

## CALCULATION OF ISOTOPIC EFFECTS OF MAGNESIUM IN EXTRACTION SYSTEMS USING CROWN ESTERS

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Taking into account the previously calculated value of the  $b$ -factor of the magnesium ion aquacomplex at different concentrations of magnesium salts, a single coefficient of isotope extraction separation ( $\alpha$ ) of an isotope pair for  $^{24}\text{Mg}$ – $^{26}\text{Mg}$  for an extraction system containing magnesium cation complexes with crown esters in the organic phase was calculated. A higher charge of the magnesium cation compared to lithium and thus stronger magnesium-oxygen bonds in the macrocycle ring may explain the reason for the lack of influence of water molecules in the coordination sphere.

Quantum chemical calculations of the oscillation frequencies of isotopic forms of the complex with crown ether were carried out using the Firefly program. The RHF/6-311++G\*\* basis was used to calculate all complexes. It is shown that the most effective macrocyclic ligand for practical separation of magnesium isotopes is benzo-15-crown-5.

**Keywords:** nonempirical quantum chemical methods, magnesium, aquacomplexes, isotope effects, isotope separation coefficients, crown ethers.