	---	---	[1]
	---	---	---	[b] 224	[b] 262	---	[b] 225	[b] 275	---	---	---	$^1A_{1g} \rightarrow {}^1T_{1u}(C)$	[2, 3, 5]
	[b] 201	---	[b] 201	---	---	[b] 206	---	---	[b] 204	[b] 222	[b] 260	$^1A_{1g} \rightarrow {}^1T_{1u}(C_1)$	[3, 5, 6]
	[b] 198	---	[b] 198	---	---	[b] 202	---	---	[b] 200	[b] 216	[b] 253	$^1A_{1g} \rightarrow {}^1T_{1u}(C_2)$	[3, 5, 6]
	[b] 194	---	[b] 195	---	---	[b] 196	---	---	[b] 196	[b] 210	[b] 244	$^1A_{1g} \rightarrow {}^1T_{1u}(C_3)$	[3, 5, 6]
	[b] 184	---	[b] 188	[b] 215	[b] 253	[b] 192	[b] 217	[b] 254	---	---	---	D′	[3, 5]
	[b] 160	---	[b] 165	[b] 192	[b] 228	[b] 173	[b] 194	[b] 229	---	---	[b] 215	D	[5, 6]
Pb^{1+}	---	---	[b] 240	[a] 300	[a] 320	---	---	---	[b] 258	[b] 291	[b] 347	---	[2, 4, 6]
Pb^0	---	---	[b] 604	---	---	---	---	---	---	---	---	$(Pb^0)_2$	[2]
	[a] 285	---	[b] 280	---	---	---	---	---	---	---	---	---	[2, 7]
	---	---	[b] 230	---	---	---	---	---	---	---	---	---	[2]

TABLE 17. *Optical absorption bands (in nm) of lead centers in alkali halides*—Continued

Center	NaCl	NaI	KCl	KBr	KI	RbCl	RbBr	RbI	CsCl	CsBr	CsI	Assignment	References
Pb Colloids	[a] 270	---	[a] 260	[a] 255	[a] 265	---	---	---	---	---	---	---	[2, 4]
Pb^-	[b] 447	[b] 564	[b] 497	[b] 541	[b] 608	---	---	---	---	---	---	T_1	[8, 9, 10]
	[b] 418	[b] 490	[b] 444	[b] 460	[b] 502	---	---	---	---	---	---	T_2	[8, 9, 10]
	[b] 360	[b] 438	[b] 388	[b] 418	[b] 459	---	---	---	---	---	---	T_3	[8, 9, 10]
	[b] 332	---	[b] 359	[b] 383	[b] 427	---	---	---	---	---	---	T_4	[8, 9, 10]
	[b] 308	[b] 396	[b] 323	[b] 342	[b] 387	---	---	---	---	---	---	T_5	[8, 9, 10]
	[b] 284	[b] 365	[b] 296	---	---	---	---	---	---	---	---	T_6	[8, 9, 10]
	[b] 260	[b] 299	[b] 280	[b] 294	[b] 306	---	---	---	---	---	---	T_7	[8, 9, 10]
	[b] 239	---	[b] 257	[b] 274	[b] 301	---	---	---	---	---	---	T_8	[8, 9, 10]
	[b] 220	---	[b] 226	[b] 238	[b] 263	---	---	---	---	---	---	T_9	[8, 9, 10]
	---	---	[b] 205	[b] 221	[b] 240	---	---	---	---	---	---	T_{10}	[8, 9, 10]
Pb^{3+}	---	---	[b] 465	---	---	---	---	---	---	---	---	---	[11]
	---	---	[b] 303	---	---	---	---	---	---	---	---	---	[11]
	---	---	[b] 216	---	---	---	---	---	---	---	---	---	[11]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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TABLE 18. *Optical absorption bands (in nm) of titanium centers in alkali halides*

Center	LiF	Assignment	References
Ti	[a] 270	---	[1]
	[a] 250	---	[1]
	[a] 240	---	[1]
	[a] 207	---	[1]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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[1] Jain, S. C., and Sootha, G. D., Phys. Stat. Sol. **22,** 505 (1967).

TABLE 19. *Optical absorption bands (in nm) of vanadium centers in alkali halides*

Center	NaCl	Assignment $^4A_{2g} \rightarrow$	References
V^{2+}	[b] 1307	$^4T_2(t_2^2)$	[1]
	[b] 1242	$^4T_2(t_2^2)$	[1]
	[b] 1221	$^4T_2(t_2^2)$	[1]
	[b] 1215	$^4T_2(t_2^2)$	[1]
	[b] 1190	$^4T_2(t_2^2)$	[1]
	[b] 1169	$^4T_2(t_2^2)$	[1]
	[b] 806	$^4T_1$(a)	[1]
	[b] 790	$^4T_1$(a)	[1]
	[b] 781	$^4T_1$(a)	[1]
	[b] 772	$^4T_1$(a)	[1]
	[b] 762	$^4T_1$(a)	[1]
	[b] 494	$^4T_1$(b)	[1]
	[b] 236	Charge transfer	[1]
	[b] 200	Charge transfer	[2]
V^{1+}	[a] 640	---	[3]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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TABLE 20. *Optical absorption bands (in nm) of chromium centers in alkali halides*

Center	NaCl	KCl	Assignment	References
Cr^{2+}	---	[b] 330	---	[1]
	[b] 240	[b] 240	---	[1]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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[1] Radhakrishna, S., and Sai, K. S. K., Phys. Stat. Sol. (b) **45,** K153 (1971).

TABLE 21. *Optical absorption bands (in nm) of manganese centers in alkali halides*

Center	NaCl	KCl	RbBr	Assignment $^6A_1(S) \rightarrow$	References
Mn^{2+}	[b] 518	[b] 521	---	$^4T_1$(G)	[1]
	[b] 460.5	[b] 443.5	---	$^4T_2$(G)	[1]
	[b] 425.3	---	---	---	[1]
	[b] 421.6 } [b] 417.5 }	[b] 418	---	$^4A_1$(G), ^4E(G)	[1]
	---	[b] 374	---	---	[1]
	[b] 370.8	{ [b] 370.8 { [b] 368.5	---	$^4T_2$(D)	[1]
	[b] 353	[b] 354	---	^4E(D)	[1]
	[b] 326	[b] 332.5	---	$^4T_1$(P)	[1]
	[b] 274 } [b] 262 }	[a] 272	{ [a] 300 { [a] 271	Charge transfer	[2, 3]
	[b] 255	[a] 260	---	$^4A_2$(F), $^4T_1$(F)	[1]
	---	[a] 245	[a] 255	Charge transfer	[2, 3]
	[b] 245.5	[a] 234	---	$^4T_2$(F)	[1]
	[b] 220	---	---	---	[3]
	[b] 194	[a] 201	[a] 230	Charge transfer	[2, 3]
Mn^{+}	[b] 278.5	---	---	$3d^54s(^7S) \rightarrow 3d^54p(^7P)$	[4]
	---	[a] 223	---	---	[5]

Table 21. *Optical absorption bands (in nm) of manganese centers in alkali halides* — Continued

Center	NaCl	KCl	RbBr	Assignment $^6A_1(S) \rightarrow$	References
Mn^{+} at the lattice site	[c] 422.8	---	---	---	[6]
	[c] 415–226.5	---	---	---	[6]
	[c] 226.5	---	---	---	[6]
Mn° at the off center position	[c] 453.0	---	---	---	[6]
	[c] 408.4	---	---	---	[6]
	[c] 355.9	---	---	---	[6]
	[c] 415–226.5	---	---	---	[6]
	[c] 232.4	---	---	---	[6]
	[c] 226.0	---	---	---	[6]
	[c] 216.7	---	---	---	[6]
Mn^{+} at the interstitial site	[c] 519.0	---	---	---	[6]
	[c] 453.0	---	---	---	[6]
	[c] 389.3	---	---	---	[6]
	[c] 415–226.5	---	---	---	[6]
	[c] 232.4	---	---	---	[6]
	[c] 226.0	---	---	---	[6]
	[c] 216.7	---	---	---	[6]
Mn° Aggregates	[a] 210.0	[a] 210.0	---	---	[7]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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[1] Mehra, A., Phys. Stat. Sol. **29**, 847 (1968).
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Table 22. *Optical absorption bands (in nm) of cobalt centers in alkali halides*

Center	LiCl	NaF	NaCl	NaBr	KCl	KBr	RbCl	Assignment $^4A_2 \rightarrow$	References
Co^{2+} in tetrahedral symmetry	---	---	[b] 1923	---	[a] 2070	---	---	$^4T_1(F)$	[1, 2]
	---	---	[b] 1727	---	[a] 1770	---	---	$^4T_1(F)$	[1, 2]
	---	---	[b] 1493	---	[a] 1531	---	---	$^4T_1(F)$	[1. 2]
	---	---	---	[a] 728	---	[b] 724	---	---	[3, 4]
	---	---	---	[a] 702	---	[b] 694	---	---	[3, 4]
	---	---	[b] 695	---	[a] 695	---	---	$^4T_1(P)$	[1, 2]
	---	---	[b] 660	---	[a] 667	---	---	$^4T_1(P)$	[1, 2]
	---	---	[b] 640	---	[a] 630	---	---	$^4T_1(P)$	[1, 2]
	---	---	---	[a] 668	---	[b] 670	---	---	[3]
	---	---	---	[a] 644	---	[b] 640	---	---	[3, 4]
	---	---	---	---	[b] 610	[b] 625	[b] 608	---	[4, 5]
	---	---	---	---	[b] 599	[b] 602	[b] 580	---	[4, 5]
	---	---	---	---	---	[b] 585	---	---	[4, 5]
	---	---	---	---	[b] 578	[b] 575	---	---	[4, 5]
	---	---	---	---	[b] 552	[b] 562	[b] 568	---	[4, 5]

TABLE 22. *Optical absorption bands (in nm) of cobalt centers in alkali halides*—Continued

