06.4-03 INTERPRETATION OF SPIN DENSITIES OBTAINED BY NEUTRON DIFFRACTION. B. Gillon[1], D. Sfez[1], P. Becker[1], J. Schweizer[2], M. Bonnet[3]
CMOA, 23 rue du Maroc, 75019 Paris
2. ILL, BP 156X, 38042 Grenoble Cedex
3. LLB, L'Orme du Merisier, 91290 Gif sur Yvette, France

I. Nitroxy Radicals. Neutron experiments, through a multipolar expansion of the spin density, reveal an equal distribution of unpaired electron among N and O atoms, in disagreement with EPR measurements. Using a unique GTO basis set and the UHF programm MONSTERGAUSS, calculations have been done on a series of radicals (H_2NO to $C_5H_{10}NO$), leading to an increase of density on N with the bulk of substituents, the effect saturating at the experimental value. EPR signal is quite insensitive to environment. Interpretation is proposed.

II. Yttrium Iron Garnet. A recent analysis of flipping ratios has shown the possibility of fitting magnetic structure factors with a limited number of parameters. But the interpretation of such a fit was ambiguous. We propose an analysis taking into account the antiferromagnetic coupling between tetrahedral and octahedral sites (which share an oxygen), which allows for the spin density in the region of oxygen ion.

06.5-01 ANALYSIS OF DEBYE-WALLER FACTORS FROM HIGHLY ANHARMONIC SYSTEMS. By S.L. Mair, CSIRO Division of Chemical Physics, P.O. Box 160, Clayton, Victoria, Australia 3168.

Analytical expressions are obtained for the Debye-Waller factor of an atom vibrating in a highly anharmonic one-particle potential. The model used for the effective one-particle potential takes the form of an array of harmonic oscillators, with origins at sites determined by the atomic environment. The resulting multi-minimum potential is particularly suitable for the interpretation of thermal vibration associated with displacive phase transitions or with mobile ions. Features in observed Debye-Waller factors, which cannot be explained by perturbation theory about the harmonic case, are predicted by the model. Analyses of neutron diffraction data from ionic conductor and ferro-electric materials are presented.

06.5-02 THE HAUNTED SITE OF $VAl_{10.4}$: HIGH RESOLUTION STUDY OF AN UNUSUAL VANADIUM ALUMINIDE.* By A. Kontio, E. D. Stevens, R. F. Boehme and P. Coppens, Department of Chemistry, State University of New York at Buffalo, Buffalo, New York, 14214 USA.

The highly symmetric structure of α-vanadium aluminide has been reinvestigated by X-ray diffraction at both room and liquid nitrogen temperatures.

The results confirm the partial occupancy of the Al(4) site. They correspond to the stoichiometric formula $VAl_{10.4}$ which differs somewhat from earlier values (P. J. Brown, Acta Cryst. (1957) 10, 133; A. E. Ray & J. F. Smith, Acta Cryst. (1957) 10, 604). The Al(4) atom is located in a spacious 16-atom cage of aluminum atoms, all of which are at a distance exceeding the Al-Al separation in the pure metal.

The highly anharmonic temperature parameters of Al(4) have been analyzed with 3rd and 4th cumulants at both temperatures. The one-particle potential derived from the cumulant values disagrees with the results of a theoretical pseudopotential treatment (A. D. Caplin & L. Kay Nicholson, J. Phys. F: Metal Phys. (1978) 8, 51), in the sense that the most probable direction of motion is opposite to that predicted by the theory.

Charge accumulation is consistently observed in the Al-Al bonds not involving Al(4) and in the VAl bonds, indicating covalent contributions to the metal-metal bonding. There is no clear observable difference between the characteristic short VAl bonds which occur in these alloys and other bonds of more normal length.

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06.5-03 PRESSURE DEPENDENCE OF GRÜNEISEN PARAMETER γ FOR ROCK-SALT CRYSTAL USING INTERACTION APPROACH. By C.L. Gupta, V.B.L. Mehrotra and M.N. Sharma, Solid State Physics Laboratory, Lucknow University, Lucknow, U.P., India.

The effect of pressure on the Grüneisen parameter γ (Grüneisen, Ann. Physik (1912) 39, 257) for the rock-salt crystal in the pressure range of 2.05 - 31.89 kbar has been studied following the two well known theories (Dugdale and MacDonald, Phys. Rev. (1953) 89, 832; Vashchenko and Zubarev, Soviet Physics.- Solid State (1963) 5, 653) in solid state Physics literature using the interaction approach and employing the notable (Born-Mayer, Z. Phys. (1932) 75, 1) potential energy function. The theoretical computed values of γ , when compared with the corresponding experimental results (Boehler et al, J. Phys. Chem. Solids (1977) 38, 233) are found satisfactory in the case of Vashchenko and Zubarev theory, thereby proving its superiority over the Dugdale and MacDonald theory.