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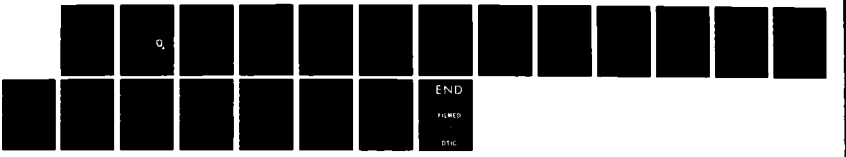

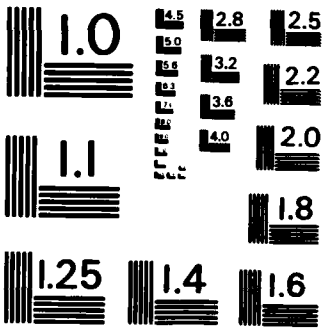

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Host Materials for Transition-Metal Ions with the nd^N Electronic Configuration

by Clyde A. Morrison
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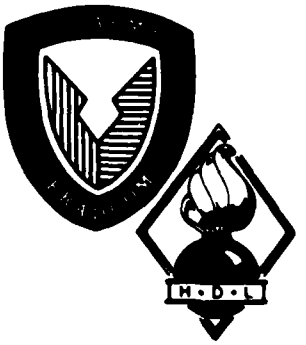

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Data are given on 12 host materials for lasers that use the transition metal ions. Included in each section are the crystallographic data, x-ray data, lattice sum parameters $A_{\widetilde{nm}}$, crystal field parameters B_{nm}(Dq), and spin-orbit constants (ζ). One section contains the phenomenological free ion parameters $F^{(k)}$, ξ, and α, which have been obtained by fitting the reported free ion data. There is a bibliography for each host which, dependent on that particular host, is more or less complete. The data contained on each host material as well as on new host materials will be added periodically.

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Contents

Tables

A1

1. INTRODUCTION

The following report contains tables that list information on various potential laser host materials for transition metal ions of the nd^N electronic configuration. Many of the fluorinated host materials were selected from a list supplied by H. P. Jenssen and A. Linz of the Massachusetts Institute of Technology (MIT). We thank them for the use of this list. Also we wish to thank D. Gabbe of MIT for supplying us with a list of fluorinated garnets (almost all the information we have on these garnets was supplied by Gabbe).

A number of host materials were selected because lasers had been reported that used $3d^N$ ions as impurities in those hosts. These host materials, with limited amounts of experimental energy levels, were reported during the early 1960's, and some later work has been done in some of these hosts. Unfortunately, much of the reported absorption data have been taken at room temperature (~300 K) and are quite unreliable because of the presence of vibronics and absorption from excited levels. Further complications arise when the data are extracted from the excitation spectra. There is a real need for low-temperature absorption spectra of many of these ions.

2. DISCUSSION OF TABLES

2.1 Crystallographic data

The crystallographic data on each host are given in the notation of the International Tables.[1] The crystallographic data are presented in a short table for each host that lists the following information:

(a) Crystal class, such as triclinic, orthorhombic

(b) Space group symbol and number from the International Tables

(c) Number of chemical formula units, Z, per unit cell

(d) Setting, if there is more than one for that space group in the International Tables

(e) Position (site type in the International Tables), site symmetry (in the Schoenflies notation), and general x, y, and z coordinates (expressed as fractions of the lattice constants) for that site type, for each constituent of the host crystal

(f) Lattice constants a, b, and c (in Å) and angles α, β, and γ (in degrees and decimal parts)

(g) Effective charges (usually the valence charge) in units of the electronic charge

(h) Electric-dipole polarizabilities, α (in $Å^3$), for each of the constituent ions

2.2 Lattice sums, A_{nm}

The data given in section 2.1 were used to obtain the point-charge,[2,3] point-dipole,[4] and self-induced[5] contributions to the lattice sum parameters A_{nm}. All the A_{nm} for $1 \leq n \leq 5$ are given and are sufficient for the analysis of the nd^N configuration. The units of A_{nm} are $cm^{-1}/Å^n$. The crystal-field parameters for a particular ion are given by $B_{nm} = \langle r^n \rangle A_{nm}$, where $\langle r^n \rangle$ is the radial expectation value[6] of r^n for the ion under consideration. At the bottom of each of the tables of A_{nm} the lattice sums $S^{(0)}$, $S^{(2)}$, and $S^{(4)}$ are given.

The $S^{(0)}$ sum yields the interconfiguration shift[7] $\Delta E = \Delta E_0 - [\langle r^2 \rangle_{n'l'} - \langle r^2 \rangle_{nl}] S^{(0)}$, and the $S^{(k)}$ sums yield the Slater integral shifts as $\Delta F^{(2)} = -\langle r^2 \rangle^2 S^{(2)}$ and $\Delta F^{(4)} = -\langle r^4 \rangle^2 S^{(4)}$; the

[1] *International Tables for X-Ray Crystallography, I, Symmetry Groups, Eds., N. F. M. Henry and K. Lonsdale, Kynoch, Birmingham, U. K. (1969).*

[2] *C. A. Morrison and R. P. Leavitt, Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Crystals, in Handbook on the Physics and Chemistry of Rare Earths, 5, K. Gschneidner and L. Erying, Eds., North-Holland, New York (1982).*

[3] *N. Karayianis and C. A. Morrison, Rare Earth Ion-host Interactions, 1. Point Charge Lattice Sum in Scheelites, Harry Diamond Laboratories, HDL-TR-1648 (October 1973) (NTIS 011252).*

[4] *C. A. Morrison, Dipolar Contributions to the Crystal Fields in Ionic Solids, Solid State Comm., 18 (1976), 153.*

[5] *C. A. Morrison, G. F. de Sá, and R. P. Leavitt, Self-Induced Multipole Contribution to the Single-Electron Crystal Field, J. Chem. Phys., 6 (1982), 3899.*

[6] *S. Fraga, K. M. S. Saxena, and J. Karwowski, Handbook of Atomic Data, Elsevier, New York (1976).*

[7] *C. A. Morrison, Host Dependence of the Rare-Earth Ion Energy Separation $4f^N - 4f^{N-1}nl$, J. Chem. Phys., 2 (1980), 1001.*

units are such that if $\langle r^k \rangle$ is in Å units, then each shift is in units of cm^{-1}.

2.3 Experimental results

In this section we report all the experimental data in terms of the Slater integrals $F^{(k)}$ and the crystal-field parameters B_{nm}. Since a number of different notations exist, we describe in detail our conversion from each set of constants to B_{nm} or $F^{(k)}$.