Center	LiCl	NaF	NaCl	NaBr	KCl	KBr	RbCl	Assignment $^4A_2 \rightarrow$	References
	———	———	———	———	^{b}549	^{b}552	^{b}552	———	[4, 5]
	———	———	———	———	^{b}544	^{b}540	^{b}542	———	[4, 5]
	———	———	———	———	^{b}535	^{b}535	^{b}535	———	[4, 5]
	———	———	———	———	^{a}529	———	———	d^2T_1	[1]
	———	———	———	———	^{b}526	———	^{b}526	———	[4, 5]
	———	———	———	———	^{b}518	———	^{b}517	———	[4, 5]
	———	———	———	———	^{b}515	———	———	———	[4, 5]
	———	———	———	———	^{b}505	———	^{b}508	———	[4, 5]
	———	———	———	———	———	^{b}483	———	b^2T_2	[1]
	———	———	———	———	———	^{b}469	———	———	[4]
	———	———	———	———	^{b}457	^{b}462	^{b}453	———	[4, 5]
	———	———	———	———	———	^{b}454	^{b}450	———	[4, 5]
	———	———	———	———	^{b}450	———	———	b^2T_1	[1]
	———	———	———	———	^{b}444	^{b}431	^{b}444	———	[4, 5]
	———	———	———	———	———	^{b}423	^{b}411	———	[4, 5]
	———	———	———	———	———	———	^{b}407	———	[5]
	———	———	———	———	^{a}271	———	———	———	[6]
	———	———	———	———	^{a}244	———	———	———	[6]
	———	———	———	———	^{a}235	———	———	———	[6]
	———	———	———	———	^{a}230	———	———	———	[1]
Co^{2+} in octahedral symmetry	———	^{b}1412	———	———	———	———	———	———	[7]
	———	^{b}1337	———	———	———	———	———	———	[7]
	———	^{b}1312	———	———	———	———	———	———	[7]
	———	^{b}1280	———	———	———	———	———	———	[7]
	———	^{b}967	———	———	———	———	———	———	[7]
	^{b}615	^{b}610	———	———	———	———	———	———	[4, 7]
	^{b}591	———	———	———	———	———	———	———	[4]
	^{b}581	———	———	———	———	———	———	———	[4]
	^{b}575	———	———	———	———	———	———	———	[4]
	^{b}562	———	———	———	^{b}562	———	———	———	[4, 8]
	^{b}550	———	———	———	^{b}551	———	———	———	[4, 8]
	^{b}543	———	———	———	———	———	———	———	[4]
	^{b}538	———	———	———	———	———	———	———	[4]
	^{b}535	———	^{b}533	———	^{b}533	———	———	———	[4, 8]
	^{b}523	———	^{b}526	———	^{b}525	———	———	———	[4, 8]
	^{b}518	———	———	———	———	———	———	———	[4]
	^{b}515	^{b}515	^{b}507	———	^{b}516	———	———	———	[4, 7, 8]
	———	^{b}500	^{b}502	———	^{b}502	———	———	———	[7, 8]
	———	^{b}465	^{b}495	———	———	———	———	———	[7, 8]
	———	———	^{b}240	———	———	———	———	———	[9]
	———	———	^{b}212	———	———	———	———	———	[9]
	———	———	^{b}193	———	———	———	———	———	[9]
Co^{+}	———	———	^{a}210	———	^{a}212	———	———	———	[10, 11]

^{a} Room temperature.
^{b} Liquid air/nitrogen temperature.
^{c} Liquid helium temperature.
^{d} Temperature between 4.2 and 77 K.

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Table 23. *Optical absorption bands (in nm) of nickel centers in alkali halides*

Center	LiF	LiCl	NaCl	NaBr	KCl	RbCl	Assignment $^3A_{2g} \rightarrow$	References
Ni^{2+}	[a]1233	---	[a]1850	---	---	---	^3E_g } $^3T_{2g}(F)$	[1, 2]
	---	---	[a]1560	---	---	---	$^3B_{2g}$	[1, 2]
	---	---	[a]1250	---	---	---	---	[1]
	[a]729	---	[a]935	---	---	---	$^3A_{2g}$, ^3E_g } $^3T_{1g}(F)$	[1, 2]
	[a]649	---	[a]792	---	---	---	$^1A_{1g}$ } $^1E_g(D)$	[1, 2]
	---	---	[a]771	---	---	---	$^1B_{1g}$	
	---	---	[a]666	---	---	---	---	[1]
	[a]454	---	[a]545	---	---	---	$^1T_{2g}(D)$	[1, 2]
	[a]405	---	[a]490	---	---	---	$^3A_{2g}$ } $^3T_{1g}(P)$	[1, 2]
	---	---	[a]476	---	---	---	^3E_g	
	---	---	[a]254	---	[a]266	---	---	[3]
	---	---	[a]246	---	---	[a]265	$3t_2 \rightarrow e_g(^3T_{2u})$	[1]
	---	[a]254	[a]242	[a]321	[a]251	---	$G(T^{**}_{2u}) \rightarrow e^*_g$	[3]
	---	[a]207	[a]216	[a]280	[a]220	---	---	[3]
	---	[a]182	[a]194	[a]240	[a]196	[a]209	{ $3t_{1u} \rightarrow 3e_g(^3T_{2u})$; $e^*_g \rightarrow a^*_{1u}$ or t^*_{1u}	[1, 3]
Ni^+	---	---	350	---	370	---	---	[4]
	---	---	310	---	340	---	---	[4]
	---	---	279	---	288	---	---	[4]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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Table 24. *Optical absorption bands (in nm) of rhodium centers in alkali halides*

Center	NaCl	Assignment	References
Rh^{3+}	[a]680	$^1A_{1g} \rightarrow {}^3T_{1g}$ or $^3T_{2g}$	[1]
	[a]515	$^1A_{1g} \rightarrow {}^1T_{1g}$	[1]
	[a]412	$^1A_{1g} \rightarrow {}^1T_{2g}$	[1]
	[a]250	Charge transfer	[1]
	[a]210	---	[1]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

Reference

[1] Jain, S. C., Agarwal, S. K., and Sootha, G. D., Phys. Stat. Sol. **40b**, K69 (1970).

Table 25. *Optical absorption bands (in nm) of palladium centers in alkali halides*

Center	NaCl	KCl	Assignment	References
Pd^{2+}	[a]272	[b]272	Charge transfer	[1, 2]
Pd^{1+}	[a]220	---	Charge transfer	[1]
Pd Colloids	---	[a]222	---	[2]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

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TABLE 26. *Optical absorption bands (in nm) of europium centers in alkali halides*

Center	NaCl	KCl	KBr	KI	Assignment	References
Eu^{2+}	---	[d]410.8	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]407.5	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]404.1	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]400.8	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]397.5	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]394.2	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]391	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]388.5	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]386.4	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]383.5	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]380.6	---	---	$4f^7 \rightarrow 4f^65d$	[1]
	---	[d]376.8	---	[b]375	$4f^7 \rightarrow 4f^65d$	[1, 2]
	---	[d]364	[b]367	[b]365	$4f^7 \rightarrow 4f^65d$	[1, 2]
	[b]343	[b]343	[b]344.8	[b]345	$4f^7 \rightarrow 4f^65d$	[2, 3]
	---	[b]328.9	[b]330	[b]330	$4f^7 \rightarrow 4f^65d$	[2, 3]
	---	---	---	[b]275	$4f^7 \rightarrow 4f^65d$	[2]
	---	[b]270.6	---	[b]270	$4f^7 \rightarrow 4f^65d$	[2, 3]
	---	---	---	[b]260	$4f^7 \rightarrow 4f^65d$	[2]
	[b]249.2	[b]249.2	[b]254.3	[b]255	$4f^7 \rightarrow 4f^65d$	[2, 3]
	---	[b]246.5	[b]248.7	---	$4f^7 \rightarrow 4f^65d$	[3]
	---	[b]240	[b]243.1	---	$4f^7 \rightarrow 4f^65d$	[3, 4]
	---	[b]234	---	[b]235	$4f^7 \rightarrow 4f^65d$	[4]
Eu^+	[a]570	---	---	---	---	[5]
	[b]400	---	---	---	---	[6]
	[a]312	---	---	---	---	[5]
	[a]272	---	---	---	---	[5]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

References

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TABLE 27. *Optical absorption bands (in nm) of samarium centers in alkali halides*

Center	NaCl	NaI	KCl	KBr	KI	RbCl	Assignment	References
Sm^{2+}	[d]627.2	[c]662.3	[c]613	[c]614	[d]629	[d]605	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	[c]584.8	[d]569.8	---	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2]
	---	[c]542.3	[c]541.8	[c]544.9	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	---	[c]504.6	[c]504	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	[c]458.5	---	---	---	---	$4f^6 \rightarrow 4f^55d$	[2]
	---	[c]432	[c]431.5	[c]432.9	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	---	[c]408	[c]408	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	[c]382	[d]387.4	---	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2]
	---	[c]371	---	---	---	---	$4f^6 \rightarrow 4f^55d$	[2]
	---	---	[c]337.7	[c]358	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	---	[c]327.5	[c]344.9	---	---	$4f^6 \rightarrow 4f^55d$	[1, 2, 3]
	---	---	[d]275.5	---	---	---	$4f^6 \rightarrow 4f^55d$	[1, 3]
	---	---	[d]268.4	---	---	---	$4f^6 \rightarrow 4f^55d$	[1, 3]

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TABLE 27. *Optical absorption bands (in nm) of samarium centers in alkali halides*—Continued

Center	NaCl	NaI	KCl	KBr	KI	RbCl	Assignment	References
	---	---	d 261.4	---	---	---	$4f^6 \rightarrow 4f^5 5d$	[1. 3]
	---	---	d 249	---	---	---	$4f^6 \rightarrow 4f^5 5d$	[1. 3]
	---	---	d 241	---	---	---	$4f^6 \rightarrow 4f^5 5d$	[1. 3]
	---	---	d 225.5	---	---	---	$4f^6 \rightarrow 4f^5 5d$	[1. 3]
	---	---	d 187.3	---	---	---	$4f^6 \rightarrow 4f^5 6s^1$	[3]
	---	---	d 173	---	---	---	$4f^6 \rightarrow 4f^5 6s^1$	[3]
Sm^+	---	---	b 1250	---	---	---	$^6H_{5/2}$	[4]
	---	---	b 1120	---	---	---	$^6H_{7/2}$	[4]
	---	---	b 961.6	---	---	---	$^6H_{9/2}$	[4]
	---	---	b 861.1	---	---	---	$^6H_{11/2}$	[4]
	---	---	b 799.2	---	---	---	$^6H_{13/2}$	[4]

a Room temperature

b Liquid air/nitrogen temperature.

c Liquid helium temperature.

d Temperature between 4.2 and 77 K.

References

[1] Bron. W. E., and Heller. W. R., Phys. Rev. **136A,** 1433 (1964).

[2] Kaplyanskii. A. A., et al.. Optics and Spectroscopy **16,** 144 (1964).

[3] Patscheke. E., Z. Physik **186,** 63 (1965).

[4] Fong. F. K., et al.. Phys. Rev. **151,** 299 (1966).

TABLE 28. *Optical absorption bands (in nm) of holmium centers in alkali halides*

Center	KCl	KBr	Assignment	References
Ho^{2+}	b310	b299	$4f^{11} \rightarrow 4f^{10} 5d$	[1]
	b269	b260	$4f^{11} \rightarrow 4f^{10} 5d$	[1]
	b245	b225	$4f^{11} \rightarrow 4f^{10} 5d$	[1]
	b234	b216	$4f^{11} \rightarrow 4f^{10} 5d$	[1]
Ho^+	---	a375	---	[1]
	---	a282	---	[1]
	---	a252	---	[1]
Ho^0	---	a220	Clusters of Ho^0	[1]

aRoom temperature.

bLiquid air/nitrogen temperature.

cLiquid helium temperature.

dTemperature between 4.2 and 77 K.

Reference

[1] Sai. K. S. K.. Ph.D. Thesis. I.I.T. Delhi. India (1971).

TABLE 29. *Optical absorption bands (in nm) of ytterbium centers in alkali halides*

Center	NaCl	KCl	KBr	Assignment	References
Yb^{2+}	---	---	^{d}377.3	---	[1]
	---	---	^{d}337	---	[1]
	---	^{b}310	^{b}300	---	[2]
	^{b}270	^{b}270	---	---	[2]
	---	^{b}245	---	---	[2]
	---	^{b}230	^{b}225	---	[2]
Yb^{3+}	^{b}270	^{b}270	---	---	[3]

^{a}Room temperature.
^{b}Liquid air/nitrogen temperature.
^{c}Liquid helium temperature.
^{d}Temperature between 4.2 and 77 K.

References

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TABLE 30. *Optical absorption bands (in nm) of uranyl centers in alkali halides*

Center	LiF	NaCl	KCl	Assignment	References
UO_2^{2+}	^{b}290	^{b}260	^{b}270	---	[1. 2]
	^{b}240	---	^{b}234	---	[1]

^{a}Room temperature.
^{b}Liquid air/nitrogen temperature.
^{c}Liquid helium temperature.
^{d}Temperature between 4.2 and 77 K.

