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108: 173883s **Determination of $R_e(M^{2+}-F^-)$ for chromium(1+), iron(1+), nickel(1+), and manganese(2+) in ionic fluoride lattices from the isotropic superhyperfine constant.** Fernandez-Rodrigo, G.; Florez, M.; Pueyo, L.; Moreno, M.; Barriuso, M. T. (Fac. Quim., Univ. Oviedo, Oviedo, Spain 33007). *Cryst. Latt. Defects Amorphous Mater.* 1987, 16(1-4), 281-7 (Eng). The det. of equil. metal-ligand distances in transition-metal fluorides fr. the obsd. isotropic superhyperfine const. A_s is analyzed in the light of cluster-type calcns. at the Hartree-Fock-Roothaan level. The $MnF_6(4-)$ wavefunctions obtained at different metal-ligand distances confirm that the covalency parameter λ_s is proportional to the $\langle 3d\sigma|2s\rangle$ metal-ligand overlap integral. This behavior is also obsd. if theor. refinements such as the core projection and the cluster-lattice interaction are included into the SCF process. Thus, this result greatly support the method previously used by M. Barriuso and M. Moreno (1984) for deriving the true $Mn^{2+}-F^-$ distances for Mn^{2+}-doped fluoride lattices from obsd. values of A_s. The present method works also very well for the unstable Cr^+, Fe^+, and Ni^+ cations. The $R_e(Fe^+-F^-)$ distances in Fe^+:LiF, Fe^+:NaF, and Fe^+:$KMgF_3$ are reported here for the first time. Ionic radii and values of $10Dq$ are also given for these unstable systems.

$(R_e(Fe^+-F^-)$ неор. расчет)

(+2) ☒

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Спектроскопия

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α-$NaUF_6$

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$(LiF)_n (FeF_3)_m$ 1997

$m, n = 1, 2$

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