2.3.1 Relation of Dq with B_{40}

In his article, McClure[8] gives the electric potential for a six-fold cubic array of charges at a distance R as

$$V = D(x^4 + y^4 + z^4 - 3/5\, r^4), \quad (1)$$

where $D = 35\, e/(4R^5)$. The potential energy, eV, can be written as

$$U = eDr^4(X^4 + Y^4 + Z^4 - 3/5), \quad (2)$$

where $X = x/r$, etc. For equivalent electrons, McClure[8] defines q by $q = 2\langle r^4 \rangle e/105$, so that

$$U = (105/2)Dq(X^4 + Y^4 + Z^4 - 3/5). \quad (3)$$

In our notation, we write the same potential as

$$U = B_{40}[C_{40} + (5/\sqrt{70})(C_{44} + C_{4-4})], \quad (4)$$

for six-fold cubic coordination with charges at $(\pm R,0,0)$, $(0,\pm R,0)$, and $(0,0,\pm R)$. The C_{nm} are given by[9]

$$C_{40} = (35Z^4 - 30Z^2 + 3)/8, \quad (5)$$

$$C_{4\pm4} = (X \pm iY)^4(35/128)^{1/2}. \quad (6)$$

Substituting (5) and (6) into (4) gives

$$C_{40} + (5/\sqrt{70})(C_{44} + C_{4-4}) = (5/2)(X^4 + Y^4 + Z^4 - 3/5). \quad (7)$$

Thus, we obtain

$$(5/2)B_{40} = (105/2)Dq,$$

or

$$B_{40} = 21Dq. \quad (8)$$

This relation (8) has been used to convert the Dq reported in the literature to B_{40} for crystals with four-fold axes (e.g., C_4, S_4, etc.). If in the cubic group the principal axis of rotation is the cube diagonal, then relation (4) becomes

$$U = B'_{40}[C_{40} + \sqrt{10}/\sqrt{7}(C_{43} - C_{4-3})], \quad (9)$$

and the reported Dq, B_{40} relation becomes

$$B'_{40} = 14\, Dq \quad (10)$$

Since the sign of Dq is generally not reported, we give the sign of B_{40} or B'_{40} that is obtained from the point charge lattice sum A_{40}.

2.3.2 Relation between Slater and Racah parameters

For d electrons, Judd[10] gives the following relations:

$$F_0 = F^{(0)}$$
$$F_2 = F^{(2)}/49$$
$$F_4 = F^{(4)}/441 \quad (11)$$

and

$$E^0 = F_0 - 7F_2/2 - 63F_4/2$$
$$E^1 = 5(F_2 + 9F_4)/2$$
$$E^2 = (F_2 - 5F_4)/2 \quad (12)$$

and Racah[11] introduces A, B, and C by

$$A = F_0 - 49F_4$$
$$B = F_2 - 5F_4$$
$$C = 35F_4 \quad (13)$$

[8] D. S. McClure, Electronic Spectra of Molecules and Ions in Crystals: II, Solid State Phys., 9 (1959), 420, Academic Press, New York.
[9] C. J. Ballhausen, Ligand Field Theory, McGraw Hill, New York (1962), 93.
[10] B. R. Judd, Operator Techniques in Atomic Spectroscopy, McGraw-Hill, New York (1963), 221.
[11] G. Racah, Theory of Complex Spectra IV, Phys. Rev., 76 (1949), 1352.

All these parameters are used and reported in the literature. We have chosen to put all the reported data in terms of $F^{(k)}$, since Hartree-Fock calculations of $F^{(k)}$ have been reported for a large number of ions.[6] In terms of A, B, and C we have

$$F^{(0)} = (5A + 7C)/5,$$

$$F^{(2)} = 7(7B + C),$$

and

$$F^{(4)} = 63C/5. \quad (14)$$

And in terms of E^k :

$$F^{(0)} = E^0 - 49E^1/10 + 63E^2/2,$$

$$F^{(2)} = 49(9E^2 - E^1)/2,$$

and

$$F^{(4)} = 441(5E^2 - E^1)/10; \quad (15)$$

and the relation between $F^{(k)}$ and F_k is given in equation (11).

2.4 References for each host material

The final section on each host material consists of a number of references to experimental and theoretical work that has been reported. This list, in most cases, is far from exhaustive and will be continuously updated as new work is reported or older references found. For a number of hosts, only x-ray data have been reported, and we have been unable to find any reference to optical data on transition elements in these hosts. On a number of host materials, references were found which contain important information on that host not contained in the tables. These references have been included.

3. SUMMARY

In this report we have provided the data on 12 host materials for lasers that use the transition metal ions. Included in each section are the crystallographic data, x-ray data, lattice sum parameters A_{nm}, crystal field parameters B_{nm} (Dq), and spin-orbit constants (ζ). One section includes the phenomenological free ion parameters $F^{(k)}$, ζ, and α, which have been obtained by fitting the reported free ion data. For each host, there is a bibliography which, dependent on that particular host, is more or less complete. We plan to update the data contained on each host material as well as on new host materials as additional information becomes available.

[6] *S. Fraga, K. M. S. Saxena, and J. Karwowski, Handbook of Atomic Data, Elsevier, New York (1976).*

ACKNOWLEDGEMENTS

We thank Norman Brandt of the Harry Diamond Laboratories' library for his cooperation in responding to our many requests for special information searches and copies of numerous documents from obscure sources. Also, we wish to thank A. Linz, H. Jenssen, and B. Aull of the Massachusetts Institute of Technology for suggesting a number of the materials referenced here. Thanks also go to A. Pinto and J. Paul of the Night Vision and Electro-Optics Laboratory for suggested materials.

LITERATURE CITED

(1) *International Tables for X-Ray Crystallography*, I, Symmetry Groups, Eds., N. F. M. Henry and K. Lonsdale, Kynoch, Birmingham, U. K. (1969).

(2) C. A. Morrison and R. P. Leavitt, *Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Crystals*, in *Handbook on the Physics and Chemistry of Rare Earths*, **5**, K. Gschneidner and L. Erying, eds., North-Holland, New York (1982).

(3) N. Karayianis and C. A. Morrison, *Rare Earth Ion-Host Interactions, 1. Point Charge Lattice Sum in Scheelites*, Harry Diamond Laboratories, HDL-TR-1648 (October 1973) (NTIS 011252).

(4) C. A. Morrison, *Dipolar Contributions to the Crystal Fields in Ionic Solids*, Solid State Comm., **18** (1976), 153.

(5) C. A. Morrison, G. F. de Sá, and R. P. Leavitt, *Self-Induced Multipole Contribution to the Single-Electron Crystal Field*, J. Chem. Phys., **76** (1982), 3899.

(6) S. Fraga, K. M. S. Saxena, and J. Karwowski, *Handbook of Atomic Data*, Elsevier, New York (1976).