References

[1] Sootha. G. D.. Radharkrishna. S.. and Agarwal. S. K.. Nuovo Cimento **64B**, 19 (1969).
[2] Agarwal. S. K.. Ph.D. Thesis. I.I.T. Delhi. India. 1970.

TABLE 31. *Optical absorption bands (in nm) of hydrogen centers in alkali halides*

Center	NaF	NaCl	NaBr	NaI	KCl	KBr	KI	RbCl	RbBr	RbI	CsBr	CsI	Assignment	References
$U(H^-)$	^{a}157	192	210	---	^{d}211.5	^{d}225	244	^{d}226	242	---	^{d}242.5	^{d}269	---	[1. 2. 3. 4.5]
$U(D^-)$	---	---	---	---	^{d}210.8	^{d}224	---	^{d}225.3	---	---	---	^{d}268.5	---	[3. 5]
U_2	---	^{d}220	^{d}259	^{d}328	^{d}235	^{d}272	^{d}337	^{d}247	^{d}280.5	^{d}345	---	---	---	[6]
U_2'	---	---	^{d}242.5	^{d}300	---	^{d}257	^{d}315	---	^{d}267	^{d}325	---	---	---	[6]
U_2''	---	---	^{d}217	^{d}255.5	---	^{d}240.5	^{d}266.5	---	^{d}251.5	^{d}272.5	---	---	---	[6]

^{a}Room temperature.
^{b}Liquid air/nitrogen temperature.
^{c}Liquid helium temperature.
^{d}Temperature between 4.2 and 77 K.

References

[1] Meistrisch. M. L.. J. Phys. Chem. Solids **29**, 1119 (1968).
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Table 32. *Optical absorption bands (in nm) of halogen centers in alkali halides*

Center	NaBr	KCl	KBr	Assignment	References
I^-	[b]193.5	[b]184.7	[b]193.8	---	[1, 2]

[a]Room temperature. [b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature. [d]Temperature between 4.2 and 77 K.

References

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[2] Rolfe, J., Appl. Phys. Letters **6**, 66 (1965).

Table 33. *Optical absorption bands (in nm) of oxygen centers in alkali halides*

Center	NaF	NaCl	KCl	KBr	Assignment	References
O_2^-	---	[b]248	[b]248	[b]248	---	[1]
	142	---	194	---	---	[2, 3]

[a]Room temperature. [b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature. [d]Temperature between 4.2 and 77 K.

References

[1] Rolfe, J., Lipsett, F. R., and King, W. J., Phys. Rev. **123**, 447 (1961).

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Table 34. *Optical absorption bands (in nm) of sulphur centers in alkali halides*

Center	KCl	KBr	Assignment	References
SH^-	[b]185.1	[b]193.6	---	[1, 2, 3]
S^-	[b]192.4	[b]203.5	---	[1, 2, 3]
S^{--}	[b]393.5	---	---	[2]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

References

[1] Fischer, F., and Grundig, H., Phys. Letters **13**, 113 (1964).
[2] Fischer, F., and Grundig, H., Z. Physik **184**, 299 (1965).
[3] Rolfe, J., Appl. Phys. Letters **6**, 66 (1965).

Table 35. *Optical absorption bands (in nm) of selenium centers in alkali halides*

Center	KCl	KBr	Assignment	References
SeH^-	[d]202.4	[d]211.4	---	[1]
	[d]193.6	[d]202.3	---	[1]
Se^-	[d]208.6	[d]219.0	---	[1]
	[d]201.6	[d]212.6	---	[1]
Se^{--}	[d]395	[d]406.5	---	[1]
	[d]364	[d]374	---	[1]

[a]Room temperature.
[b]Liquid air/nitrogen temperature.
[c]Liquid helium temperature.
[d]Temperature between 4.2 and 77 K.

Reference

[1] Fischer, F., Z. Physik **187**, 262 (1965).

TABLE 36. *Optical absorption bands (in nm) of OH/OD centers in alkali halides*

Center	NaF	NaCl	KCl	KBr	Assignment	References
OH^-	151.2	[b] 185	[c] 205	[b] 214	---	[1, 2, 3, 4]
OD^-	---	---	[d] 203	---	---	[4]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

References

[1] Meistrisch, M. L., J. Phys. Chem. Solids **29,** 1119 (1968).
[2] Etzel, H. W., and Patterson, D. A., Phys. Rev. **112,** 1112 (1958).
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[4] Fischer, F., Sol. Stat. Comm. **2,** 51 (1964).

TABLE 37. *Optical absorption bands (in nm) of amide centers in alkali halides*

Center	KCl	KBr	KI	Assignment	References
NH_2^-	[d] 253.9	[d] 272.2	[d] 295.0	0–0	[1]
ND_2^-	[d] 251.8	[d] 268.5	[d] 294.0	0–0	[1]

[a] Room temperature
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

References

[1] Windheim, R., and Fischer, F., Z. Physik **197,** 309 (1966).

TABLE 38. *Optical absorption bands (in nm) of nitrite centers in alkali halides*

Center	NaBr	KCl	KBr	KI	Assignment	References
NO_2^-	*[c] 397.2	*[c] 398.8	*[c] 401.1	*[c] 401.1	Zero-phonon transition	[1, 2]

*This band shows vibrational progression with separations (~ 1010 cm^{-1} and 600 cm^{-1}).
[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

References

[1] Timusk, T., and Staude, W., Phys. Rev. Letters **13,** 373 (1964).
[2] Avarmaa, R., and Rebane, L., Phys. Stat. Sol. **35,** 107 (1969).

TABLE 39. *Optical absorption bands (in nm) of chromate centers in alkali halides*

Center	KCl	KBr	KI	Assignment	References
CrO_4^{2-}	*[b] 335	*[b] 355	*[b] 365	$t_1 \rightarrow e$	[1, 2]
	---	[b] 285	---	---	[1, 2]
	[b] 270	[b] 270	[b] 270	$t_1 \rightarrow t_2$	[1, 2]
	[b] 240	[b] 246	---	---	[1, 2]

*This absorption band shows a vibrational progression with a separation of 800 cm^{-1}. The peak position reported here corresponds to the strongest peak in the progression.
[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

References

[1] Jain, S. C., Warrier, A. V. R., and Agarwal, S. K., Chem. Phys. Letters **14,** 211 (1972).
[2] Jain, S. C., Warrier, A. V. R., and Agarwal, S. K., J. Phys. Chem. Solids **34,** 209 (1973).

TABLE 40. *Optical absorption bands (in nm) of permanganate centers in alkali halides*

Center	KBr	KI	Assignment	References
MnO_4^{1-}	*[c] 600	*[c] 650	$t_1 \rightarrow e$	[1. 2]
	*[c] 520	*[c] 540	$t_1 \rightarrow e$	[1. 2]
	[c] 390	---	$t_2 \rightarrow e$	[1]
	[c] 336	---	$t_2 \rightarrow e$	[1]
	[c] 305	---	---	[1]
	[c] 230	---	$t_1 \rightarrow t_2$	[1]
	[c] 200	---	---	[1]

*These bands show vibrational progression with separations of 760 cm^{-1} and 780 cm^{-1}. The peak position corresponds to the strongest peak in the progression.

[a] Room temperature.

[b] Liquid air/nitrogen temperature.

[c] Liquid helium temperature.

[d] Temperature between 4.2 and 77 K.

References

[1] Jain. S. C., Pooley. D., and Singh. Risal. J. Phys. C. **5**, L307 (1972).

[2] Jain. S. C., Singh. Risal. and Agarwal S. K., (to be published).

TABLE 41. *Optical absorption bands (in nm) of manganate centers in alkali halides*

Center	KCl	KBr	KI	Assignment	References
MnO_4^{2-}	[b] 850	[b] 850	[b] 850	$e \rightarrow t_2$	[1]
	*[b] 600	*[b] 600	″[b] 600	$t_1 \rightarrow e$	[1. 2]
	[b] 430	[b] 430	[b] 430	$t_1 \rightarrow t_2$	[2]
	[b] 340	[b] 340	[b] 340	$t_1 \rightarrow t_2$	[2]
	[b] 290	[b] 290	[b] 290	$t_1 \rightarrow t_2$	[2]

*This band shows vibrational progression with a separation of 740 cm^{-1}. The peak position given here corresponds to the strongest peak in the progression.

[a] Room temperature.

[b] Liquid air/nitrogen temperature.

[c] Liquid helium temperature.

[d] Temperature between 4.2 and 77 K.

References

[1] Jain. S. C.. Singh. Risal. and Agarwal. S. K., (to be published).

[2] Jain. S. C.. Sootha. G. D., and Agarwal. S. K.. J. Phys. Chem. Solids **32**, 897 (1971).

TABLE 42. *Optical absorption bands (in nm) of ferricyanide centers in alkali halides*

Center	NaCl	KCl	Assignment $t_{2g}^5(^2T_{2g})\rightarrow$	References
$Fe(CN)_6^{3-}$	[a] 505	[a] 500	$t_{2g}^4e_g^1(^4T_{1g})$	[1]
	[a] 420	[a] 414	$t_{1u}^5t_{2g}^6(^2T_{1u})$	[1]
	[a] 376	[a] 377	$t_{2g}^5a_{1g}^1(^2A_{1g})$	[1]
	[a] 357	[a] 348	$t_{2g}^4e_g^1(^4T_{2g})$	[1]
	[a] 338	[a] 323	$t_{2g}^4e_g^1(^2A_{2g}, {}^2T_{1g})$	[1]
	[a] 302	[a] 296	$t_{1u}^5t_{2g}^5e_g^1$	[1]
	[a] 262	[a] 274	$t_{2g}^4e_g^1(^2E_g)$	[1]
---	[a] 258		$t_{1u}^5t_{2g}^5e_g^1$	[1]
---	[a] 248		$t_{1u}^5t_{2g}^5e_g^1$	[1]
---	[a] 200		$t_{1u}^5t_{2g}^5e_g^1$	[1]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

References

[1] Jain. S. C.. Warrier. A. V. R.. and Sehgal. H. K.. J. Phys. C. **6**, 193 (1973).

TABLE 43. *Optical absorption bands (in nm) of cobalticyanide centers in alkali halides.*

Center	NaCl	KCl	Assignment $t_{2g}^6(^1A_{1g})\rightarrow$	References
$Co(CN)_6^{3-}$	[a] 484	[a] 480	$t_{2g}^5e_g^1(^3T_{1g})$	[1]
	[a] 409	[a] 400	$t_{2g}^5e_g^1(^3T_{2g})$	[1]
	[a] 361	[a] 353	$t_{2g}^5e_g^1(^1T_{1g})$	[1]
	[a] 316	[a] 310		
	[a] 280	[a] 277	$t_{2g}^5e_g^1(^1T_{2g})$	[1]
	[a] 260	[a] 258		
	---	[a] 201	t_{1u}	[1]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

Reference

[1] Jain. S. C.. Warrier. A. V. R.. and Sehgal. H. K.. J. Phys. C. **5**, 1511 (1972).

PART II.

