Structure of a Cs(18-crown-6)N(CN)$_2$·H$_2$O Complex:
Assembly of the Dimeric 2:2 Anion Paired Encapsulate by Means of $\mu^2$-Bridging Water Molecules

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The new macrocyclic complex of composition Cs(18-crown-6)N(CN)$_2$·H$_2$O 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; $\beta = 92.66(1)^\circ$, $V = 2083(2)$ 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)($\mu^2$-H$_2$O){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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