(7) C. A. Morrison, *Host Dependence of the Rare-Earth Ion Energy Separation* $4f^N - 4f^{N-1}nl$, J. Chem. Phys., **72** (1980), 1001. In the expression for the Slater-parameter host-dependent shift, a factor (k+1) was omitted. This omission has been reported by: M. V. Eremin and A. A. Kornienko, *Effect of Covalency on Slater Parameters and the Correlation Crystal Field in Transient-Metal Compounds*, Opt. Spectrosc., **53** (1982), 45.

(8) D. S. McClure, *Electronic Spectra of Molecules and Ions in Crystals: II*, Solid State Phys., **9** (1959), 420, Academic Press, New York.

(9) C. J. Ballhausen, *Ligand Field Theory*, McGraw Hill, New York (1962), 93.

(10) B. R. Judd, *Operator Techniques in Atomic Spectroscopy*, McGraw-Hill, New York (1963), 221.

(11) G. Racah, *Theory of Complex Spectra IV*, Phys. Rev., **76** (1949), 1352.

Table 1. $Y_3Al_5O_{12}$ (YAG)

(A) Crystallographic data on $Y_3Al_5O_{12}$.

Cubic Ia3d, 230, Z = 8

Ion	Site	Symm.	x[a]	y	z	q	$\alpha(Å^3)$[b]
Al_1	16(a)	C_{3i}	0	0	0	3	0.0530
Al_2	24(d)	S_4	3/4	0	1/4	3	0.0530
Y	24(c)	D_2	0	1/4	1/8	3	0.870
O	96(h)	C_1	−0.0306	0.0512	0.1500	−2	1.349

[a] *X-ray data, a = 12.000 Å, reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al ion in 24(d) (S_4) site in $Y_3Al_5O_{12}$.

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	6,355	−2,604	14,013	17,765
ReA_{32}	−27,522	8,609	−11,957	−30,870
ImA_{32}	37,839	−11,913	6,332	32,258
A_{40}	−25,089	11,879	−8,516	−21,726
ReA_{44}	−3,763	1,614	1,964	−185.1
ImA_{44}	−9,108	4,740	−2,875	−7,243
ReA_{52}	−2,931	2,287	−3,498	−4,142
ImA_{52}	4,328	−3,207	3,640	4,762
$\|A_{44}\|$	9,855	—	—	7,245

(C) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al ion in 16(a) (C_{3i}) site in $Y_3Al_5O_{12}$ (rotated so that the z-axis is parallel to the (111) crystallographic axis).

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	6,836	−1,107	−13,553	−7,823
A_{40}	−20,054	8,166	3,273	−8,615
ReA_{43}	2,813	−1,422	6,253	7,644
ImA_{43}	−22,370	8,639	2,348	−11,383
$\|A_{43}\|$	22,546	—	—	13,711

(D) Experimental (cm^{-1}) values of B_{40}, $F^{(2)}$, and $F^{(4)}$ for nd^N ions in $Y_3Al_5O_{12}$

Ion	B_{40}	$F^{(2)}$	$F^{(4)}$	T	Site	Ref.	nd^N
Cr^{+3}	−23,730	53,438	34,978	300	C_{3i}	3,16	$3d^3$
Cr^{+3}	−23,072	55,806	36,806	300	C_{3i}	4	$3d^3$
Cr^{+3}	−24,150	53,760	40,320	—	C_{3i}	10	$3d^3$
Cr^{+3}	−23,380	—	—	—	C_{3i}	6	$3d^3$
Cr^{+3}	−22,960	54,600	40,950	77	C_{3i}	11	$3d^3$
Mn^{+3}	−27,650	59,500	32,130	300	C_{3i}	3,10	$3d^4$
Mn^{+4}	−27,874	53,540	43,456	300	C_{3i}	4	$3d^3$
Mn^{+4}	−44,100	—	—	—	—	5	$3d^3$
Fe^{+3}	−26,950	39,690	15,876	300	C_{3i}	3,10	$3d^5$
Fe^{+3}	−17,682	49,224	36,477	—	C_{3i}	5,8	$3d^5$
Fe^{+3}	−21,756	51,023	42,979	—	S_4	5,8	$3d^5$
Co^{+3}	−25,200	56,630	34,020	300	C_{3i}	3,10	$3d^6$
Co^{+3}	−17,430	—	—	—	S_4	12	$3d^6$
Co^{+2}	−9,660	—	—	—	S_4	12	$3d^7$
Co^{+2}	−12,880	—	—	—	C_{3i}	12	$3d^7$
Ni^{+3}	−27,580	42,000	22,680	300	C_{3i}	3,10	$3d^7$
Rh^{+3}	−28,840	40,600	21,924	—	C_{3i}	5	$4d^6$
Pd^{+3}	−23,730	39,326	21,218	—	C_{3i}	5	$4d^7$
Pt^{+3}	−23,100	44,520	30,744	—	C_{3i}	5	$5d^7$
V^{+3}	−23,800	—	—	—	C_{3i}	5	$3d^2$
V^{+3}	−17,850	—	—	—	S_4	5	$3d^2$
V^{+4}	−30,800	—	—	—	C_{3i}	5	$3d^1$
V^{+4}	−26,250	—	—	—	S_4	5	$3d^1$

Table 1(D) References

(1) F. Euler and J. A. Bruce, *Oxygen Coordinates of Compounds with Garnet Structure*, Acta Cryst. **19** (1965), 971.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) P. A. Arsenov and D. T. Sviridov, *Absorption Spectra of Yttrium Aluminum Garnet (YAG) with Contaminant Ions of the Iron Group*, Sov. Phys. Crystallogr. **14** (1970), 578.

(4) *D. T. Sviridov, R. K. Sviridova, N. I. Kulik, and V. B. Glasko, Optical Spectra of the Iso-Electronic Ions V^{2+}, Cr^{3+} and Mn^{4+} in an Octahedral Coordination*, J. Appl. Spectrosc. **30** (1979), 334.

(5) Landolt-Bornstein, *Numerical Data and Functional Relationships in Science and Technology, New Series*, **12**, Supplement and Extension to **4**, Part a, Garnets and Perovskites, Springer-Verlag, New York (1978), 301.

(6) R. W. McMillan, *Optical Absorption Spectrum of Cr^{3+} in Yttrium Aluminum Garnet*, J. Opt. Soc. Am. **67** (1977), 27.

(7) M. J. Weber and L. A. Riseberg, *Optical Spectra of Vanadium Ions in Yttrium Aluminum Garnet*, J. Chem. Phys. **55** (1971), 2032.

(8) T. F. Veremeichik, B. N. Grechusnikov, T. M. Varina, D. T. Sviridov, and I. N. Kalinkina, *Absorption Spectra and Calculation of Energy-Level Diagram of Fe^{3+} and Mn^{2+} Ions in Single Crystals of Yttrium Aluminum Garnet, Orthoclase, and Manganese Silicate*, Sov. Phys. Crystallogr. **19** (1975), 742.