Vibrational Frequencies of Internal Modes of Complex Ions Doped in Alkali Halide Crystals

TABLE 44. *Point group symmetry, normal modes and their activity in infrared absorption and Raman scattering for the molecular ions investigated.*

No. of atoms	Point group symmetry	Modes and their symmetry and activity in infrared and Raman[a]	Molecular impurities investigated
2	$D_{\infty h}$	ν_s (Σ_g^+; R)	N_2^-, O_2^-, S_2^-, Se_2^-
2	$C_{\infty v}$	ν_s (Σ^+; IR, R)	OH^-, OD^-, CN^-, SH^-, SeH^-, SSe^-
3	$D_{\infty h}$	ν_{1s} (Σ_g^+; R) ν_{2b} (Π_u; IR) ν_{3s} (Σ_u^+; IR)	N_3^-, BO_2^-
3	$C_{\infty v}$	ν_{1s} (Σ^+; IR, R) ν_{2b} (Π; IR R) ν_{3s} (Σ^+; IR, R)	NCO^-, NCS^-
3	C_{2v}	ν_{1s}(A_1; IR, R) ν_{2b}(A_1; IR, R) ν_{3s}(B_2; IR, R)	NO_2^-, NH_2^-, ND_2^-, H_2O NHD^- S_3^-
4	C_{3v}	ν_{1s}(A_1, IR, R) ν_{2b}(A_1; IR, R) ν_{3s}(E, IR, R) ν_{4b}(E; IR, R)	ClO_3^-, IO_3^-, SeO_3^{2-}
4	D_{3h}	ν_{1s}(A'; R) ν_{2b}(A''; IR) ν_{3s}(E'; IR, R) ν_{4b}(E'; IR, R)	NO_3^-, CO_3^{2-}, BO_3^{3-}
5	T_d	ν_{1s}(A_1; R) ν_{2b}(E; R) ν_{3s}(T_2; IR, R) ν_{4b}(T_2; IR, R)	NH_4^+, ND_4^+, BH_4^-, BD_4^-, BF_4^-, ClO_4^-, MnO_4^-, SO_4^{2-}, SeO_4^{2-}, CrO_4^{2-}, MnO_4^{2-}, MoO_4^{2-}, BeF_4^{2-}
13	O_h	ν_{1s}(A_{1g}; R) ν_{3s}(E_g; R) ν_{6s}(T_{1u}; IR)	$Co(CN)_6^{3-}$, $Co(CN)_6^{4-}$, $Co(CN)_6^{5-}$, $Fe(CN)_6^{3-}$, $Fe(CN)_6^{4-}$, $Fe(CN)_6^{5-}$

[a]Subscripts 's' and 'b' for the modes indicate stretching and bending respectively. IR and or R in the parenthesis after the modes means whether that particular mode is infrared and or Raman active.

TABLE 45. *Internal vibration frequencies of homonuclear diatomic molecular ions doped in alkali halide crystals.*

These ions have only one vibrational mode $\nu_s\left(\sum_g^+\right)$ which is Raman active and infrared inactive. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}. ESR and uniaxial stress experiments [1] suggest that O_2^-, S_2^- and Se_2^- are aligned along ⟨110⟩ direction in FCC alkali halides.

Crystal : Impurity	Frequency (cm^{-1}) $\nu_s\left(\sum_g^+\right)$	Temperature K	Remarks	References
KCl : N_2^-	1836 ± 3	RT	Raman	[2]
KBr : N_2^-	1821 ± 3	RT	Raman	[2]
KI : N_2^-	1870 ± 3	RT	Raman	[2]
NaCl : O_2^-	1144 ± 1	RT	Raman	[2, 3, 4]
NaBr : O_2^-	1131 ± 1	RT	Raman	[2, 3, 4]
KCl : O_2^-	1145 ± 1	RT	Raman	[2, 3, 4]
KBr : O_2^-	1135 ± 1	RT	Raman	[2, 3, 4]
KI : O_2^-	1123 ± 1	RT	Raman	[2, 3, 4]
RbCl : O_2^-	1141 ± 1	RT	Raman	[2, 3, 4]
RbBr : O_2^-	1132 ± 1	RT	Raman	[2, 3, 4]
NaBr : S_2^-	610 ± 1	RT	Raman	[2]
NaI : S_2^-	592 ± 1	RT	Raman	[2]
KBr : S_2^-	612 ± 2	RT	Raman	[2]
KI : S_2^-	594 ± 1	RT	Raman	[2]
RbBr : S_2^-	611 ± 1	RT	Raman	[2]
RbI : S_2^-	598 ± 1	RT	Raman	[2]
NaI : Se_2^-	333 ± 1	RT	Raman	[2]
KI : Se_2^-	325 ± 1	RT	Raman	[2]

RT—Room temperature.

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TABLE 46. *Internal vibrational frequencies of heteronuclear diatomic molecular ions in alkali halides.*

These ions have only one vibrational mode $\nu_s(\Sigma_g^+)$ which is both Raman and IR active. The accuracy. when given by the authors. is quoted. In other cases the accuracy is estimated to be ±1 cm^{-1}. except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ±0.5 cm^{-1}. Stress and dichroism experiments suggest that the molecular axis in the ⟨100⟩ direction for CN^- and perhaps also for OH^- in FCC alkali halides[1] and ⟨110⟩ or possibly ⟨111⟩ in BCC alkali halides[3]. The free ion frequencies are:

$\nu_s = 3596$ cm^{-1} for OH^-. $\nu_e = 2680$ cm^{-1} for OD^- and $\nu_s = 2042$ cm^{-1} for CN^-.

Crystal : Impurity	Frequency (cm^{-1}) $\nu_s(\Sigma_g^+)$	Temperature K	Remarks	References
NaCl : CN^-	2106.8	10	Raman	[2]
NaBr : CN^-	2087±1	100	IR	[3]
NaI : CN^-	2074±1	100	IR	[3]
KCl : CN^-	2087.7	8.5	Raman	[2]
KBr : CN^-	2078	2	IR	[4]
KI : CN^-	2067	2	IR	[4]
RbCl : CN^-	2081	2	IR	[4]
RbBr : CN^-	2070±1	100	IR	[3]
RbI : CN^-	2063±1	100	IR	[3]
CsCl : CN^-	2078±1	100	IR	[3]
CsBr : CN^-	2066±1	100	IR	[3]
CsI : CN^-	2053±1	100	IR	[3]
NaCl : OH^-	3654.5±0.5	4.5	IR	[6]
NaBr : OH^-	3626±0.5	4.5	IR	[6]
KCl : OH^-	3641±0.5	4.5	IR	[6]
KBr : OH^-	3618±0.5	4.5	Raman and IR	[5. 6]
KI : OH^-	3603	4.5	IR	[6]
RbCl : OH^-	3632±0.5	4.5	IR	[6]
NaCl : OD^-	2689	4.5	Raman	[5]
KCl : OD^-	2684.5±0.5	4.5	IR	[6. 7]
KBr : OD^-	2668±0.5	4.5	IR	[6]
KCl : SH^-	*2585	RT	IR	[8]
KBr : SH^-	*2569	RT	IR	[8]
KCl : SeH^-	*2294	RT	IR	[9]
NaI : SSe^-	462±1	RT	Raman	[10]
KI : SSe^-	464±1	RT	Raman	[10]

RT Room temperature.

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TABLE 47. *Internal vibrational frequencies (cm^{-1}) of linear triatomic molecular ions with $D_{\infty h}$ point group, doped in alkali halides.*

These ions have one mode $\nu_1\left(\sum_g^+, s\right)$ which is only Raman active and two modes $\nu_2\left(\prod_u^+, b\right)$ and $\nu_3\left(\sum_u^+, s\right)$ only infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}, N_3^- and BO_2^- enters substitutionally into the lattice at the anion site such that molecular axis is along ⟨111⟩ in FCC alkali halides [1, 2]. The free ion values are known only for N_3^- ions and are $\nu_1 = 1344$ cm^{-1}, $\nu_2 = 645$ cm^{-1} and $\nu_3 = 2041$ cm^{-1}

Crystal : Impurity	Frequency (cm^{-1})			Temperature K	Remarks	References
	$\nu_1\left(\sum_g^+\right)$	$\nu_2\left(\prod_u^+\right)$	$\nu_3\left(\sum_u^-\right)$			
NaCl : N_3^-	---	640.3 ± 0.1	2083.1 ± 0.1	120	IR	[1]
NaBr : N_3^-*	---	---	2064.5	---	IR	[2]
NaI : N_3^-*	---	---	2037.0	---	IR	[2]
KCl : N_3^-	---	643.0 ± 0.1	2051.2 ± 0.1	120	IR	[1]
KBr : N_3^-	---	641.5 ± 0.1	2038.2 ± 0.1	120	IR	[1]
KI : N_3^-	---	639.7 ± 0.1	2022.1 ± 0.1	120	IR	[1]
RbCl : N_3^-*	---	---	2040.0	---	IR	[2]
RbBr : N_3^-*	---	---	2029.0	---	IR	[2]
RbI : N_3^-*	---	---	2016.2	---	IR	[2]
CsCl : N_3^-*	---	---	2043.0	---	IR	[2]
CsBr : N_3^-*	---	---	2026.0	---	IR	[2]
CsI : N_3^-*	---	---	2006.0	---	IR	[2]
KCl : BO_2^-						
$^{10}B^{16}O^{16}O$	---	610	2043	---	IR	[3]
$^{10}B^{16}O^{17}O$	---	---	2038	---	IR	[3]
$^{10}B^{16}O^{18}O$	---	---	2029	---	IR	[3]
$^{11}B^{16}O^{16}O$	---	590	1972	---	IR	[3]
$^{11}B^{16}O^{17}O$	---	---	1968	---	IR	[3]
$^{11}B^{16}O^{18}O$	---	---	1959	---	IR	[3]
KBr : BO_2^-						
$^{10}B^{16}O^{16}O$	---	607	2029	---	IR	[3]
$^{10}B^{16}O^{17}O$	---	---	2023	---	IR	[3]
$^{10}B^{16}O^{18}O$	---	---	2016	---	IR	[3]
$^{11}B^{16}O^{16}O$	---	587	1959	---	IR	[3]
$^{11}B^{16}O^{17}O$	---	---	1953	---	IR	[3]
$^{11}B^{16}O^{18}O$	---	---	1946	---	IR	[3]
KI : BO_2^-						
$^{10}B^{16}O^{16}O$	---	607	2016	---	IR	[4]
$^{10}B^{16}O^{18}O$	---	---	2000	---	IR	[4]
$^{11}B^{16}O^{16}O$	---	587	1946	---	IR	[4]

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TABLE 48. *Vibrational frequencies of triatomic linear molecular ions doped in alkali halides.*

These ions have three modes, $\nu_1(\Sigma^+)$, $\nu_2(\Pi)$ and $\nu_3(\Sigma^+)$ which are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}. NCO^- and NCS^- enter the alkali halide lattice substitutionally replacing the anion such that the molecular axis is along ⟨111⟩ in FCC alkali halides [1] and along ⟨100⟩ in BCC alkali halides [5]. The free ion frequencies are:

$\nu_1 = 1207$ cm^{-1}, $\nu_2 = 637$, 628 cm^{-1} and $\nu_3 = 2165$ cm^{-1} for NCO^- and $\nu_1 = 743$ cm^{-1}, $\nu_2 = 470$ cm^{-1} and $\nu_3 = 2066$ cm^{-1} for NCS^-.

