Structure of a $Cs(18\text{-crown-}6)N(CN)_2 \cdot H_2O$ Complex: Assembly of the Dimeric 2:2 Anion Paired Encapsulate by Means of μ^2-Bridging Water Molecules

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The new macrocyclic complex of composition $Cs(18\text{-crown-}6)N(CN)_2 \cdot H_2O$ has been prepared and characterized by X-ray crystallography (monoclinic, space group $P2_1/n$, with a = 11.218(3), b = 8.563(7), c = 21.704(2) Å; β = 92.66(1)°, V = 2083(2) Å^3, Z = 4; final R = 0.034 and R_w = 0.038 for 2529 independent reflections with $I > 3\sigma(I)$). The complex adopts a molecular dimeric array $[Cs(18c6)(\mu^2\text{-}H_2O)\{N(CN)_2\}]_2$(2:2 anion-paired encapsulate). The dimerization of $Cs(18c6)^+$ moieties takes place surprisingly not *via* the nitrilic nitrogen atoms, but *via* the water molecules (Cs-O 3.139(5), 3.334(5) Å), which is an unprecedented example in the chemistry of $M(18c6)^+$ complexes. The caesium atom adopts nine-fold coordination (Cs-O (ether) 3.099(5) - 3.280(5) Å). One cyano group of the counter anion completes the coordination environment of the caesium atom (Cs-N 3.420(8) Å), while the second one is involved in hydrogen bonding.

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