(9) I. N. Douglas, *Optical Spectra of Chromium Ions in Crystals of Yttrium Aluminum Garnet*, Phys. Stat. Sol. **a9** (1972), 635.

(10) B. K. Sevast'yanov, D. T. Sviridov, V. P. Orekhovo, L. B. Pasternak, R. K. Sviridova, and T. F. Vermeichik, *Optical Absorption Spectra of Excited Cr^{3+} Ions in Yttrium Aluminum Garnet*, Sov. J. Electron. **2** (1973), 339.

(11) D. L. Wood, J. Ferguson, K. Knox, and J. F. Dillon, Jr., *Crystal-Field Spectra of $d^{3,7}$ Ions III. Spectrum of Cr^{3+} in Various Octahedral Crystal Fields*, J. Chem. Phys. **39** (1963), 890.

Table 1(D) References (cont'd)

(12) D. L. Wood and J. P. Remeika, *Optical Absorption of Tetrahedral Co^{3+} and Co^{2+} in Garnets*, J. Chem. Phys. **46** (1967), 3595.

(13) G. A. Slack, D. W. Oliver, R. M. Chrenko, and S. Roberts, *Optical Absorption of $Y_3Al_5O_{12}$ from 10- to 55,000-cm^{-1} Wave Numbers*, Phys. Rev. **177** (1969), 1308.

(14) J. P. Hurrell, S. P. S. Porto, I. F. Chang, S. S. Mitra, and R. P. Bauman, *Optical Phonons of Yttrium Aluminum Garnet*, Phys. Rev. **173** (1968), 851.

(15) J. A. Hodges, R. A. Serway, and S. A. Marshall, *Electron-Spin Resonance Absorption Spectrum of Platinum in Yttrium Aluminum Garnet*, Phys. Rev. **151** (1966), 196.

(16) Z. T. Azamatov, P. A. Arsenev, T. Yu. Geraskina, and M. V. Chukichev, *Properties of Chromium Ions in the Lattice of Yttrium Aluminum Garnet (YAG)*, Phys. Stat. Sol. (a), 1 (1970), 801.

(B) Lattice sum data.

1. Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site (C_{3i}) in the Pa3 form of K_2NaAlF_6.

A_{nm}	Monopole	Dipole
A_{20}	20,464	4,881
A_{40}	−15,791	−13,471
ReA_{43}	14,510	12,897
ImA_{43}	3,769	3,277

2. Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site (O_h) in the Fm3m form of K_2NaAlF_6.

A_{nm}	Monopole	Dipole	Self-Induced	Total
A_{40}	23,267	15,593	−12,274	26,586
A_{44}	13,905	9,319	−7,335	15,888

$S^{(0)} = 16{,}750\ cm^{-1}/Å^2$
$S^{(2)} = 15{,}425\ cm^{-1}/Å^4$
$S^{(4)} = 2{,}551.3\ cm^{-1}/Å^8$

Table 2. K_2NaAlF_6

(A) Crystallographic data on the two forms of K_2NaAlF_6.

1. Cubic Pa3, 205, Z = 4, elpasolite.

Ion	Site	Symm.	x[a]	y	z	q	α(Å^3)[b]
Na	4(b)	C_{3i}	1/2	1/2	1/2	1	0.147
K	8(c)	C_3	1/4	1/4	1/4	1	0.827
Al	4(a)	C_{3i}	0	0	0	3	0.0530
F	24(d)	C_1	0.22	0.03	0.01	−1	1.04

[a] X-ray data, a = 8.11 Å, reference 1.
[b] Reference 2.

2. Cubic Fm3m, 225, Z = 4, elpasolite.

Ion	Site	Symm.	x[a]	y	z	q	α(Å^3)[b]
Al	4(a)	O_h	0	0	0	3	0.0530
Na	4(b)	O_h	1/2	1/2	1/2	1	0.147
K	8(c)	T_d	1/4	1/4	1/4	1	0.827
F	24(e)	C_{4v}	0.219	0	0	−1	1.04

[a] X-ray data, a = 8.119 Å, reference 6.
[b] Reference 2.

Table 2 References

(1) R. W. G. Wyckoff, *Crystal Structures*, **3**, Interscience, New York (1968), 374.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) C. D. Adam, *ENDOR Determination of Covalency in K_2NaAlF_6, Cr^{3+}*, J. Phys. C: Solid State Phys. **14** (1981), L105.

(4) P. Greenough and A. G. Paulusz, *The $^2E_g \rightarrow {}^4A_{2g}$ Phosphorescence Spectrum of the Cr^{3+} Ion in K_2NaAlF_6*, J. Chem. Phys. **70** (1979), 1967.

(5) K. Grjotheim, J. G. Holm, and S. A. Mikhaiel, *Equilibrium Studies in the Systems K_3AlF_6-Na_3AlF_6 and K_3AlF_6-Rb_3AlF_6*, Acta Chem. Scand. **27** (1973), 1299.

(6) L. R. Morss, *Crystal Structure of Dipotassium Sodium Fluoroaluminate (Elpasolite)*, J. Inorg. Nucl. Chem. **36** (1974), 3876.

Table 3. $Na_3Al_2Li_3F_{12}$ Cryolithionite (Garnet)

(A) Crystallographic data on $Na_3Al_2Li_3F_{12}$.

Cubic Ia3d, 230, Z = 8.

Ion	Site	Symm.	x[a]	y	z	q	α(Å^3)[b]
Na	24(c)	D_2	1/8	0	1/4	1	0.179
Al	16(a)	C_{3i}	0	0	0	3	0.0530
Li	24(d)	S_4	3/8	0	1/4	1	0.0321
F	96(h)	C_1	−0.02888	0.04268	0.13989	−1	0.731

[a] X-ray data, a = 12.122 Å, from reference 1.
[b] Reference 2.

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site (C_{3i}) in $Na_3Al_2Li_3F_{12}$ (rotated so that the z-axis is along the (111) crystallographic axis).