Crystal : Impurity	Frequency (cm^{-1})			Temperature K	Remarks	References
	$\nu_1(\Sigma^+)$	$\nu_2(\Pi)$	$\nu_3(\Sigma^+)$			
NaCl : NCO^-						
$^{14}N^{12}C^{16}O^-$	---	633.2±0.3	2211.2±0.3	298	IR	[1]
$^{14}N^{13}C^{16}O^-$	---	---	2153.1±0.3	298	IR	[1]
NaBr : NCO^-	1217.6	637.3	2219	---	IR	[2]
NaI : NCO^-	1210.6	636.4	2195	---	IR	[2]
KCl : NCO^-						
$^{14}N^{12}C^{16}O^-$	1211	---	2182	100	IR	[4]
$^{14}N^{13}C^{16}O^-$	---	613.2±0.3	2153.1±0.3	298	IR	[1]
KBr : NCO^-						
$^{14}N^{12}C^{16}O^-$	1206	629.98	2170	100	IR	[3, 4]
$^{14}N^{13}C^{16}O^-$	---	612.78	2115	100	IR	[3]
$^{15}N^{12}C^{16}O^-$	---	626.64	2154	100	IR	[3]
$^{14}N^{12}C^{18}O^-$	---	625.23	2163	100	IR	[3]
$^{14}N^{13}C^{18}O^-$	---	---	2104±0.3	298	IR	[1]
$^{15}N^{13}C^{16}O^-$	---	---	2097	100	IR	[3]
$^{15}N^{12}C^{18}O^-$	---	---	2144	100	IR	[3]
KI : NCO^-						
$^{14}N^{12}C^{16}O^-$	1200.8±0.3	628.0±0.3	2155.8±0.3	298	IR	[1]
$^{14}N^{13}C^{16}O^-$	---	610.0±0.3	2099.0±0.3	298	IR	[1]
$^{14}N^{12}C^{18}O^-$	---	---	2148.2±0.3	298	IR	[1]
$^{15}N^{12}C^{16}O^-$	---	---	2138.7±0.3	298	IR	[1]
RbCl : NCO^-	1211.8	635.1	2201	---	IR	[2]
RbBr : NCO^-	1207	633.5	2191	---	IR	[2]
RbI : NCO^-	1202.4	632.4	2179	---	IR	[2]
CsCl : NCO^-	1212.4	633.2	2205	---	IR	[2]
CsBr : NCO^-	1206	632	2187	---	IR	[2]
CsI : NCO^-	1200	630	2170	---	IR	[2]
NaI : NCS^-*	---	---	2050	40	IR	[5]
KI : NCS^-*	---	---	2038	40	IR	[5]
RbI : NCS^-*	---	---	2028	40	IR	[5]
CsI : NCS^-*	---	---	2038	40	IR	[5]

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TABLE 49. *Vibrational frequencies* (cm^{-1}) *of bent triatomic molecular ions doped in alkali halides.*

These ions have three modes $\nu_1(A_1)$, $\nu_2(A_1)$ and $\nu_3(B_2)$ which are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The NO_2^- ion enters substitutionally into the lattice at the anion site such that the 2-fold axis of the ion points in the ⟨110⟩ directions in FCC alkali halides. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}. The free ion values are:

$\nu_1 = 1328$ cm^{-1}, $\nu_2 = 828.2$ cm^{-1} and $\nu_3 = 1261$ cm^{-1} for NO_2^-
$\nu_1 = 3210$ cm^{-1}, $\nu_2 = 1532$ cm^{-1} and $\nu_3 = 3266$ cm^{-1} for NH_2^-
$\nu_1 = 2355$ cm^{-1}, $\nu_2 = 1131$ cm^{-1} and $\nu_3 = 2429$ cm^{-1} for ND_2^-
$\nu_1 = 2387$ cm^{-1}, $\nu_2 = 1247$ cm^{-1} and $\nu_3 = 3236$ cm^{-1} for NHD^- and
$\nu_1 = 3657$ cm^{-1}, $\nu_2 = 1595$ cm^{-1} and $\nu_3 = 3756$ cm^{-1} for H_2O.

Crystal:Impurity	Frequency (cm^{-1})			Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(A_1)$	$\nu_3(B_2)$			
NaCl:NO_2^-	1346	636	1304	2	IR	[1]
NaBr:NO_2^-	1327±2	828±2	1283±2	6	R	[2]
KCl:NO_2^-	1329	805	1290	2	IR	[1]
KBr:NO_2^-						
$^{14}N^{16}O_2^-$	1316.2±0.5	798.1±0.5	1275±0.5	8	IR	[3]
$^{14}N^{16}O^{18}O^-$	1303.9±0.5	779±0.5	1256.6±0.5	8	IR	[3]
$^{15}N^{16}O^{16}O^-$	1294.2±0.5	793±0.5	1249.5±0.5	8	IR	[3]
$^{15}N^{16}O^{18}O^-$	---	---	1230.4	8	IR	[3]
$^{15}N^{18}O^{18}O^-$	---	---	1221.5	8	IR	[3]
KI:NO_2^-	1308	806±2	1253	5	IR	[1]
NaCl:S_3^-	531±1	---	---	300	IR, R	[4]
NaBr:S_3^-	523±1	---	---	300	IR, R	[4]
KCl:S_3^-	527±1	---	540±2	300	IR, R	[4]
KBr:S_3^-	523±1	---	585±2	300	IR, R	[4]
KI:S_3^-	543±1	---	585±2	300	IR, R	[4]
RbCl:S_3^-	528±1	---	---	300	IR, R	[4]
RbBr:S_3^-	555±1	---	---	300	IR, R	[4]
RbI:S_3^-	544±1	---	---	300	IR, R	[4]
KCl:NH_2^-	3202	1532	3258	20	[a] IR	[5]
KBr:NH_2^-	3185	1508	3235	20	[a] IR	[5]
KI:NH_2^-	3154	1500	3202	20	[a] IR	[5]
KCl:NHD^-	2379	1355	3218	20	[a] IR	[5]
KBr:NHD^-	2371	1330	3202	20	[a] IR	[5]
KCl:ND_2^-	2353	1137	2419	20	[a] IR	[5]
KBr:ND_2^-	2339	1121	2412	20	[a] IR	[5]
KI:ND_2^-	2323	1113	2395	20	[a] IR	[5]
KCl:H_2O	3435	1630	3400	20	IR	[6]
KBr:H_2O	3472	1625	3425	20	IR	[6]
KI:H_2O	3570	1690	3390	20	IR	[6]

[a] The absorption maxima expressed in eV in the paper is converted to wave number (cm^{-1}) by using the conversion factor 1 eV = 8065 cm^{-1}.

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TABLE 50. *Vibrational frequencies of nonplanar tetra-atomic (C_{3v}) molecular ions doped in alkali halide crystals.*

These ions have four modes $\nu_1(A_1)$, $\nu_2(A_1)$, $\nu_3(E)$ and $\nu_4(E)$ which are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}. ClO_3^-, IO_3^- and SeO_3^{2-} ions go substitutionally into the lattice at the anion site such that the 3-fold axis of the ion coincides with ⟨111⟩ direction [1–3] in FCC alkali halides. The free ion frequencies are:

$\nu_1 = 930$, $\nu_2 = 610$, $\nu_3 = 982$ and $\nu_4 = 479$ cm^{-1} for ClO_3^-
$\nu_1 = 754$, $\nu_2 = 373$, $\nu_3 = 774$ and $\nu_4 = 355, 330$ cm^{-1} for IO_3^-
$\nu_1 = 807$, $\nu_2 = 432$, $\nu_3 = 737$ and $\nu_4 = 374$ cm^{-1} for SeO_3^{2-}.

Crystal:Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(A_1)$	$\nu_3(E)$	$\nu_4(E)$			
NaCl:ClO_3^-							
$^{35}ClO_3^-$	---	---	1027.5	---	---	IR	[1]
$^{37}ClO_3^-$	---	---	1017.5	---	---	IR	[1]
KCl:ClO_3^-							
$^{35}ClO_3^-$	---	---	1016	---	---	IR	[1]
$^{37}ClO_3^-$	---	---	1006	---	---	IR	[1]
KBr:ClO_3^-							
$^{35}ClO_3^-$	947.60	628.01	1004.45	493.82	176	IR	[1]
$^{37}ClO_3^-$	940.60	623.08	994.35	492.28	176	IR	[1]
KI:ClO_3^-							
$^{35}ClO_3^-$	937.60	620.88	990.36	487.12	176	IR	[1]
$^{37}ClO_3^-$	930.80	615.98	980.28	485.53	176	IR	[1]
KI:IO_3^-							
$I^{16}O_3^-$	791.05 ± 0.15	381.7 ± 0.15	806.75 ± 0.15	323.7 ± 0.15	130	IR	[2]
$I^{18}O_3^-$	749.75 ± 0.15	365.6 ± 0.15	767.25 ± 0.15	307.15 ± 0.15	130	IR	[2]
KBr:SeO_3^{2-}	845.5	---	780 ± 1	---	293	[a]IR	[3]
	---	---	763 ± 1	---	293	[a]IR	[3]
	---	---	752.5 ± 1	---	293	[a]IR	[3]
	---	---	749 ± 1	---	293	[a]IR	[3]

[a] Charge compensating defect occupying the nearest neighbour positions lowers the site symmetry of the ion resulting in the splitting of ν_3.

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TABLE 51. *Vibrational frequencies (cm^{-1}) of planar tetraatomic molecular ions (D_{3h}) doped in alkali halide crystals.*

These ions have four modes $\nu_1(A')$ Raman active, $\nu_2(A'')$ infrared active and $\nu_3(E')$ and $\nu_4(E')$ both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}. NO_3^-, CO_3^{2-}, and BO_3^{3-} enter the lattice substitutionally at the anion site such that the plane of the ion is perpendicular to the ⟨111⟩ direction [1, 2, 6] in FCC alkali halides.

Crystal: Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A')$	$\nu_2(A'')$	$\nu_3(E')$	$\nu_4(E')$			
NaCl:NO_3^-	---	---	1423 ± 1	---	77	IR	[1]
NaBr:NO_3^-	---	---	1398 ± 1	---	77	IR	[1]
NaI:NO_3^-	---	---	1391 ± 1	---	77	IR	[1]
KCl:NO_3^-	---	---	1398 ± 1	---	77	IR	[1]
KBr:NO_3^-							
$^{14}N^{16}O_3^-$	1054.8 ± 0.5	841.3 ± 0.5	1382.2 ± 0.5	715.6 ± 0.5	8	IR	[2]
$^{14}N^{16}O_2^{18}O^-$	1034.9	837.8	1383.2	---	8	IR	[2]
$^{14}N^{16}O^{18}O_2^-$	---	834.3	1377.2	---	8	IR	[2]
$^{14}N^{18}O_3^-$	944.4	830.6	1363.4	---	8	IR	[2]
$^{15}N^{16}O_3^-$	1055.1	820.0	1352.4	714.4	8	IR	[2]
$^{15}N^{16}O_2^{18}O^-$	---	816.4	1352.3 1338.7	---	8	IR	[2]
$^{15}N^{16}O^{18}O_2^-$	---	---	1344.7 1329.3	---	8	IR	[2]
$^{15}N^{18}O_3^-$	---	---	1329.3	---	8	IR	[2]
KI:NO_3^-	---	---	1372 ± 1	---	77	IR	[1]
KCl:CO_3^{2-}	---	882	1476 1420 1391	---	300	[a]IR	[4]
KCl:CO_3^{2-}, Ca^{2+}	---	---	1520 1398	---	300	[a]IR	[3]
KCl:CO_3^{2-}, Sr^{2+}	1073	880	1493 1473 1420 1380	---	300	[a]IR	[4]
KCl:CO_3^{2-}, Pb^{2+}	1049	864	1551 1333	736 681	---	[a]IR	[5]
KBr:CO_3^{2-}	---	883	1475 1459 1402 1380	---	300	[a]IR	[4]
KBr:CO_3^{2-}, Pb^{2+}	1043	863	1556 1319	731 677	---	[a]IR	[5]
KI:CO_3^{2-}	---	885	1485 1398 1368	---	300	[a]IR	[4]
KBr:BO_3^{3-}	952	735	1247 1222	---	300	[a]IR	[6]
KBr:H_3BO_3	1040	---	1450 1400	---	300	[a]IR	[6]

[a] Because of the charge compensating defect in the neighbourhood of the ion the symmetry is lowered resulting in the splitting of ν_3 and ν_4.

