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Unified view of the hydrogen-bond structure of water in the hydration shell of metal ions (Li^+, Mg^{2+}, La^{3+}, Dy^{3+}) as observed in the entire 100–3800 cm^{-1} regions

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Highlights

- Water in the hydration shell of a high charge density metal ion has a heterogeneous structure.
- Water adopts “enhanced” as well as “reduced” H-bonding in the extended hydration shell of high charge density metal ions.
- The first hydration shell water is a strong H-bond donor and weak H-bond acceptor.
- Librational freedom of water is restricted in the hydration shell due to stronger and stiffer intermolecular H-bonding.