A_{nm}	Monopole	Total
A_{20}	−2,050.90	732.86
A_{40}	14,469.88	−15,454.32
A_{43}	−16,491.07	18,471.61

Table 3 References

(1) R. W. G. Wyckoff, *Crystal Structures*, **3**, Interscience, New York (1968), 222.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

Table 4. Free ion data

Free ion $F^{(2)}$, $F^{(4)}$, and ζ and α for nd^N ions (cm^{-1}).

nd^N	Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	Ref.
$3d^2$	Sc^{1+}	35,469	19,832	63.18	27	1
$3d^2$	Ti^{2+}	53,061	30,920	126.4	56.4	1
$3d^2$	Ti^{2+}	54,870	32,034	129.4	20.80	2
$3d^2$	Ti^{2+}	53,322[a]	29,000[a]	120.4[b]	—	3
$3d^2$	V^{3+}	67,200	40,522	219.6	75	1
$3d^2$	Cr^{4+}	75,831	47,061	337.9	—	1
$3d^3$	V^{2+}	55,153	20,954	186.3	199	1
$3d^3$	V^{2+}	59,669	35,882	176.7	24.58	2
$3d^3$	V^{2+}	57,437[a]	36,363[a]	167.8[b]	—	4
$3d^3$	Cr^{3+}	75,950	30,076	295.6	437	1
$3d^3$	Cr^{3+}	70,905[a]	45,986[a]	296.4[b]	—	5
$3d^3$	Mn^{4+}	80,332	47,754	437.0	91	1
$3d^4$	Cr^{2+}	59,121[a]	46,179[a]	234.3[b]	—	5
$3d^4$	Cr^{2+}	62,300	38,934	263.2	61.0	1
$3d^4$	Cr^{2+}	64,467	39,730	239.4	28.36	2
$3d^4$	Mn^{3+}	81,970	46,998	387.7	12	1
$3d^4$	Mn^{3+}	71,593[a]	55,647[a]	361.8[b]	—	6
$3d^4$	Fe^{4+}	87,269	56,183	564.6	85	1
$3d^5$	Mn^{2+}	67,685	40,698	351.4	74.8	7
$3d^5$	Mn^{2+}	69,266	43,578	317.5	32.14	2
$3d^6$	Fe^{2+}	79,149	49,153	440.5	81	1
$3d^6$	Fe^{2+}	74,064	47,426	411.0	35.92	2
$3d^6$	Co^{3+}	84,377[a]	60,291[a]	584.6[b]	—	8
$3d^7$	Co^{2+}	77,532	50,123	560.3	65	1
$3d^7$	Co^{2+}	78,863	51,274	519.9	39.70	2
$3d^8$	Ni^{2+}	86,933	60,871	701.7	42	1
$3d^8$	Ni^{2+}	83,661	55,122	644.2	43.48	2

[a]The Slater parameters are obtained by fitting the centroids of the reported experimental data for a given nd^N configuration.
[b]The ζ values are obtained by fitting the lowest J multiplet of the Hund ground state of the nd^N configuration.

Table 4 References

(1) W.-K. Li, *Magnetic Interactions in Transition Metal Ions, Part I. Electronic Configurations d^2, d^3, and d^4*, Atomic Data **2** (1970), 45.
W.-K. Li, *Magnetic Interactions in Transition Metal Ions, Part II. Bivalent Cations of the First Transition Series*, Atomic Data **2** (1970), 58.

(2) A. Pasternak and Z. B. Goldschmidt, *Spin-Dependent Interactions in the $3d^N$ Configurations of the Third Spectra of the Iron Group*, Phys. Rev. **A6** (1972), 55.
The parameters are given in the form

$F^{(2)} = 69{,}266 + 4{,}798.5(N - 5)$

$F^{(4)} = 43{,}578 + 3{,}848(N - 5)$

$\alpha = 32.14 + 3.78(N - 5)$

$\zeta = 348.3 + 85.8(N - 5) + 7.7[(N - 5)^2 - 4]$

(3) C. Corliss and J. Sugar, *Energy Levels of Titanium, Ti I through Ti XXII*, J. Phys. Chem. Ref. Data **8** (1979), 1.

(4) J. Sugar and C. Corliss, *Energy Levels of Vanadium, V I through V XXIII*, J. Phys. Chem. Ref. Data **7** (1978), 1191.

(5) J. Sugar and C. Corliss, *Energy Levels of Chromium, Cr I through Cr XXIV*, J. Phys. Chem. Ref. Data **6** (1977), 317.

(6) C. Corliss and J. Sugar, *Energy Levels of Manganese, Mn I through Mn XXV*, J. Phys. Chem. Ref. Data **6** (1977), 1253.

(7) T. M. Dunn and W.-K. Li, *Magnetic Interactions for the Electronic Configuration d^5*, J. Chem. Phys. **46** (1967), 2907.

(8) J. Sugar and C. Corliss, *Energy Levels of Cobalt, Co I through Co XXVII*, J. Phys. Chem. Ref. Data **10** (1981), 1097.

Table 5. Cs_2TlF_6

(A) Crystallographic data (two forms reported) on Cs_2TlF_6.

1. Cubic Fm3m, 225, Z = 4.

Ion	Site	Symm.	x[a]	y	z	q	$\sigma(Å^3)$[b]
Ti	4(a)	O_h	0	0	0	+4	0.506
Cs	8(c)	T_d	1/4	1/4	1/4	+1	2.492
F	24(e)	C_{4v}	0.195	0	0	−1	0.731

[a]X-ray data, a = 8.96 Å, the F position is not reported for Cs_2TlF_6 and is taken from Cs_2MnF_6, reference 1.
[b]Reference 3.

2. Hexagonal $P\bar{3}m1$, 164, Z = 1.

Ion	Pos.	Symm.	x[a]	y	z	q	$\sigma(Å^3)$[b]
Ti	1(a)	D_{3d}	0	0	0	+4	0.506
Cs	2(d)	C_{3v}	1/3	2/3	0.691	+1	2.492
F	6(i)	C_s	0.167	0.167	0.206	−1	0.731

[a]X-ray data, a = 6.15 Å, c = 4.96 Å, the Cs and F positions are not reported for Cs_2TlF_6 and are taken from Cs_2ZrF_6, reference 2.
[b]Reference 3.

(B) Lattice sums.

1. Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Ti site (O_h) in the cubic form of Cs_2TiF_6.

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{40}	25,400	32,148	−14,102	43,445
A_{44}	15,179	19,212	−8,428	25,963

$S^{(0)} = 18,682\ cm^{-1}/Å^2$
$S^{(2)} = 17,743\ cm^{-1}/Å^4$
$S^{(4)} = 3,148.1\ cm^{-1}/Å^8$

2. Lattice sums, $A_{nm}(cm^{-1}/Å^n)$, for the Ti site (D_{3d}) in the hexagonal form of Cs_2TiF_6.

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	−5,629	−3,291	1,172	−7,748
A_{40}	−5,090	−3,546	1,986	−6,651
A_{43}	10,051	6,316	−3,059	13,308

$S^{(0)} = 8,919\ 9\ cm^{-1}/Å^2$
$S^{(2)} = 5,251.8\ cm^{-1}/Å^4$
$S^{(4)} = 460.86\ cm^{-1}/Å^8$

Table 5 References

(1) R. W. G. Wyckoff, *Crystal Structures*, 3, Interscience, New York (1968), 341.

(2) R. W. G. Wyckoff, *Crystal Structures*, 3, Interscience, New York (1968), 350.