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TABLE 52. *Vibrational frequencies of penta-atomic tetrahedral molecular ions (T_d) doped in alkali halides.*

These ions have four modes of which $\nu_1(A_1)$ and $\nu_2(E)$ are only Raman active, while $\nu_3(T_2)$ and $\nu_4(T_2)$ are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ±1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ±0.5 cm^{-1}. These tetrahedral ions enter the lattice substitutionally such that the four bonds are directed along the ⟨111⟩ directions in FCC alkali halides [2, 3]. In BCC alkali halides the tetrahedral ions occupy the anion site such that the site symmetry is reduced to D_{2d} [1–3]. The free ion frequencies are:

$\nu_1 = 3040$, $\nu_2 = 1680$, $\nu_3 = 3145$ and $\nu_4 = 1400$ cm^{-1} for $^{14}NH_4^+$
$\nu_1 =$ — , $\nu_2 = 1646$, $\nu_3 = 3137$ and $\nu_4 = 1399$ cm^{-1} for $^{15}NH_4^+$
$\nu_1 = 2214$, $\nu_2 = 1215$, $\nu_3 = 2346$ and $\nu_4 = 1065$ cm^{-1} for ND_4^+
$\nu_1 = 2264$, $\nu_2 = 1210$, $\nu_3 = 2244$ and $\nu_4 = 1080$ cm^{-1} for BH_4^-
$\nu_1 = 1570$, $\nu_2 = 855$, $\nu_3 = 1696$ and $\nu_4 = 823$ cm^{-1} for BD_4^-
$\nu_1 = 769$, $\nu_2 = 353$, $\nu_3 = 984$ and $\nu_4 = 524$ cm^{-1} for $^{11}BF_4^-$
$\nu_1 = 769$, $\nu_2 = 353$, $\nu_3 = 1016$ and $\nu_4 = 529$ cm^{-1} for $^{10}BF_4^-$
$\nu_1 = 928$, $\nu_2 = 459$, $\nu_3 = 1119$ and $\nu_4 = 625$ cm^{-1} for ClO_4^-
$\nu_1 = 845$, $\nu_2 = 355$, $\nu_3 = 910$ and $\nu_4 = 395$ cm^{-1} for MnO_4^-
$\nu_1 = 983$, $\nu_2 = 450$, $\nu_3 = 1105$ and $\nu_4 = 611$ cm^{-1} for SO_4^{2-}
$\nu_1 = 833$, $\nu_2 = 335$, $\nu_3 = 875$ and $\nu_4 = 432$ cm^{-1} for SeO_4^{2-}
$\nu_1 = 847$, $\nu_2 = 348$, $\nu_3 = 884$ and $\nu_4 = 368$ cm^{-1} for CrO_4^{2-}
$\nu_1 = 894$, $\nu_2 = 381$, $\nu_3 = 833$ and $\nu_4 = 318$ cm^{-1} for MoO_4^{2-}

Crystal:Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(E)$	$\nu_3(T_2)$	$\nu_4(T_2)$			
CsCl:NH_4^-							
$^{14}NH_4^-$	---	---	3129	1432	---	IR	[1]
$^{15}NH_4^+$	---	---	3118	1426	---	IR	[1]
CsBr:NH_4^+	---	---	3132	1422	---	IR	[1]
CsI:NH_4^+	---	---	3136	1411.5	---	IR	[1]
CsCl:ND_4^+							
$^{14}ND_4^+$	---	---	2349	1084	---	IR	[1]
$^{15}ND_4^+$	---	---	2331	1077.3	---	IR	[1]
CsBr:ND_4^-	---	---	2350	1077.3	---	IR	[1]
CsI:ND_4^-	---	---	2350	1070.9	---	IR	[1]
NaCl:BH_4^-	---	---	2376 ± 3	1166 ± 3	120	IR	[2]
NaBr:BH_4^-	---	---	2284 ± 3	1123 ± 3	300	IR	[2]
NaI:BH_4^-	---	---	2278 ± 3	1109 ± 3	300	IR	[2]
KCl:BH_4^-	---	---	2321 ± 3	1142 ± 3	300	IR	[2]
KBr:BH_4^-	---	---	2290 ± 3	1125 ± 3	300	IR	[2]
KI:BH_4^-	---	---	2256 ± 3	1107 ± 3	300	IR	[2]
CsBr:BH_4^-	---	---	2340 ± 3	1090 ± 3	120	IR	[2]
CsI:BH_4^-	---	---	2298 ± 3	1070 ± 3	120	IR	[2]
KCl:BD_4^-	---	---	1696 ± 3	863 ± 3	300	IR	[2]
KBr:BD_4^-	---	---	1678 ± 3	856 ± 3	300	IR	[2]
KI:BD_4^-	---	---	1657 ± 3	842 ± 3	300	IR	[2]
CsBr:BD_4^-	---	---	1748 ± 3	835 ± 3	120	IR	[2]
CsI:BD_4^-	---	---	1707 ± 3	820 ± 3	120	IR	[2]
NaI:BF_4^-							
$^{10}BF_4^-$	---	---	1120.5 ± 0.5	530.0 ± 0.5	300	IR	[3]
$^{11}BF_4^-$	---	---	1079 ± 0.5	528.0 ± 0.5	300	IR	[3]
KCl:BF_4^-							
$^{10}BF_4^-$	---	---	1131.0 ± 0.5	538.0 ± 0.5	300	IR	[3]
$^{11}BF_4^-$	---	---	1090.5 ± 0.5	536.5 ± 0.5	300	IR	[3]

TABLE 52. *Vibrational frequencies of penta-atomic tetrahedral molecular ions* (T_d) *doped in alkali halides.* — Continued

Crystal:Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(E)$	$\nu_3(T_2)$	$\nu_4(T_2)$			
KBr:BF_4^-							
$^{10}BF_4^-$	---	---	1124.0 ± 0.5	532.5 ± 0.5	300	IR	[3]
$^{11}BF_4^-$	---	---	1084.0 ± 0.5	531.0 ± 0.5	300	IR	[3]
KI:BF_4^-							
$^{10}BF_4^-$	---	---	1116.5 ± 0.5	528.0 ± 0.5	300	IR	[3]
$^{11}BF_4^-$	---	---	1076.5 ± 0.5	526.5 ± 0.5	300	IR	[3]
CsBr:BF_4^-							
$^{10}BF_4^-$	---	---	1120 ± 1	535 ± 1	300	IR	[3]
$^{11}BF_4^-$	---	---	1080 ± 1	533 ± 1	300	IR	[3]
CsI:BF_4^-							
$^{10}BF_4^-$	---	---	1109 ± 1	529 ± 1	300	IR	[3]
$^{11}BF_4^-$	---	---	1070 ± 1	527 ± 1	300	IR	[3]
KCl:ClO_4^-	---	---	1133.7	642.6	176	IR	[4]
KBr:ClO_4^-							
$^{35}ClO_4^-$	---	---	1122.60	636.18	176	IR	[4, 5]
$^{37}C10_4^-$	---	---	1109.40	633.18	176	IR	[5]
KI:ClO_4^-	---	---	1111.00	631.78	176	IR	[4, 5]
RbBr:ClO_4^-	---	---	1118.35	634.78	176	IR	[4]
RbI:ClO_4^-	---	---	1100.10	631.36	176	IR	[4]
KBr:MnO_4^-	840	---	923 ± 1	---	300	IR, R	[6]
KI:MnO_4^-	840	---	913 ± 1	---	300	IR, R	[6]
RbBr:MnO_4^-	---	---	923.5	404.5	77	IR	[7]
KCl:SO_4^{2-}, ⊟	---	---	1172 1119 1113	---	300	[a]IR	[8]
KCl:SO_4^{2-}, Ca^{2+}	982	---	1186 1157 1090	651 629 616	300	[b]IR	[8, 9, 10]
KCl:SO_4^{2-}, Sr^{2+}	---	---	1184 1152 1089	---	300	[b]IR	[10]
KCl:SO_4^{2-}, Ba^{2+}	979	---	1186 1147 1083	640 628 619	300	[b]IR	[9, 10]
KCl:SO_4^{2-}, Zn^{2+}	---	---	1185 1156 1090	---	300	[b]IR	[10]
KCl:SO_4^{2-}, Cd^{2+}	---	---	1185 1156 1090	---	300	[b]IR	[10]
KC1:SO_4^{2-},Pb^{2-}	969	---	1197 1150 1048	---	300	[b]IR	[9, 10]

TABLE 52. *Vibrational frequencies of penta-atomic tetrahedral molecular ions (T_d) doped in alkali halides.* — Continued

Crystal:Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(E)$	$\nu_3(T_2)$	$\nu_4(T_2)$			
KBr:SO_4^{2-}, Ca^{2+}							
$^{34}SO_4^{2-}$	975	---	1172 1135 1067	---	77	[b]IR	[9]
$^{32}SO_4^{2-}$	977	---	1185 1154 1082	---	77	[b]IR	[9]
KCl:SeO_4^{2-}, M^{2+}							
$^{82}SeO_4^{2-}$	---	---	925.5 ± 1 904.5 ± 1 860.5 ± 1	---	120	[b]IR	[11]
$^{80}SeO_4^{2-}$	836	---	928 ± 1 907 ± 1 862.5 ± 1	---	120	[b]IR	[11]
$^{78}SeO_4^{2-}$	---	---	930.5 ± 1 909.5 ± 1 865.0 ± 1	---	120	[b]IR	[11]
$^{77}SeO_4^{2-}$	---	---	931.5 ± 1 910.5 ± 1 866.0 ± 1	---	120	[b]IR	[11]
$^{76}SeO_4^{2-}$	---	---	933 ± 1 912 ± 1 867.5 ± 1	---	120	[b]IR	[11]
KBr:SeO_4^{2-}, M^{2+}							
$^{82}SeO_4^{2-}$	---	---	917.5 ± 1 897.5 ± 1 851.5 ± 1	---	120	[b]IR	[11]
$^{80}SeO_4^{2-}$	828.5	---	920 ± 1 899.5 ± 1 854 ± 1	---	120	[b]IR	[11]
$^{78}SeO_4^{2-}$	---	---	922.5 ± 1 902.0 ± 1 856.0 ± 1	---	120	[b]IR	[11]
$^{77}SeO_4^{2-}$	---	---	924 ± 1 903 ± 1 857 ± 1	---	120	[b] IR.	[11]
$^{76}SeO_4^{2-}$	---	---	925.5 ± 1 904.5 ± 1 858.5 ± 1	---	120	[b] IR,	[11]
KCl : CrO_4^{2-}	---	---	913 ± 1	---	300	IR	[12]
KCl : CrO_4^{2-}.⊟	860	---	939 ± 1 896 ± 1 887 ± 1	---	300	[a] IR,	[12]

TABLE 52. *Vibrational frequencies of penta-atomic tetrahedral molecular ions (T_d) doped in alkali halides.* — Continued

