

³⁵Cl and ⁷⁹Br NQR Spectra and the Secondary Bonding of Chalcogen Halide Complexes

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The ³⁵Cl and ⁷⁹Br NQR spectra of chalcogen halide complexes of aluminium, gallium, titanium, zirconium, hafnium, niobium, tantalum, molybdenum, tungsten, rhenium, iron, ruthenium, osmium, iridium, rhodium, platinum, palladium and gold are discussed.

Three structure types of these complexes have been distinguished by X-ray structure analysis: type I with AX₂ ligand and [MX_nA_m] coordination polyhedron; type II with AX₃ ligand and [MX_{n+m}] coordination polyhedron; type III, dimeric complexes with M-X-M bridge (where X = Cl, Br and A = S, Se, Te). The formation of secondary M-X-A or M-X-M bonds is characteristic of most structures. The spectra were interpreted by a Townes-Dailey approximation with allowance for the electronic configuration of the metal, mutual influence of ligands and structure features of complexes. Systematic investigation of a big series of chalcogen halide complexes-analogues allowed the following changes in ³⁵Cl and ⁷⁹Br NQR frequencies on secondary bonding to be established for intraligand halogen atoms: A decrease in frequency for type I complexes and an increase in frequency for type II complexes; for halogen atoms in the coordination polyhedron: a decrease in frequency for p metals and transition metals with $d > 6$, and an increase in frequency for metals with $d < 6$.

Key words: Electronic Configuration; Mutual Influence of Ligands; Coordination Polyhedron; Peripheral Polyhedron.