(3) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(4) N. B. Manson, G. A. Shah, B. Howes, and C. D. Flint, $^4A_g \leftrightarrow {}^2E_g$ *Transition of* Mn^{4+} *in* $Cs_2TiF_6{:}MnF_6^{2-}$, Molec. Phys. **34** (1977), 1157.

Table 6. $NH_4Al(SO_4)_2$

(A) Crystallographic data on $NH_4Al(SO_4)_2$.

Trigonal P321, 150, Z = 1.

Ion	Site	Symm.	x[a]	y	z	q	$\alpha(Å^3)$[b]
NH_4	1(a)	D_3	0	0	0	1	2.684
Al	1(b)	D_3	0	0	1/2	3	0.0530
S	2(d)	C_3	1/3	2/3	0.222	6	4.893
O_1	2(d)	C_3	1/3	2/3	0.016	−2	1.349
O_2	6(g)	C_2	0.328	0.344	0.317	−2	1.349

[a] *X-ray data, a = 4.724 Å, c = 8.225 Å, the positions for S, O_1, and O_2 in $NH_4Al(SO_4)_2$ are not given. Those listed above are for the same ions in $KAl(SO_4)_2$, reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site (D_3) in $NH_4Al(SO_4)_2$.

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	13,668	−42,591	−2,720.0	−41,994.49
A_{33}	10,708	−17,390	−1,961.9	—
A_{40}	−4,089.1	25,994	4,005.7	25,293.63
A_{43}	8,105.7	−36,041	840.80	3,661.09
A_{53}	5,996.4	−15,968	−2,489.0	—

$S^{(0)} = 15,593\ cm^{-1}/Å^2$
$S^{(2)} = 7,176.6\ cm^{-1}/Å^4$
$S^{(4)} = 444.17\ cm^{-1}/Å^8$

(C) Experimental parameters.

Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	B_{40}	Ref.
Cr^{3+}	—	—	186	—	38,156	3

Table 6 References

(1) R. W. G. Wyckoff, *Crystal Structures*, 3, Interscience, New York (1968), 168.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) S. V. J. Lakshaman, B. C. Venkatareddy, and J. Lakshmanarao, *Crystal Field, Spin Orbit and Excitation Interactions in the Spectrum of Chromium-Doped Ammonium Aluminum Sulphate*, Physica **98B** (1979), 65.

Table 7. MgF_2

(A) Crystallographic data on MgF_2.

Tetragonal $P4_2/mnm$, 136, Z = 2.

Ion	Site	Symm.	x[a]	y	z	q	$\alpha(Å^3)$[b]
Mg	2(a)	D_{2h}	0	0	0	+2	0.0809
F	4(f)	C_{2v}	0.303	0.303	0	−1	0.731

[a] *X-ray data, a = 4.623 Å, c = 3.052 Å, from reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Mg site (D_{2h}) of MgF_2.

A_{nm}	Monopole	Dipole	*Self-induced*	Total
A_{20}	−576.3	3,745	−592.7	2,576
A_{22}	2,447	−1,807	−327.8	312.6
A_{40}	−3,020	−381.7	660.3	−2,742
A_{42}	−10,015	−212.2	3,965	−6,262
A_{44}	4,458	−513.4	−2,057	1,887

$S^{(0)} = 8,871\ cm^{-1}/Å^2$
$S^{(2)} = 6,315\ cm^{-1}/Å^4$
$S^{(4)} = 656.0\ cm^{-1}/Å^8$

Table 7 References

(1) R. W. G. Wyckoff, *Crystal Structures*, **1**, Interscience, New York (1968), 251.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Optical Maser Oscillation from Ni^{2+}* in MgF_2 Involving Simultaneous Emission of Phonons, Phys. Rev. Lett. **11** (1963), 318.

(4) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Spontaneous and Stimulated Emission from Co^{2+}* Ions in MgF_2 and ZnF_2, Appl. Phys. Lett. **5** (1964), 21.

(5) L. F. Johnson and H. J. Guggenheim, *Phonon-Terminated Coherent Emission from V^{2+}* Ions in MgF_2, J. Appl. Phys. **38** (1964), 483.

(6) R. R. Sharma and S. Sundaram, *Transition Metal Ions in Crystals: A Refined Treatment and Deduction of Coulomb and Exchange Interaction Constants*, Solid State Commun. **33** (1979), 381.

(7) S. I. Yun, L. A. Kappers, and W. A. Sibley, *Enhancement of Impurity Ion Absorption due to Radiation-Produced Defects*, Phys. Rev. **B5** (1973), 773.

(8) W. A. Sibley, S. I. Yun, and L. N. Feuerhelin, *Radiation Defect and 3d Impurity Absorption in MgF_2 and $KMgF_3$ Crystals*, J. Phys. (Paris) **34** (1973), C9-503.

(9) L. F. Johnson, H. J. Guggenheim, and R. A. Thomas, *Phonon-Terminated Optical Masers*, Phys. Rev. **149** (1966), 179.

(10) M. D. Sturge, F. R. Merritt, L. F. Johnson, H. J. Guggenheim, and J. P. Van der Ziel, *Optical and Microwave Studies of Divalent Vanadium in Octahedral Fluoride Coordination*, J. Chem. Phys. **54** (1971), 1405.

Table 8. MnF_2

(A) Crystallographic data on MnF_2.

Tetragonal $P4_2/mnm$, 136, Z = 2.

Ion	Site	Symm.	x[a]	y	z	q	a[b]
Mn	2(a)	D_{2h}	0	0	0	+2	0.122
F	4(f)	C_{2v}	0.305	0.305	0	−1	0.731

[a] *X-ray data, a = 4.8734 Å, c = 3.3099 Å, from reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$ for the Mn site (D_{2h}) in MnF_2.

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	901.5	1,815.67	−459.22	2,258
A_{22}	2638	−847.40	−300.87	1,490
A_{40}	−1670	−125.49	266.58	−1,529
A_{42}	−7263	−61.74	2,376.30	−4,948
A_{44}	3218	−222.98	−1,239.99	1,755

$S^{(0)} = 6,070\ cm^{-1}/Å^2$
$S^{(2)} = 3,813\ cm^{-1}/Å^4$
$S^{(4)} = 307.3\ cm^{-1}/Å^8$

(C) Experimental parameters.

Ion	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref.
Co^{2+}	—	—	—	−17,220	6

Table 8 References

(1) R. W. G. Wyckoff, *Crystal Structures*, **1**, Interscience, New York (1968), 251.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Optical Maser Oscillation from Ni^{+2}* in MgF_2 Involving Simultaneous Emission of Phonons, Phys. Rev. Lett. **11** (1963), 318.

(4) L. F. Johnson, H. J. Guggenheim, and R. A. Thomas, *Phonon-Terminated Optical Masers*, Phys. Rev. **149** (1966), 179.