Crystal:Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(E)$	$\nu_3(T_2)$	$\nu_4(T_2)$			
KCl : CrO_4^{2-}. Ca^{2+}	860	---	944±1 929±1 881±1	---	300	[b] IR,	[13]
KBr : CrO_4^{2-}	---	---	908	---	300	IR	[12]
KBr : CrO_4^{2-}.⊟	856	---	927±1 894±1 888±1	---	300	[a] IR	[12]
KBr : CrO_4^{2-}. Mg^{2+}	856	---	937±1 925±1 880±1	---	77	[b] IR	[14]
KBr : CrO_4^{2-}. Ca^{2+}	855	---	936±1 924±1 880±1	433 416 399	77	[b] IR	[13, 14]
KBr : CrO_4^{2-}. Sr^{2+}	853	---	938±1 922±1 878±1	428 --- 399	77	[b] IR	[14]
KBr : CrO_4^{2-}. Ba^{2+}	849	---	940±1 921±1 872±1	427 414 401	77	[b] IR	[14]
KBr : CrO_4^{2-}. Pb^{2+}	837	---	941±1 920±1 843±1	415 391 378	77	[b] IR	[14]
KI : CrO_4^{2-}	---	---	907	---	300	[b] IR	[12]
KI : CrO_4^{2-}, ⊟	855	---	926±1 891±1 884±1	---	300	[a] IR	[12]
KI : CrO_4^{2-}, Ca^{2+}	855	---	928±1 920±1 875±1	---	300	[b] IR	[12]
KBr : MnO_4^{2-}	830	---	860±1	---	300	IR, R	[6]
KBr : MnO_4^{2-}, ⊟	830	---	870±1 842±1 836±1	---	300	[a] IR	[6]
KBr : MnO_4^{2-}. Ca^{2+}	830	---	890±1 880±1 846±1	---	300	[b] IR	[6]
KBr : MoO_4^{2-}	898	---	855±1	---	300	IR, R	[15]
KBr : MoO_4^{2-}, ⊟	898	---	876±1 844±1 834±1	---	300	[a] IR	[15]

TABLE 52. *Vibrational frequencies of penta-atomic tetrahedral molecular ions (T_d) doped in alkali halides.* — Continued

Crystal:Impurity	Frequency (cm^{-1})				Temperature K	Remarks	References
	$\nu_1(A_1)$	$\nu_2(E)$	$\nu_3)T_2)$	$\omega_4(T_2)$			
KCl:BeF_4^{2-}	---	---	837.4±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Mg^{2+}	---	---	910.4±1 870.4±1 770.0±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Ca^{2+}	---	---	909.0±1 870.3±1 770.2±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Sr^{2+}	---	---	909.6±1 862.6±1 768.1±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Ba^{2+}	---	---	910.9±1 853.4±1 762.7±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Zn^{2+}	---	---	909.0±1 869.0±1 780.0±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Cd^{2+}	---	---	910±1 --- 768±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Mn^{2+}	---	---	909.8±1 870.0±1 770.0±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Sn^{2+}	---	---	910.1±1 870.0±1 770.0±1	---	300	[b]IR	[16]
KCl : BeF_4^{2-}. Pb^{2+}	---	---	909.8±1 868.0±1 757.6±1	---	300	[b]IR	[16]

[a] Here the charge compensation is by an anion vacancy in one of the twelve nearest neighbour anion sites, reducing the symmetry from T_d to C_s resulting in the splitting of $\nu_3(T_2)$ into $\nu_3(A')+\nu_3(A')+\nu_3(A'')$. Here $\nu_3(A'')<\nu_3(A')$. ⊟ denotes anion vacancy.

[b] Here charge compensation is by a divalent cation in one of the six nearest neighbour cation sites, reducing the symmetry of the ion to C_{2v} resulting in the splitting of $\nu_3(T_2)$ into $\nu_3(A_1)+\nu_3(B_1)+\nu_3(B_2)$. Here $\nu_3(B_2)>\nu_3(A_1)>\nu_3(B_1)$. M^{2+} denotes unknown divalent cation impurity.

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TABLE 53. *Vibrational frequencies of octahedral complexes doped in alkali halide crystals.*

The $\nu_1(A_{1g})$ and $\nu_3(E_g)$ stretching modes are only Raman active and the stretching mode $\nu_6(T_{1u})$ is only infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be ± 1 cm^{-1}, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than ± 0.5 cm^{-1}. $Co(CN)_6^{n-}$ and $Fe(CN)_6^{n-}$ ($n=3, 4, 5$) ions enters the lattice substitutionally such that the metal ion occupies the cation site and the six CN^- ions occupying the six nearest neighbour anion sites in FCC alkali halides.

Crystal : Impurity	Frequency (cm^{-1})			Temperature K	Remarks	References
	$\nu_1(A_{1g})$	$\nu_3(E_g)$	$\nu_6(T_{1u})$			
NaCl : $Co(^{12}CN)_6^{3-}$	---	---	2142 ± 1 2137 ± 1 2130 ± 1 2124 ± 1 2121 ± 1	300	[a] IR	[1]
NaCl : $Co(^{13}CN)_6^{3-}$	---	---	2094 ± 1 2089 ± 1 2085 ± 1 2078 ± 1	300	[a] IR	[1]
KCl : $Co(^{12}CN)_6^{3-}$	---	---	2128 ± 1 2126 ± 1 2118 ± 1 2111 ± 1 2109 ± 1	300	[a] IR	[1]
KCl : $Co(^{13}CN)_6^{3-}$	---	---	2085 ± 1 2076 ± 1	300	[a] IR	[1]
NaCl : $Co(CN)_6^{4-}$	---	---	2094 ± 1 2086 ± 1 2081 ± 1 2076 ± 1	300	[a, b] IR	[1]
KCl : $Co(CN)_6^{4-}$	---	---	2085 ± 1 2076 ± 1 2067 ± 1 2063 ± 1	300	[a, b] IR	[1]
NaCl : $Co(CN)_6^{5-}$	---	---	1976 ± 1	300	[b] IR	[1]
KCl : $Co(CN)_6^{5-}$	---	---	1959 ± 1	300	[b] IR	[1]
NaCl : $Fe(CN)_6^{3-}$	2131	2127	2121 ± 1 2115 ± 1 2110 ± 1	300	[a] IR	[2]
KCl : $Fe(CN)_6^{3-}$	2126	2121	2109 ± 1 2103 ± 1 2099 ± 1	300	[a] IR	[2]
NaCl:$Fe(CN)_6^{4-}$	---	---	2073 ± 1 2064 ± 1 2050 ± 1 2047 ± 1	300	[a] IR	[2]
KCl:$Fe(CN)_6^{4-}$	---	---	2059 ± 1 2048 ± 1 2032 ± 1 2028 ± 1	300	[a] IR	[2]

TABLE 53. *Vibrational frequencies of octahedral complexes doped in alkali halide crystals*—Continued

Crystal:Impurity	Frequency (cm^{-1})			Temperature K	Remarks	References
	$\nu_1(A_{1g})$	$\nu_3(E_g)$	$\nu_6(T_{1u})$			
NaCl:$Fe(CN)_6^{5-}$	---	---	1967±1	300	[b] IR	[2]
KCl:$Fe(CN)_6^{5-}$	---	---	1947±1	300	[b] IR	[2]

[a] Since there are charge compensating defects in the neighbourhood of the ions. the symmetry of the complex is lowered resulting in the splitting of $\nu_6(T_{1u})$ mode giving rise to more than one band.
[b] These species are produced by X-irradiating the NaCl and KCl crystals containing $Co(CN)_6^{3-}$ and $Fe(CN)_6^{3-}$ ions.

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PART III.

External Vibrational Frequencies of Impurity Centers Doped in Alkali Halide Crystals

TABLE 54a. *Frequencies of external modes (in cm^{-1}) due to U-centers in alkali halides*

Center	LiF	NaF	NaCl	NaBr	NaI	KCl	KBr	KI	RbCl	RbBr	CsCl	CsBr	CsI	Assignment	References
$U(H^-)$	[d] 1024	[d] 859.5	[b] 563	[b] 498	[d] 426.8	[d] 502	[d] 444	[b] 446	[d] 476	[d] 426	[d] 424	[d] 365.5	[d] 283	Localized mode	[1, 2, 3, 4, 5]
$U(D^-)$	[d] 746	[d] 615	[b] 408	[b] 361	[d] 318.5	[b] 360	[d] 318	---	[b] 340	---	[d] 302	[d] 263	[d] 219	Localized mode	[1, 2, 3, 4, 5]
$U_1(H)$	---	---	---	---	---	---	[d] 794	[d] 718	---	---	---	---	---	Localized mode	[6, 7]
$U_1(D)$	---	---	---	---	---	---	[d] 567.1	[d] 518	---	---	---	---	---	Localized mode	[6, 7]
$H^- Na^+$	---	---	---	---	---	[d] 531	---	---	---	---	---	---	---	Localized mode	[8]
	---	---	---	---	---	[d] 490	---	---	---	---	---	---	---	Localized mode	[8]
	---	---	---	---	---	[d] 443	---	---	---	---	---	---	---	Localized mode	[8]
$H^- K^+$	---	---	[d] 686	---	---	---	---	---	[d] 493	[d] 442	---	---	---	Localized mode	[8, 9]
	---	---	[d] 514	---	---	---	---	---	[d] 468	[d] 387	---	---	---	Localized mode	[8, 9]
	---	---	---	---	---	---	---	---	[d] 432	---	---	---	---	Localized mode	[8, 9]
$H^- - Rb^+$	---	---	---	---	---	[d] 550	[d] 489	---	---	---	---	---	---	Localized mode	[8]
	---	---	---	---	---	[d] 511	[d] 453	---	---	---	---	---	---	Localized mode	[8]
	---	---	---	---	---	[d] 483	[d] 427	---	---	---	---	---	---	Localized mode	[8]
$H^- - Cs^+$	---	---	---	---	---	[b] 617.5	---	---	---	---	---	---	---	Localized mode	[9]
	---	---	---	---	---	[b] 526	---	---	---	---	---	---	---	Localized mode	[9]
	---	---	---	---	---	[b] 455.5	---	---	---	---	---	---	---	Localized mode	[9]
$H^- - F^-$	---	---	---	---	---	[b] 519	---	---	---	---	---	---	---	Localized mode	[9]
	---	---	---	---	---	[b] 493	---	---	---	---	---	---	---	Localized mode	[9]
$H^- - Br^-$	---	---	---	---	---	[d] 525	---	---	---	---	---	---	---	Localized mode	[8]
	---	---	---	---	---	[d] 494	---	---	---	---	---	---	---	Localized mode	[8]
$H^- - I^-$	---	---	---	---	---	[b] 569	---	---	---	---	---	---	---	Localized mode	[9]
	---	---	---	---	---	[b] 513	---	---	---	---	---	---	---	Localized mode	[9]
	---	---	---	---	---	[b] 483	---	---	---	---	---	---	---	Localized mode	[9]

[a] Room temperature. [b] Liquid air/nitrogen temperature. [c] Liquid helium temperature. [d] Temperature between 4.2 and 77 K.