(5) Von Werner H. Baur, *Uber die Verfeinerung der Kristallstrukturbestimmung einieger Vertreter des Rutiltyps, II. Die Difluoride von Mn, Fe, Co, Ni, und Zn*, Acta. Cryst. **11** (1958), 488.

(6) L. F. Blunt, *Optical Absorption of Cobalt in Manganese Fluoride*, J. Chem. Phys. **44** (1966), 2317.

Table 8 References (cont'd)

(7) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Exchange Splitting of the Ground State of Ni^{2+} Ions in Antiferromagnetic MnF_2, $KMnF_3$, and $RbMnF_3$*, Phys. Rev. Lett. **17** (1966), 13.

Table 9. ZnF_2

(A) Crystallographic data on ZnF_2.

Tetragonal $P4_2/mnm$, 136, Z = 2.

Ion	Site	Symm.	x[a]	y	z	q	$\alpha(Å^3)$[b]
Zn	2(a)	D_{2h}	0	0	0	+2	0.676
F	4(f)	C_{2v}	0.303	0.303	0	−1	0.731

[a] *X-ray data, a = 4.7034 Å, c = 3.1335 Å, from reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Zn site (D_{2h}) in ZnF_2.

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	−304.8	2,855	−593.0	1,957
A_{22}	2,659	−1,379	−346.0	934.0
A_{40}	−249.1	−268.3	430.1	−2,329
A_{42}	−9,011	−135.5	3,350	−5,796
A_{44}	−4,046	−383.2	1,786	−1,876

$S^{(0)} = 8,214.0\ cm^{-1}/Å^2$
$S^{(2)} = 5,417.7\ cm^{-1}/Å^4$
$S^{(4)} = 508.50\ cm^{-1}/Å^8$

Table 9 References

(1) R. W. G. Wyckoff, *Crystal Structures*, 1, Interscience, New York (1968), 251.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) L. F. Johnson, H. F. Guggenheim, and R. A. Thomas, *Phonon-Terminated Optical Masers*, Phys. Rev. **149** (1966), 179.

(4) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Spontaneous and Stimulated Emission from Co^{2+} Ions in MgF_2 and ZnF_2*, Appl. Phys. Lett. **5** (1964), 21.

Table 10. MgO

(A) Crystallographic data on MgO.

Cubic Fm3m, 225, Z = 4.

Ion	Site	Symm.	x[a]	y	z	q	$\alpha(Å^3)$[b]
Mg	4(a)	O_h	0	0	0	+2	0.0809
O	4(b)	O_h	1/2	1/2	1/2	−2	1.349

[a] *X-ray data, a = 4.2112, from reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Mg site (O_h) in MgO.

A_{nm}	Monopole	Self-induced	Total
A_{40}	20,084	−5,812	14,271
A_{44}	12,002	−3,474	8,528.8

$S^{(0)} = 11,851\ cm^{-1}/Å^2$
$S^{(2)} = 7,523.7\ cm^{-1}/Å^4$
$S^{(4)} = 621.35\ cm^{-1}/Å^8$

(C) Experimental parameters.

Ion	$F^{(2)}$	$F^{(4)}$	α	B_{40}	Ref.
Cr^{3+}	50,906	37,825	70	33,579	5
V^{2+}	42,429	30,239	60	30,429	5
Cr^{2+}	—	—	—	14,000	14
Ni^{2+}	—	—	—	18,060	15[a]
Ni^{2+}	—	—	—	−17,115	16

[a] *Refers to experimental optical data by A. G. Shenstone, J. Opt. Soc. Am. 44 (1954), 749.*

Table 10 References

(1) R. W. G. Wyckoff, *Crystal Structures*, 1, Interscience, New York (1964), 88.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) L. F. Johnson, R. E. Dietz, and H. J. Guggenheim, *Optical Maser Oscillation from Ni^{2+}* in MgF_2 Involving Simultaneous Emission of Phonons, Phys. Rev. Lett. **11** (1963), 318.

(4) L. F. Johnson, H. J. Guggenheim, and R. A. Thomas, *Phonon-Terminated Optical Masers*, Phys. Rev. **149** (1966), 179.

(5) D. T. Sviridov, R. K. Sviridova, N. I. Kulik, and V. B. Glasko, *Optical Spectra of the Isoelectronic Ions V^{2+}, Cr^{3+},* and Mn^{4+} in an Octahedral Coordination, J. Appl. Spectrosc. **30** (1979), 334.

(6) M. D. Sturge, *Optical Spectrum of Divalent Vanadium in Octahedral Coordination*, Phys. Rev. **130** (1963), 639.

(7) M. D. Sturge, *Strain-Induced Splitting of the ^2E State of V^{2+}* in MgO, Phys. Rev. **131** (1963), 1456.

(8) V. Hochlis, K. A. Muller, and P. Wysling, *Paramagnetic Resonance and Relaxation of Cu^{2+}* and Ni^{3+} in MgO and CaO: The Determination of Jahn-Teller Energy Splittings, Phys. Lett. **15** (1965), 5.

(9) P. Wysling, K. A. Muller, and V. Hochlis, *Paramagneti Resonance and Relaxation of Ag^{2+} and Pd^{3+} in MgO and CaO*, Helv. Phys. Acta. **38** (1965), 358.

Table 10 References (cont'd)

(10) W. Low and M. Weger, *Paramagnetic Resonance and Optical Spectra of Divalent Iron in Cubic Fields, I. Theory*, Phys. Rev. **118** (1960), 1119.

(11) W. Low and M. Weger, *Paramagnetic Resonance and Optical Spectra of Divalent Iron in Cubic Fields, II. Experimental Results*, Phys. Rev. **118** (1960), 1130.

(12) F. S. Ham, W. M. Schwartz, and M. C. M. O'Brien, *Jahn-Teller Effects in the Far-Infrared, EPR, and Moessbauer Spectra of MgO:Fe^{2+}*, Phys. Rev. **185** (1969), 548.

(13) M. C. M. O'Brien, *The Jahn-Teller Coupling of $3d^6$ Ions in a Cubic Crystal*, Proc. Phys. Soc. **86** (1965), 847.

(14) C. Greskovich and V. S. Stubican, *Divalent Chromium in Magnesium-Chromium Spinels*, J. Phys. Chem. Solids **27** (1966), 1379.

(15) W. Low, *Paramagnetic and Optical Spectra of Divalent Nickel in Cubic Crystalline Fields*, Phys. Rev. **109** (1958), 247.

(16) R. Pappalardo, D. L. Wood, and R. C. Linares, Jr., *Optical Absorption Spectra of Ni-Doped Oxide Systems. I*, J. Chem. Phys. **35** (1961), 1460.

(17) P. Wysling, *Paramagnetic Resonance and Relaxation of Ag^{2+} and Pd^{3+} in MgO and CaO*, Helv. Phys. Acta. **38** (1965), 358.