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TABLE 54b. *Frequencies of external modes (in cm^{-1}) due to point impurities in alkali halides*

Center	NaCl	NaBr	NaI	KCl	KBr	KI	RbCl	RbBr	Assignment	References
$^7Li^+$	[d] 154	—	—	—	—	—	—	—	Lattice mode around impurity	[1]
	[d] 141	—	—	—	—	—	—	—	Lattice mode around impurity	[1]
	[d] 114	—	—	—	—	—	—	—	Lattice mode around impurity	[1]
	[c] 43.7	—	—	[c] 42.1	[c] 16.07	—	—	—	Resonant mode	[1, 2, 3, 4]
$^6Li^+$	[c] 45.3	—	—	[c] 39.5	[c] 17.71	—	—	—	Resonant mode	[1, 2, 3, 4]
Na^-	—	—	—	—	—	[c] 63	—	—	Resonant mode	[5]
K^-	[d] 143	—	—	—	—	—	—	—	Lattice mode around impurity	[1]
	[d] 122	—	—	—	—	—	—	—	Lattice mode around impurity	[1]
	[d] 87	—	—	—	—	—	—	—	Lattice mode around impurity	[1]
Cs^-	—	—	—	—	—	[c] 83.5	—	—	Gap mode	[5]
$^{65}Cu^+$	[c] 48	—	—	—	—	—	—	—	A_{1g}, T_{2g}	[6]
	[c] 40	—	—	—	—	—	—	—	E_g	[6]
	[c] 23.57	—	—	—	—	—	—	—	Resonant mode	[3]
Ag^+	187.5	—	—	—	—	—	—	—	A_{1g}, E_g, T_{2g}	[8]
	183.7	—	—	—	—	—	—	—	A_{1g}, E_g	[8]
	183	—	—	—	—	—	—	—	E_g	[8]
	179.2	—	—	—	—	—	—	—	A_{1g}	[8]
	178.5	—	—	—	—	—	—	—	T_{2g}	[8]
	164.7	—	—	—	—	—	—	—	A_{1g}	[8]
	163.8	—	—	—	—	—	—	—	T_{2g}	[8]
	159	—	—	—	—	—	—	—	E_g	[8]
	156	—	—	—	—	—	—	—	T_{2g}	[8]
	155	—	—	—	—	—	—	—	T_{1u}	[1, 8]
	143	—	—	—	—	—	—	—	A_{1g}	[8]
	142.5	—	—	—	—	—	—	—	T_{2g}	[8]
	142	—	—	—	—	—	—	—	E_g	[8]
	131	—	—	—	—	—	—	—	T_{1u}	[1, 8]
	130.8	—	—	—	—	—	—	—	T_{2g}	[8]
	[d] 122.4	—	—	—	—	—	—	—	A_{1g}	[8]
	[d] 121.5	—	—	—	—	—	—	—	T_{2g}	[8]
	120.5	—	—	—	—	—	—	—	T_{1u}	[1, 8]
	[d] 119.7	—	—	—	—	—	—	—	E_g	[8]
	[d] 113	—	—	—	—	—	—	—	T_{2g}	[8]
	[d] 111.5	—	—	—	—	—	—	—	E_g	[8]
	[d] 104.8	—	—	—	—	—	—	—	A_{1g}, T_{2g}	[8]
	[d] 103.5	—	—	—	—	—	—	—	E_g	[8]
	[d] 99.5	—	—	—	—	—	—	—	E_g	[8]
	[d] 59.4	—	—	—	—	—	—	—	E_g	[8]
	—	—	—	—	—	—	[c] 36.1	—	Resonant mode	[1, 2, 7, 8]
	—	—	—	—	—	—	[c] 26.4	—	Resonant mode	[1, 2, 7, 8]
	[d] 53	48	36.7	[c] 38.6	[c] 33.5	[c] 17.5	[c] 21.4	—	Resonant mode	[1, 2, 7, 8]

TABLE 54b. *Frequencies of external modes (in cm^{-1}) due to point impurities in alkali halides*—Continued

Center	NaCl	NaBr	NaI	KCl	KBr	KI	RbCl	RbBr	Assignment	References
Mg^{2+}	120	---	---	---	---	---	---	---	---	[9]
Ca^{2+}	110	---	---	---	---	---	---	---	---	[9]
Tl^{+}	---	---	---	[a] 138	---	---	---	---	E_g	[10]
	---	---	---	[a] 135	[a] 123	[a] 113	---	---	E_g	[10]
	---	---	---	[a] 113	[a] 109	---	---	---	E_g	[10]
	---	---	---	[a] 110	---	---	---	---	T_{2g}	[10]
	---	---	---	[a] 80	[a] 82	---	---	---	E_g, A_{1g}	[10]
	---	---	---	---	[a] 71	---	---	---	E_g	[10]
	---	---	---	---	[a] 70	---	---	---	T_{2g}	[10]
	---	---	---	---	---	[a] 67	---	---	T_{1u}	[10]
	---	---	---	---	---	[a] 62	---	---	T_{2g}	[10]
	---	---	---	---	---	[a] 60	---	---	E_g	[10]
	---	---	---	---	---	[a] 51	---	---	E_g	[10]
	---	---	---	---	---	[a] 50	---	---	T_{2g}	[10]
F^-	[d] 144	---	---	---	---	78	---	---	Gap mode	[2]
	[d] 112	---	---	---	---	70	---	---	Gap mode	[2]
	[d] 59.5	---	---	---	---	---	---	---	---	[1]
Cl^-	---	---	---	---	---	77	---	---	Gap mode	[2]
Br^-	[d] 140	---	---	---	---	---	---	---	---	[1]
	[d] 117	---	---	---	---	---	---	---	---	[1]
	[d] 85	---	---	---	---	---	---	---	---	[1]
	---	---	---	---	---	73.8	---	---	Gap mode	[2]
I^-	[d] 140	---	---	---	---	---	---	---	---	[1]
	[d] 120	---	---	---	---	---	---	---	---	[1]
	[d] 71	---	---	---	---	---	---	---	---	[1]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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TABLE 55a. *Frequencies of external modes (in cm^{-1}) due to molecular impurities in alkali halides*

Center	NaCl	NaBr	NaI	KCl	KBr	KI	RbCl	RbBr	RbI	Assignment	References
NCO^-	[b]86	[b]165	[b]172	[b]194	[b]183.6	[b]172.5	[b]109	[b]153.6	[b]114.5	---	[1]
	---	[b]136	[b]105	[b]147	[b]167.5	[b]152.5	[b]101	[b]141	[b]101	---	[1]
	---	[b]127	[b]91	[b]115	[b]157	[b]133	[b]87	[b]31	[b]87	---	[1]
	---	[b]123	[b]35	[b]52	[b]122	[b]119	[b]36	---	[b]62	---	[1]
	---	[b]117	---	---	[b]105	[b]82.2	---	---	[b]57	---	[1]
	---	[b]106	---	---	[b]99.7	[b]77.8	---	---	[b]24	---	[1]
	---	[b]90	---	---	[b]97.4	[b]59	---	---	---	---	[1]
	---	---	---	---	[b]84	[b]31	---	---	---	---	[1]
	---	---	---	---	[b]79	---	---	---	---	---	[1]
	---	---	---	---	[b]41	---	---	---	---	---	[1]
N_3^-	---	[b]124	[b]105	---	[b]178	[b]145	---	[b]155	[b]126	---	[1]
	---	---	---	---	[b]97	[b]80	---	---	---	---	[1]
BO_2^-	---	---	---	---	[b]169	[b]139	---	---	---	---	[1]
	---	---	---	---	[b]102	[b]88	---	---	---	---	[1]
NO_2^-	---	---	---	---	---	[d]89.2	---	---	---	Gap mode	[2]
	---	---	---	---	---	[d]88	---	---	---	Gap mode	[2]
	---	---	---	---	---	[d]79.4	---	---	---	Gap mode	[2]
	---	---	---	---	---	[d]78	---	---	---	Gap mode	[2]
	---	---	---	---	---	[d]72.8	---	---	---	Gap mode	[2]
	---	---	---	---	---	[d]71.1	---	---	---	Gap mode	[2]
NO_3^-	---	---	---	---	[b]175	[b]182	---	---	---	---	[1]
	---	---	---	---	[b]143	[b]111	---	---	---	---	[1]
	---	---	---	---	[b]103	[b]89	---	---	---	---	[1]
	---	---	---	---	[b]93	[b]74	---	---	---	---	[1]
CN^-	[b]189	[b]197	[b]165	---	---	---	---	---	---	---	[1]
	[b]147	[b]154	[b]126	---	---	---	---	---	---	---	[1]
	[b]132	[b]122	[b]93	---	---	---	---	---	---	---	[1]
	---	[b]114	---	---	---	---	---	---	---	---	[1]
	---	[b]109	---	---	---	---	---	---	---	---	[1]
	---	---	---	---	---	[c]83	---	---	---	Gap mode	[3, 4]
	---	---	---	---	---	[c]68	---	---	---	Translational mode	[3]
	[b]45	[b]35	[b]26	---	---	[c]43	---	---	---	---	[1, 3]
	---	---	---	[c]12	[c]12	[c]11	[d]19	---	---	Librational mode	[1, 3, 5]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.

[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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TABLE 55b. *Frequencies of external modes (in cm^{-1}) due to OH^- and OD^- in alkali halides*

Center	NaCl	NaI	KCl	KBr	KI	RbCl	CsBr	Assignment	References
OH^-	[c] 390	427	[c] 297.5	[c] 312.7	[c] 284	[c] 272	289	Librational mode	[1, 2, 3]
	---	---	---	---	[c] 86.9	---	---	Gap mode	[4]
	---	---	---	---	[c] 86.2	---	---	Gap mode	[4]
	---	---	---	[c] 86	[c] 77	---	---	---	[4, 5]
	---	---	---	[c] 68	[c] 69.5	---	---	---	[4, 5]
	[c] 12.2	---	[c] 32	[c] 37.5	---	[c] 30	---	Non-Devonshire line	[4, 6, 7]
	[c] 22	---	---	---	---	---	---	---	[7]
	[c] 15.6	---	---	---	---	---	---	---	[7]
	[c] 9.3	---	---	---	---	---	---	---	[7]
	[c] 2	---	---	---	---	---	---	---	[7]
OD^-	---	---	[c] 232	[c] 236.3	[c] 215	---	---	Librational mode	[1, 2]
	---	---	---	[c] 86	---	---	---	---	[5]
	---	---	---	[c] 68	---	---	---	---	[5]
	---	---	---	[c] 35	---	---	---	Non-Devonshire line	[5]

[a] Room temperature.
[b] Liquid air/nitrogen temperature.
[c] Liquid helium temperature.
[d] Temperature between 4.2 and 77 K.

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FORM NBS-114A (1-71)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBS-NSRDS-52	2. Gov't Accession No.	3. Recipient's Accession No.
4. TITLE AND SUBTITLE Electronic Absorption and Internal and External Vibrational Data of Atomic and Molecular Ions Doped in Alkali Halide Crystals			5. Publication Date July 1974 6. Performing Organization Code
7. AUTHOR(S) S.C. Jain, A.V.R. Warrier, and S.K. Agarwal			8. Performing Organization
9. PERFORMING ORGANIZATION NAME AND ADDRESS NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234			10. Project/Task/Work Unit No. 11. Contract/Grant No.
12. Sponsoring Organization Name and Address Same as No. 9.			13. Type of Report & Period Covered Final 14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 74-600010

16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)

Spectral data for more than 70 atomic and molecular ions doped in alkali halide crystals are tabulated. The tables include electronic absorption data, listings of internal vibrational frequencies of doped complex ions, and tabulations of the frequencies of external modes. The data that appear in the tables were selected on the basis of the consistency among different authors, the types of instruments, and the temperature of measurement. In addition to the data, the tables include the spectroscopic assignments given by the authors in the references cited.

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Atomic ions; doped alkali halide crystals; external vibrational modes; internal vibrational modes; molecular ions.

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