Table 11. $Be_3Al_2(SiO_3)_6$ (Beryl, Emerald)

(A) Crystallographic data on $Be_3Al_2(SiO_3)_6$.

Hexagonal P6/mcc, 192, Z = 2.

Ion	Site	Symm.	x[a]	y	z	q	α(Å^3)[b]
Al	4(c)	D_3	1/3	2/3	1/4	+3	0.0530
Be	6(f)	D_2	1/4	0	1/4	+2	0.0125
Si	12(i)	C_s	0.382	0.118	0	+4	0.0165
O_1	12(i)	C_s	0.294	0.242	0	−2	1.349
O_2	24(m)	C_1	0.499	0.143	0.138	−2	1.349

[a] *X-ray data, a = 9.206 Å, c = 9.205 Å, from reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Al site (D_3) in $Be_3Al_2(SiO_3)_6$.

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	−16,578	13,630	1,289	−1,659
A_{33}	−14,113	−12,941	12,339	−14,716
A_{40}	−16,436	−23,937	6,117	−34,257
A_{43}	20,357	29,273	−8,341	41,288
A_{53}	−14,004	−13,056	11,543	−15,516

Table 11 References

(1) R. W. G. Wyckoff, *Crystal Structures*, **4**, Interscience, New York (1968), 277.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

(3) A. A. Akhumyan, Zh. A. Arakelyan, G. V. Bukin, R. M. Martirosyan, and V. K. Ogneva, *Quantum Parametric Amplifier Utilizing Synthetic Emerald Crystals*, Sov. J. Quantum Electron. **9** (1979), 61.

(4) A. A. Akhumyan, R. M. Martirosyan, and N. G. Pogosyan, *Quantum Amplification of Millimeter Waves by Synthetic Emerald Crystals*, Sov. Tech. Phys. Lett. **7** (1981), 371.

(5) R. M. Martirosyan, M. O. Manvelyan, G. A. Mnatsakanyan, and V. S. Sevastyanov, *Spin-Lattice Relaxation of Cr^{3+} Ions in Emerald*, Sov. Phys. Solid State **22** (1980), 563.

(6) L. V. Nikol'skaya and M. I. Samoilovich, *Optical Absorption Spectra of Beryls in the Near-Infrared (900-2500 nm)*, Sov. Phys. Crystallogr. **24** (1979), 604.

(7) V. P. Solntsev, A. S. Lebedev, V. S. Pavlyuchenko, and V. A. Klyakhin, *Copper Centers in Synthetic Beryl*, Sov. Phys. Solid State **8** (1976), 805.

(8) B. V. Shul'gin, M. V. Vasilenko, V. P. Palvanov, and A. V. Kruzhalov, *Electronic Spectra and Structure of Beryl and Chrysoberyl*, Zh. Prik. Spekt. **34** (1981), 116.

(9) M. V. Vasilenko, A. V. Kruzhalov, and G. V. Bukin, *Excitation Spectra of Synthetic Emerald in the Vacuum Ultraviolet Region*, in *Proceedings of the All-Union Conference on Physics of Dielectrics and New Areas for Their Use* [in Russian], Karaganda (1978), 87.

(10) J. Buchert and R. R. Alfano, *Emerald—A New Gem Laser Material*, Laser Focus (September 1983), 117.

(11) P. J. Beckwith and E. J. Troup, *The Optical and Infrared Absorption of V^{3+} in Beryl ($Be_3Al_2Si_6O_{18}$)*, Phys. Stat. Sol. **a16** (1973), 181.

Table 12. $Na_3Li_3Sc_2F_{12}$

(A) Crystallographic data on $Na_3Li_3Sc_2F_{12}$.

Cubic Ia3d, 230, Z = 8.

Ion	Pos.	Symm.	x[a]	y	z	q	α[b]
Sc	16(a)	C_{3i}	0	0	0	3	0.540
Na	24(e)	D_2	1/4	1/8	0	1	0.147
Li	24(d)	S_4	1/4	3/8	0	1	0.0321
F	96(f)	C_1	−0.0343	0.0499	0.1407	−1	0.731

[a] *X-ray data, a = 12.607 Å, from reference 1.*
[b] *Reference 2.*

(B) Lattice sum, $A_{nm}(cm^{-1}/Å^n)$, for the Sc site (C_{3i}) in $Na_3Li_3Sc_2F_{12}$ (rotated so that the z axis is along the (111) crystallographic direction).

A_{nm}	Monopole	Total
A_{20}	−107.71	−307.29
A_{40}	10,176	−11,064
A_{43}	−11,848	13,385

$S^{(0)} = 10{,}262\ cm^{-1}/Å^2$
$S^{(2)} = 7{,}978.8\ cm^{-1}/Å^4$
$S^{(4)} = 947.55\ cm^{-1}/Å^8$

Table 12 References

(1) R. de Pape, J. Portier, J. Grannec, G. Gauthier, and P. Hagenmuller, *Sur quelques nouveaux grenats fluorés*, C. R. Acad. Sc. Paris **269** (1969), 1120, Series C.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

Table 13. $Na_3Li_3In_2F_{12}$

(A) Crystallographic data on $Na_3Li_3In_2F_{12}$.

Cubic Ia3d, 230, Z = 8.

Ion	Site	Symm.	x[a]	y	z	q	α^b
In	16(a)	C_{3i}	0	0	0	3	0.574
Na	24(c)	D_2	1/4	1/8	0	1	0.179
Li	24(d)	S_4	1/4	3/8	0	1	0.0321
F	96(f)	C_1	−0.0349	0.0507	0.1422	−1	0.731

[a] *X-ray data, a = 12.693, from reference 1.*
[b] *Reference 2.*

(B) Lattice sums, $A_{nm}(cm^{-1}/Å^n)$, for the In site (C_{3i}) in $Na_3Li_3In_2F_{12}$ (rotated so that the z axis is along the (111) crystallographic axis).

A_{nm}	Monopole	Total
A_{20}	−123.31	−482.55
A_{40}	−9150.3	−10,065
A_{43}	10,803	12,202

$S^{(0)} = 9{,}228.1\ cm^{-1}/Å^2$
$S^{(2)} = 6{,}898.8\ cm^{-1}/Å^4$
$S^{(4)} = 760.65\ cm^{-1}/Å^8$

Table 13 References

(1) R. de Pape, J. Portier, J. Grannec, G. Gauthier, and P. Hagenmuller, *Sur quelques nouveaux grenats fluorés*, C. R. Acad. Sc. Paris **269** (1969), 1120, Series C.

(2) P. C. Schmidt, A. Weiss, and T. P. Das, *Effect of Crystal Fields and Self-Consistency on Dipole and Quadrupole Polarizabilities of Closed-Shell Ions*, Phys. Rev. **B19** (1979), 5525.

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